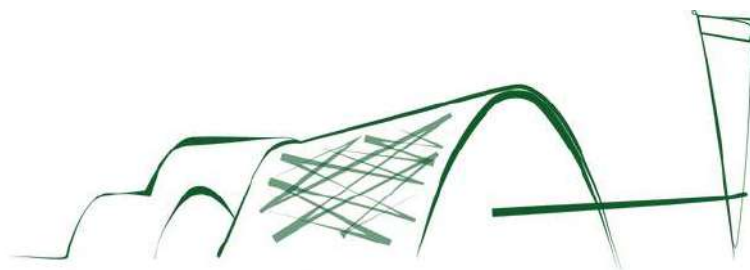




10th Brazilian Conference on Natural Products
XXXVI RESEM



4-7 November, 2025
Belo Horizonte, MG

Abstracts

Metabolomics
and
RESEM

Chemical
Ecology

Biological and
Pharmacologic
al Activity of
NP

Biosynthesis
and Molecular
Biology of NP

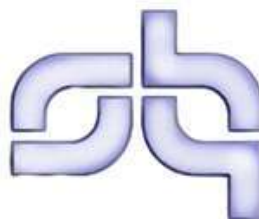
Biodiversity
&
Natural Products

Recent Advances
on Isolation and
Structure
Elucidation of NP

Manufacturing
and Quality
Control of
Herbal Drugs
and Essential
Oils

Organic
Synthesis and
Structural
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10th Brazilian Conference on Natural Products (BCNP)

**XXXVI Annual Meeting on Evolution,
Systematics, and Micromolecular Ecology
(RESEM)**

BOOK OF ABSTRACTS (Livro de Resumos)

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Belo Horizonte, Minas Gerais State, Brazil.

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WELCOME FROM THE ORGANIZING COMMITTEE

On behalf of the Organizing Committee and the Universidade Federal de Minas Gerais (UFMG) community, we are pleased to welcome all participants to the 10th Brazilian Conference on Natural Products (BCNP) and the XXXVI Meeting on Micromolecular Evolution, Systematics, and Ecology (RESEM). We extend a particularly warm welcome to our distinguished guests, many of whom have traveled long distances to join us for this event.

The Brazilian Conference on Natural Products (BCNP) was established in 2007 by the Natural Products Division of the Brazilian Chemical Society. Since then, it has become a landmark scientific meeting, bringing together researchers from Brazil and abroad to discuss advances, challenges, and future perspectives in natural products chemistry.

As is well known, the high costs of international conferences often limit participation by Brazilian researchers, especially students. In this context, the BCNP and RESEM play a fundamental role by bringing leading scientists from around the world to Brazil, fostering direct interaction with national experts, early-career researchers, and students. The realization of this edition with the expected scientific quality was made possible through the generous financial support of the Brazilian funding agencies FAPEMIG, CAPES, and CNPq, and we are particularly pleased to note the significant increase in student participation compared to previous meetings.

These scientific encounters promote high-level discussions, stimulate collaborations, and inspire innovative research, strengthening the international visibility of Brazilian science and contributing to the development of new products and technologies.

This year, we are honored to host the conference at UFMG, a special occasion in the year when the university celebrates its 98th anniversary. UFMG has a long-standing tradition of academic excellence and a strong commitment to regional and national development, standing out for its cutting-edge research, technological innovation, and engagement with public policy, inclusive education, and sustainability.

In designing the scientific program, we sought not only to invite distinguished scientists to deliver the Plenary Lectures but also to highlight young researchers from different regions of Brazil in the Invited Lectures, thereby providing them with the opportunity to share their work and engage with the broader natural products community. We sincerely hope that this program will encourage interaction, exchange of experiences, and mutual learning.

We are also pleased to announce that a Special Issue of the journal *Frontiers in Natural Products*, entitled "Highlights from the 10th Brazilian Conference on Natural Products (BCNP) and the XXXVI Meeting on Micromolecular Evolution, Systematics and Ecology (RESEM)", will be published, featuring selected contributions arising from this Conference.

We would like to express our sincere gratitude to the members of the Organizing and Scientific Committees, whose dedication, commitment, and teamwork were essential to the success of this event.

A special acknowledgment is due to the BCNP at School initiative, organized in collaboration with Professor Fernando Silva from the Faculty of Education. In partnership with the Science Club Trem Bão, this program sought to engage young students at the beginning of their academic journey. At least 10% of the registrations were offered free of charge to public high school students, and one afternoon of the Conference was dedicated to science outreach activities, including experiments, games, and interactive experiences focused on the Cerrado biome, its biodiversity, and its environmental importance.

Finally, we invite all participants not only to enjoy the scientific program but also to experience the rich and traditional cuisine of Minas Gerais, a true expression of the region's culture and hospitality.

We wish you an inspiring and memorable conference.

Prof. Dr. *Lúcia Pinheiro Santos Pimenta*
Chair, Organizing Committee

Prof.Dr. *Grasiely Faria de Sousa*
Secretary General, Organizing Committee



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10th Brazilian Conference on Natural Products
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OPENING CONFERENCE



10th Brazilian Conference on Natural Products XXXVI RESEM

4-7 November 2025, Belo Horizonte, MG, Brazil

SYNERGIES BETWEEN CLIMATE ACTION AND NATURE CONSERVATION

Mercedes Bustamante^{1*}

mercedesmcb@gmail.com

1-Departamento de Ecologia, Universidade de Brasília, DF, Brazil.

The climate and nature crises are deeply connected. A changing climate negatively impacts biodiversity, while the loss of nature amplifies the climate breakdown, reducing adaptation potential. Despite these interactions, global strategies to halt these crises are formulated separately within two international conventions (the Convention on Biological Diversity and the UN Framework Convention on Climate Change) and often within different departments or ministries. Highlighting the synergies in the responses to climate change and biodiversity decline can support bridging the implementation gaps between the global convention and governmental and social actions. Consideration of the mutual effects is also central to achieving the Sustainable Development Goals (SDGs), as goals related to nature conservation provide the basis for social, economic, and institutional goals. Human societies' well-being depends intimately on the living components of natural and managed systems. Designing synergistic solutions that conserve biodiversity and ecosystem functions and fight climate change demands strong evidence and special attention to local contexts and vulnerable social groups. Focusing on the synergies in the responses to climate change and biodiversity decline can support bridging the implementation gaps while achieving the SDGs.



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PLENARY LECTURE ABSTRACT



10th Brazilian Conference on Natural Products

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4-7 November 2025, Belo Horizonte, MG, Brazil

ACCESSING THERAPEUTIC NATURAL PRODUCTS VIA A BIO-BASED APPROACH

Amy E. Fraley*, Anita Berg¹, Chad Papenfuhs²

amy.fraley@pharma.ethz.ch

*Institute of Pharmaceutical Sciences, Department of Chemistry and Applied Biosciences,
Eidgenössische Technische Hochschule (ETH) Zürich, Vladimir-Prelog-Weg 4, CH-8093 Zürich,
Switzerland*

Botanical extracts have been used in traditional medicine for centuries, however many times the source plants are protected or difficult to access. We are discovering new, laboratory-cultivable sources for bioactive natural products typically used in medical supplements. In this work, we aim to provide an alternative, more sustainable production system for these therapeutic compounds while also revealing the molecular mechanisms behind their production.

Keywords: diterpenes, terpene cyclase, cytochrome P450, plant natural products, biosynthesis



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10th Brazilian Conference on Natural Products XXXVI RESEM

4-7 November 2025, Belo Horizonte, MG, Brazil

Silent Warriors: Natural Products Are No Longer Just Promising

Francisco A. Macías¹, Francisco J. Rodríguez-Mejías¹, Daniela Rosa^{1,2}, Aurelio Scavo³,
Carlos Rial¹, Fatima Duarte², José M. G. Molinillo¹, Rosa M. Varela¹.

famacias@uca.es

1- Allelopathy Group, Department of Organic Chemistry, Facultad de Ciencias, Institute of Biomolecules (INBIO), University of Cadiz, C/ Avenida República Saharaui, s/n, 11510 Puerto Real, Spain.

2- Alentejo Biotechnology Center for Agriculture and Agro-Food (CEBAL)/Polytechnic Institute of Beja (IPBeja), 7801-908 Beja, Portugal.

3- Department of Veterinary Sciences, University of Messina, Polo Universitario dell'Annunziata, Messina, Italy.

Allelopathy has emerged as a promising approach to develop new agrochemicals based on natural products, offering sustainable alternatives to classical herbicides in the face of rising weed resistance and increasing environmental concerns. However, for more than four decades, research in this area has largely resulted in "potential" compounds or products. While many of these have advanced to trials in controlled cultivation zones or even across several hectares, very few have reached the stage of commercial application.

This presentation will showcase several **real alternatives** that, having successfully passed key stages such as chemical optimization, greenhouse testing, and off-target evaluation, are now genuinely close to being marketed as commercial bioherbicides.

One example focuses on *Cynara cardunculus* fractions enriched in major sesquiterpene lactones such as cynaropicrin and grosheimin. These fractions were obtained through ultrafiltration-based enrichment, then formulated using both micro- and nanoencapsulation strategies. The resulting product can be produced at scales of hundreds of grams and has shown strong performance in field trials.¹

A second example involves the formulation of aminophenoxazinones, microbial degradation products of benzoxazinoids, whose phytotoxic activity has been debated for decades due to their striking bioactivity. Through nanoformulation and derivatization, we have succeeded in applying these compounds directly to crop fields. Even at application rates of just a few hundred grams, we observed up to a **50% increase in wheat yield**, effective control of a broad spectrum of weeds, and **no detectable bioaccumulation in soil**.²



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These natural products are no longer just promises. **They are fully equipped warriors ready for battle.**

Keywords: Allelopathy, biocommunicators, natural products, bioherbicides

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ANTI-OBESITY AND LONGEVITY PROMOTION PROPERTIES OF DIETARY PLANTS AND HERBS

Milen I. Georgiev^{1,2}

¹ Department of Plant Cell Biotechnology, Center of Plant Systems Biology and Biotechnology, 4000 Plovdiv, Bulgaria

² Laboratory of Metabolomics, Institute of Microbiology, Bulgarian Academy of Sciences, 139 Ruski Blvd., 4000 Plovdiv, Bulgaria

Obesity presents a significant challenge to the modern society, imposing a substantial burden on health systems and individuals alike. Nowadays, more than a billion people globally are considered obese, a condition that does not solely refer to weight management but rather to mitigating its far-reaching consequences on healthspan and lifespan [1]. Individuals diagnosed with obesity are predisposed to comorbidities including type 2 diabetes, cardiovascular disease, and metabolic complications often referred to as metabolic syndrome. Most importantly, obesity is associated with a reduction in disease-free years, an excess risk of premature death, and accelerated aging [1, 2].

On the other hand, we live in a rapidly aging world, with an expectancy of more than a 2 billion people aged 65 years (or older) by 2050, alongside a rising proportion of age-related diseases. Thus, both obesity and ageing are, *per se*, different sides of the same coin and represent healthcare burden on our society [1, 2]. The development of strategies targeting both of these processes now becomes a challenge for science. Central to this pursuit is the recognition that metabolic health serves as a cornerstone for both healthy weight maintenance and prolonged lifespan [2]. Additionally, key molecular pathways attributed to nutrient signalling that are implicated in obesity progression, intersect with those fundamental to longevity, suggesting potential shared targets for intervention [2].

Utilizing the model organism *Caenorhabditis elegans* (nematode), along with combining omics and molecular pharmacology approaches, our research focuses on the discovery of natural products that target these shared pathways [1-4]. Through our approach, we aim not only to mitigate the adverse effects of obesity but also to uncover novel strategies for promoting healthy aging and longevity.

Acknowledgements: MIG acknowledges financial support from the European Regional Development Fund through Programme Research Innovation and Digitalisation for Smart Transformation, Grant agreement № BG16RFPR002-1.014-0003-C01.





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4-7 November 2025, Belo Horizonte, MG, Brazil

QUALITY CONTROL OF PLANT MATERIALS

Miriam Anders Apel¹

miriam.apel@ufrgs.br

1- Departamento de Produção de Matéria-Prima, UFRGS, RS, Brazil.

The quality control of herbal drugs and essential oils is a fundamental step to ensure the efficacy, safety, and quality of herbal products and commercial oils. This process involves a series of analyses aimed at ensuring that the plant raw material (medicinal plant or parts thereof, such as leaves, roots, flowers, as well as their derivatives) complies with the standards established by official compendia, such as the Brazilian Pharmacopoeia. The lack of quality control in herbal drugs is a critical issue, as it can compromise therapeutic efficacy, patient safety, and the credibility of herbal medicines. Among the problems caused by the lack of quality control are: incorrect identification of the plant, contamination, adulteration, and variation in the chemical composition of the raw materials.

Keywords: quality control, medicinal plants, Brazilian Pharmacopoeia.



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***WOMEN'S HEALTH UNVEILED: EXPLORING THE HIDDEN LINKS BETWEEN
THE MICROBIOME, METABOLOME, AND KEY INFLUENCERS***

Denise Medeiros Selegato

Molecular Systems Biology Unit

European Molecular Biology Laboratory, Heidelberg

denise.selegato@embl.de

The field of medical research has long been criticized for its systemic neglect of women's health, resulting in significant knowledge gaps that persist today. Historically, women have been underrepresented in clinical trials, with fewer than 30% of participants in early-phase studies being women. This exclusion, often justified by concerns about hormonal fluctuations and potential pregnancy risks, has perpetuated a "one-size-fits-all" approach to medicine that assumes male physiology as the default. Consequently, critical aspects of women's health remain poorly understood, including the vaginal microbiome, drug metabolism, pregnancy outcomes, and diseases such as endometriosis. The vaginal microbiome, for example, plays a crucial role in reproductive health by maintaining an acidic environment dominated by *Lactobacillus* species. However, much remains unknown about how host and environmental factors influence their composition and how imbalances contribute to conditions like bacterial vaginosis, infertility, and pregnancy complications. Similarly, diseases unique to or more prevalent in women, such as endometriosis, are also under-researched. Here, we show three case studies on the use of targeted and untargeted metabolomics to address some of these disparities: (1) the citizen science project ISALA, that investigates the vaginal microbiome and metabolome of healthy women and the production of secondary metabolites by their microbial population, (2) the AROMA project, that tries to understand infertility by the chemical profiling of embryo supernatants during in vitro fertilization (IVF) and (3) the ENDO project that tries to find chemical biomarkers for the diagnoses of ovarian and peritoneal endometriosis in plasma. Overall, addressing these disparities is essential to advancing our understanding of women's health and improving medical outcomes for half the population.

Keywords: *women's health, microbiome, untargeted metabolomics, IVF, endometriosis*

Acknowledgements: *Isala project has been done in collaboration with the group of Prof. Dr. Sarah Leber from the University of Antwerp, Belgium (<https://isala.be/en/>); AROMA and ENDO have been done in collaboration with Prof. Dr. med. Ariane Germeyer, Dr. med. Sabine Kess and Dr. med. Réka Kollarics from the Clinic for Gynecological Endocrinology and Fertility Disorders from Heidelberg University, Germany.*





***FROM BIOACTIVE NATURAL PRODUCTS TO MEGABYTES: HARNESSING AI'S
POTENTIAL AND METABOLOMICS FOR THE DIGITAL TRANSFORMATION OF
PHARMACOGNOSY***

Jean-Luc Wolfender^{1,2}, A. Kirchhoffer^{1,2}, Arnaud Gaudry^{1,2}, Luis Quiros-Guerrero^{1,2}, Olivier
Marco Pagni³, Florence Mehl³, Frederic Burdet³, Laurence Marcourt^{1,2}, Bruno David⁴,
Antonio Grondin⁴, Adriano Rutz^{1,2}, Emerson Ferreira Queiroz^{1,2}, Pierre-Marie Allard^{1,2,5},
Louis-Félix Nothias^{1,2,6}

Jean-luc.wolfender@unige.ch

¹Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, CMU, 1211
Geneva, Switzerland, ²School of Pharmaceutical Sciences, University of Geneva, CMU, 1211 Geneva,
Switzerland, ³Vital-IT, SIB Swiss Institute of Bioinformatics, 1015 Lausanne, Switzerland, ⁴Green
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Toulouse, France, ⁵Department of Biology, University of Fribourg, 1700 Fribourg, Switzerland,
⁶Université Côte d'Azur, CNRS, ICN, Nice, France.

The integration of omics, digital technologies and artificial intelligence (AI) is gradually leading to a transformative change in pharmacognosy, enabling unprecedented insights into the plant and microorganisms chemodiversity through detailed metabolome profiling [1]. In this context, modern LC-MS platforms deliver extensive qualitative insights into natural extracts, yet key challenges remain unresolved [2]. These include ensuring accurate metabolite annotations, linking spectral data to bioactive compound quantities, and deriving 3D molecular structures critical for predicting bioactivity. Our research leverages metabolomic datasets from thousands of biodiverse plant and fungal extracts [3]. We are trying to understand how the massive amount of information collected and the taxonomic links can be used to answer questions about confidence/redundance in MS annotation [4]. Managing this flood of data requires innovative solutions, such as semantic web-based knowledge graphs (KGs), which organize complex relationships and enable advanced querying for pattern discovery [5]. This work addresses practical hurdles in automating chemical composition assessment and highlights the synergistic potential of KGs and AI in natural products metabolomics. By combining digitised data with the traditional roots of pharmacognosy, we aim to streamline NP research, accelerate new natural ingredient development and open up new paths for drug discovery.

Acknowledgements: J-LW, L-FN and P-MA are thankful to the Swiss National Science Foundation for the funding of the project (SNF N° CRSII5_189921/1).

Keywords: *Metabolomics, knowledge graph, artificial intelligence.*

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INVITED LECTURE ABSTRACT

DECIPHERING THE ROLE OF SECONDARY METABOLITES IN THE CHEMICAL INTERACTION BETWEEN PHYTOPATHOGENS AND THE CITRUS HOST

Taícia Fill^{1*}

¹Chemistry Institute, Universidade Estadual de Campinas – UNICAMP

* email: taicia@unicamp.br

Abstract

The world's citriculture has witnessed large-scale productivity decay due to microbial infections. The secondary metabolites produced during infection, especially by pathogens, are an important aspect of complex phytopathogen–host interactions and can be crucial for virulence and disease viability. Therefore, the production of natural products (NPs) can facilitate the colonization of plant tissue and successfully modulate the host's physiology. Here, we comprehensively explore microbial secondary metabolites produced during infection by the most important citrus pathogens and give insights concerning the biological role of NPs in some of the most important citrus diseases, such as Huanglongbing and blue mold disease.

Keywords: Metabolomics, natural products, pathogen-host interaction

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BIOSYNTHESIS OF METABOLITES PRODUCED BY MARINE AND BY MARINE-DERIVED FUNGI

rgsberlinck1010@outlook.com

Living organisms present defense traits against predators and pathogenic agents. The production and/or accumulation of defensive chemical substances derived from secondary metabolism represents one of the most successful forms of adaptation in virtually all organisms that do not possess an immune system. However, increasing evidence shows that microorganisms are often the actual source of many of these substances. Recent studies clearly indicate that secondary metabolites originally isolated from marine invertebrates are, in fact, produced by associated microorganisms, whether symbionts or those in mutualistic relationships.

Although research aimed at establishing the true origin of secondary metabolites accumulated by marine invertebrates has advanced considerably, much less progress has been made in understanding the true microbial diversity associated with marine invertebrates and vertebrates. The investigation of microorganisms associated with marine organisms that are not filter-feeding has been far less explored, possibly due to the assumption that many of these organisms lack chemical defenses. However, this is a questionable premise, since microorganisms associated with non-filtering organisms can, in fact, contribute significantly to their survival success.

Among the marine microorganism strains studied in this presentation, marine and marine-derived fungi and bacteria associated with diverse macroorganisms have been the most interesting groups due to their metabolic diversity expressed under cultivation conditions. Among the metabolite groups of our interest, we have investigated the biosynthetic origin of aminopyrones produced by a fungus of the genus *Aspergillus*, terpenes produced by the *Biatriospora* sp. CBMAI 1333 sp. strain, non-ribosomal peptides produced by a bacterium of the genus *Pseudovibrio*, and alkaloids produced by a *Penicillium*. More recently, a series of polyketides produced by a fungal strain belonging to the genus *Peroneutypa* were isolated, whose biosynthesis appears to involve a cyclization through a [4+2] cycloaddition reaction, in addition to additional polyketides with singular chemical structures. These investigations demonstrate the chemical diversity of microorganisms originating from the marine environment, with unique biosynthetic pathways.





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4-7 November 2025, Belo Horizonte, MG, Brazil

BIOPROSPECTING NATIVE PLANTS FROM THE LEGAL AMAZON: GREEN EXTRACTION METHODS AND BIOACTIVE POTENTIAL

Elisandra Scapin*

scapin@uft.edu.br

**Curso de Engenharia Ambiental, Programa de Pós-Graduação em Ciências do Ambiente - Ciamb, Programa de Pós-graduação em Biodiversidade e Biotecnologia - BIONORTE, Universidade Federal do Tocantins, Palmas, Tocantins, CEP 77001-090, Brazil.*

Brazilian biodiversity, particularly from the Legal Amazon, represents a strategic source of bioactive compounds with therapeutic and cosmetic potential. Our research group has focused on underexplored native species, emphasizing chemical characterization, biological activity evaluation, and the application of sustainable methodology. *Hancornia speciosa* Gomes exhibited high levels of phenolics, flavonoids, and strong antioxidant activity in leaves, stem, and bark. These extracts were applied in lauryl-free shampoo formulations, which showed physicochemical stability, functional properties, and potential as green phytocosmetics¹. In *Cariniana rubra*, ultrasound-assisted extraction of the bark resulted in high yields and elevated phenolic content, confirmed by chromatographic analyses. Extracts displayed significant antioxidant activity, reinforcing the efficiency of sustainable methodologies and their cosmeceutical potential². Extracts from *Dipteryx alata* leaves, obtained by ultrasound and Soxhlet methods, revealed flavonoids, tannins, phytosterols, and alkaloids, along with notable antioxidant and antimicrobial activity against oral microorganisms³. These findings highlight its applicability in dentistry and cosmetics, promoting the sustainable use of this culturally and economically important species³. *Couroupita guianensis* leaf extracts contained phenolics such as caffeic acid, rutin, and quercetin, associated with antioxidant and antibacterial properties against oral pathogens, indicating promise for oral health phytotherapeutics. *Parkia platycephala*, an endemic Cerrado species and symbolic tree of Tocantins, showed remarkable antioxidant and anticholinesterase activities in bark, flower, and seed extracts⁵. Compounds such as gallic acid, ferulic acid, and flavonoids were identified, suggesting potential for neuroprotective agents targeting Alzheimer's disease⁵. Collectively, these studies reinforce the value of Brazilian biodiversity as a platform for innovation in health, cosmetics, and biotechnology. They also emphasize the importance of adopting green extraction methodologies to enhance yields, reduce environmental impacts, and foster a sustainable bioeconomy in the Legal Amazon.

Keywords: Mangaba, Phytochemical profiling, Jequitibá Vermelho, Green extraction methods, Amazonian biodiversity.

References: ¹PANONTIN, J. F. et al. Chemical composition, antioxidant activity and development of a facial serum formulation from the extract of *Hancornia speciosa*. *Natural Product Research*, v. 36, n. 1, p. 1-9, 2022.

²BIGGI-MACIEL, A. et al. Efficient extraction of phenolic compounds from *Cariniana rubra* Gardener ex Miers from the Legal Amazon: ultrasound-assisted optimization, chemical characterization, and antioxidant potential.



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Chemistry & Biodiversity, p. 1-15, 2025. ³SCAPIN, E. et al. Phytochemical analysis, toxicity and evaluation of antioxidant and antimicrobial activities of leaves of *Dipteryx alata* Vogel. *Brazilian Journal of Biology*, v. 84, e278004, p. 1-10, 2024. ⁴AUGUSCO, M. A. C. et al. Extracts from the leaf of *Couroupita guianensis* (Aubl.): phytochemical, toxicological analysis and evaluation of antioxidant and antimicrobial activities against oral microorganisms. *Plants*, v. 12, n. 2327, p. 1-17, 2023. ⁵FERNANDES, R. M. N. et al. *Parkia platycephala* from Cerrado: phytochemical bioprospecting, toxicity and in vitro bioactivities of bark and flower extracts. *Brazilian Journal of Biology*, v. 83, e275733, p. 1-10, 2023.





10th Brazilian Conference on Natural Products
XXXVI RESEM

4-7 November 2025, Belo Horizonte, MG, Brazil

EXTREMOPHILIC FUNGI: DIVERSITY AND BIOPROSPECTING OF BIOACTIVE METABOLITES

Luiz Henrique Rosa^{1*}

lhrosa.lr@gmail.com

*1-Departamento de Microbiologia, Instituto de Ciências Biológicas
Universidade Federal de Minas Gerais, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG,
Brazil.*

The global diversity of extremophilic fungi remains poorly understood and is critical in various regions of the planet. This lecture will present research on the biodiversity of extremophilic fungi found in different ecosystems of Antarctica, the Arctic, and along Brazil's Blue Amazon, as well as their potential to produce metabolites with diverse biological activities.

Keywords: *Antarctica, Arctic, Bioprospecting, Fungi, Secondary metabolites.*



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4-7 November 2025, Belo Horizonte, MG, Brazil

BIOPROSPECTING BRAZILIAN BIODIVERSITY FOR ANTI-SARS-COV-2 NATURAL COMPOUNDS

Suzana G. Leitão

sgleitao@farmacia.ufrj.br

1-Laboratório de Fitoquímica e Farmacognosia, Faculdade de Farmácia, Universidade Federal do Rio de Janeiro, 21.941-902, Ilha do Fundão, Rio de Janeiro, Brasil.

Since the emergence of the COVID-19 pandemic caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), the discovery of compounds with antiviral potential from medicinal plants has been extensively researched [1]. Plant secondary metabolites have promising pharmacological activities due to their specific mechanisms of action in biological systems. In a context which viral infections are part of modern society, aggravated by globalization, the discovery of new antiviral substances is essential. In this sense, the Phytochemistry and Pharmacognosy (UFRJ/BR) and the Phytochemistry and Countercurrent Chromatography (UFRJ/BR) Laboratories engaged in the study of Brazilian plant species towards different Sars-CoV-2 targets, through in vitro and in silico methods. The two laboratories hold a bank with about 200 samples, among extracts, fractions, and isolated substances of Brazilian plant species, which have been used in several studies following the random and ethnopharmacological approaches, which were used in a metabolomics investigation guided by in vitro and chemometric analyses, to identify potential agents in the tackling of COVID-19 and SARS-CoV-2. Extracts from representatives of 8 families and 28 species, were screened against three of SARS-CoV-2 most important targets: the proteases 3CLpro and PLpro, related to virus replication, and the interaction between the Spike protein and its receptor ACE2, related to viral cell attachment and entry, complemented by in silico analyses, resulting in several publications, which will be discussed [1-5].

Acknowledgements to CAPES, CNPq and FAPERJ.

Keywords: SARS-CoV-2, Medicinal Plants, chemometrics, proteases, COVID-19, mass spectrometry

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Design of Bio-Inspired Peptides for GPCR Drug Discovery

Christian W. Gruber

Medical University of Vienna, Center for Physiology and Pharmacology, Schwarzspanierstr. 17,
1090 Vienna, Austria

Peptides are highly diverse signaling molecules that regulate numerous physiological processes, primarily through G protein-coupled receptors (GPCRs) - the largest class of cell surface receptors and a major drug target family. Despite their therapeutic potential, peptide-based drugs for GPCRs have been hampered by poor metabolic stability, low oral bioavailability, and off-target effects due to limited receptor selectivity. To overcome these limitations, we harness biodiversity-driven resources – including animal venom peptides, plant defense peptide libraries, and invertebrate peptide hormones – to discover novel GPCR ligands that target human neuropeptide signaling systems based on their evolutionary similarity. Through peptidomics discovery (including mining of large genetic datasets) and functional/biological screening, we have identified receptor ligands with enhanced subtype selectivity and biased signaling profiles. Advanced methods such as *de novo* design, cyclization, and late-stage modifications have yielded stabilized peptide candidates, particularly for the κ -opioid receptor. Lead compounds demonstrate analgesic efficacy *in vivo* and represent promising candidates for treating chronic abdominal pain and inflammatory diseases.



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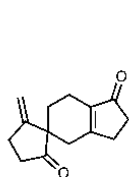
SYNTHETIC STRATEGIES AND CONCEPTS INSPIRED BY NATURAL PRODUCTS

Andrew Lawrence

a.lawrence@ed.ac.uk

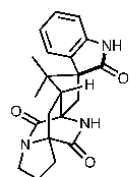
School of Chemistry, University of Edinburgh, Joseph Black Building, Edinburgh, EH9 3FJ, UK

Our research effort is primarily focused on the total synthesis of natural products, exploring new strategies and concepts in chemical synthesis, and developing new synthetic methodology. This presentation will be an account of our research into how molecular complexity is rapidly and selectively generated in biosynthetic pathways. This will include our recent development of new synthetic strategies towards complex natural products (see completed targets below) and the exploration of new concepts in asymmetric synthesis.



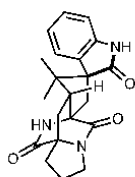
ulodione A
2 steps

Angew. Chem. Int. Ed.
2022, e202207004



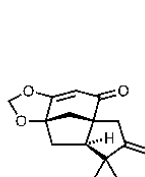
brevianamide X
8 steps

Chem. Sci. 2022,
13, 1313–1322



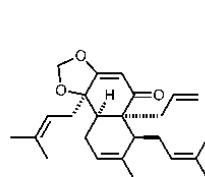
brevianamide Y (& Z)
7 steps

Chem. Sci. 2022,
13, 1313–1322



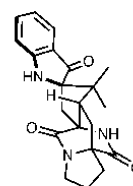
tricycloillicinone
5 steps (formal)

Org. Lett. 2021,
23, 3248–3252



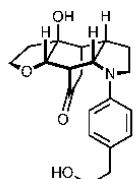
cycloillicinone
4 steps

Org. Lett. 2021,
23, 3248–3252



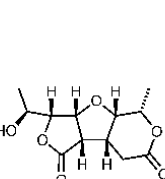
brevianamide A (& B)
7 steps

Nat. Chem. 2020,
12, 615–619



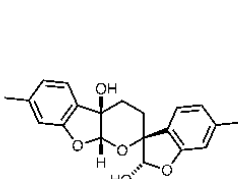
incargranine A
4 steps

Org. Biomol. Chem.
2019, 17, 1698–1702



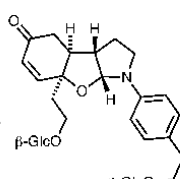
angiopterlactone B
4 steps

Org. Lett. 2017,
19, 2199–2201



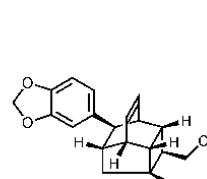
thymarnicol
6 steps

Angew. Chem. Int. Ed.
2017, 56, 6813–6817



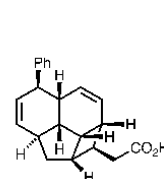
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Angew. Chem. Int. Ed.
2016, 55, 8421–8425



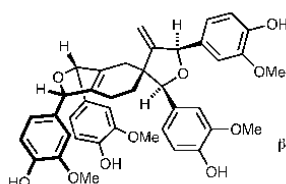
kingianic acid E
8 steps

Chem. Sci. 2015,
6, 3886–3890



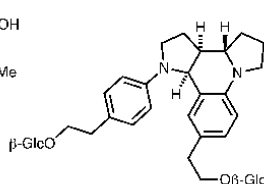
endiandric acid A
8 steps

Chem. Sci. 2015,
6, 3886–3890



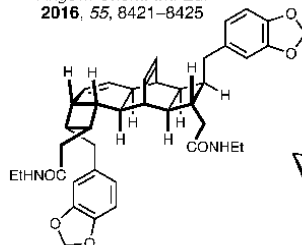
ramonanin A (B-D)
7 steps

Angew. Chem. Int. Ed.
2015, 54, 1795–1798



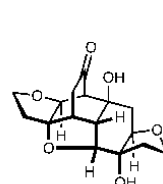
incargranine B
6 steps

Angew. Chem. Int. Ed.
2013, 52, 13273–13275



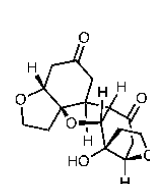
kingianin A (D & F)
10 steps

Angew. Chem. Int. Ed.
2013, 52, 4221–4224



incarvilleatone
4 steps

Org. Lett. 2012,
14, 4537–4539



incarviditone
4 steps

Org. Lett. 2012,
14, 4537–4539

Keywords: total synthesis, biomimetic synthesis, enantioconvergent reactions, dimeric natural products



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10th Brazilian Conference on Natural Products XXXVI RESEM

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ROUND TABLE REVOLUTIONIZING DATA SHARING ADVANCES NP RESEARCH

Jean-Luc Wolfender^{1,2} in the name ‘The NoBS Consortium’ and Norberto Peporine Lopes³

Jean-luc.wolfender@unige.ch

¹*Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, CMU, 1211 Geneva, Switzerland,* ²*School of Pharmaceutical Sciences, University of Geneva, CMU, 1211 Geneva, Switzerland,* ³*Núcleo de Pesquisas em Produtos Naturais e Sintéticos, Departamento de Ciências BioMoleculares, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, 14040-903 Ribeirão Preto-SP, Brazil*

Presentation The noBS Consortium:

Rooted in natural product chemistry, pharmacognosy, and chemical ecology, our consortium was founded in 2019 to link expertise in the analysis of natural and bioactive molecules, health products and drugs, including metabolomic, chemical, ecological and pharmaceutical analysis.

Our ultimate goal is to advance all natural product related fields, including the biomedical sciences, by harnessing the power of FAIR sharing of raw data spectroscopic data, particularly NMR data, computational spectroscopy, and theoretical chemistry via the development and dissemination of modern analytical chemistry technologies. We seek to build capacity by integrating this information with other spectral/ structural raw data.

The aim of this session is to briefly present the noBS Consortium’s perspective on data sharing in natural product (NP) research: ideally, all spectroscopic data used for NP identification should be searchable and openly accessible by the community to accelerate discoveries across NPs, chemical ecology, and biomedical sciences. By fostering FAIR (Findable, Accessible, Interoperable, and Reusable) data sharing—particularly for raw spectral and structural datasets—the consortium seeks to eliminate information silos and enable new findings through community-driven access and collaborative research.

For more information <https://nobs.naturalproducts.net/>

Keywords: NMR, Spectroscopic data sharing in Natural Product Research, noBS Consortium



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***IN VITRO AND IN VIVO PHARMACOLOGICAL ACTIVITIES OF ESSENTIAL OILS
FROM AMAZONIAN SPECIES***

Pablo Luis Baia Figueiredo¹

pablo.figueiredo@uepa.br

1- Departamento de Ciências Naturais, UEPA, PA, Brazil.

The Amazon is home to a remarkable diversity of aromatic plants, making it a key source of essential oils with significant pharmacological potential. This lecture will delve into the fundamental aspects of researching these natural resources, from the collection and taxonomic identification of botanical material to the standardization of selection and chemical analysis processes. We will present results from in vitro and in vivo assays, showcasing compelling biological activities such as antioxidant, anti-inflammatory, and analgesic effects, as well as acute toxicity assessments. We will spotlight Amazonian species such as *Hyptis crenata*, *Ayapana triplinervis*, and *Lippia alba*, each with a unique chemical profile that contributes to their consistent pharmacological activities. Lastly, we will underscore how the study of these aromatic plants not only enriches our scientific understanding of regional biodiversity but also paves the way for the development of therapeutic and biotechnological alternatives based on Amazonian resources.

Keywords: *essential oils; Amazonian species; experimental pharmacology; medicinal chemistry.*



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**DEVELOPMENT OF SKINCARE FORMULATION FROM A MALPIGHIACEAE
PLANT WITH ANTI-AGING PROPERTIES**

Lorena Ramos Freitas de Sousa

lorennarf@ufcat.edu.br

*Laboratório de Bioquímica e Química Orgânica (LaBiOrg), Instituto de Química, IQ, UFCAT, Av.
Dr. Lamartine Pinto de Avelar, 1120 Setor Universitário, CEP: 75704-020, Catalão, Goiás, Brazil.*

The topical application of antioxidant agents combined with enzyme inhibitors in cosmetic formulations helps reduce hyperpigmentation and delay skin aging. Elastase and tyrosinase are key enzymes targeted in the development of active ingredients with anti-aging and skin-brightening properties.^[1,2] Natural products (NPs) are widely used in cosmetics, and many of their secondary metabolites have demonstrated notable enzyme-inhibitory potential.^[1-3] We have been investigating the sustainable use of active ingredients derived from plants collected in the Cerrado biome for the development of phytocosmetic formulations.^[4] One species belonging to the Malpighiaceae family has shown anti-elastase potential and low cytotoxicity. An active extract obtained from its leaves was incorporated into cosmetic formulations such as a cream and facial gel at BIOCAP company. Accelerated stability tests revealed that the extract remains promising when incorporated into cosmetic formulations.

Keywords: *Malpighiaceae, skincare formulation, elastase*

References: [1] Calleja-Agius, J.; BRINCAT, M.; BORG, M. Skin connective tissue and ageing. *Best. Pract. Res. Clin. Obstet. Gynaecol.* 27: 727-740, 2013.

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Acknowledgements: BIOCAP, National Council for Scientific and Technological Development (CNPq) (Process 403611/2020-2, MAI/DAI Program at UFCAT), Goiás State Research Support Foundation (FAPEG, 202310267001406) and FUNAPE.





***DRUG DISCOVERY AT CNPEM: NEW TOOLS AND OPPORTUNITIES FOR THE
NATURAL PRODUCT COMMUNITY***

Daniela B. B. Trivella^{1*}

daniela.trivella@lnbio.cnpem.br

*1-Brazilian Biosciences National Laboratory (LNBio), Brazilian Center for Research in energy and
Material (CNPEM), 13083-100, Campinas, SP - Brazil.*

In this talk the Drug Discovery platform in operation at CNPEM will be presented, along with the open access methods developed by the team. A special focus will be given to the Bank of Molecules collaborative program, the software “NP³ MS workflow”¹² and the “NP³ ligand”³ package. The Bank of Molecules is an open collaborative Program aimed to empower Brazilian natural product bioprospection, with activities done in synchrony at CNPEM and at partner laboratories. All academic groups are invited to be part of this Program. The “NP³ MS workflow” is an open access software used to accelerate bioprospection, enhancing molecular mapping using untargeted metabolomics and data analytics approaches. The NP³ ligands open package consists of a chemically labeled database (LigPCDS⁴⁵) of protein ligands and a software application (NP³ BlobLabel⁶) that work on trained deep learning models, based on LigPCDS, to decipher chemical structures - even of previously unknown molecules. The “NP³ ligand” package is based on protein crystallography data and can be used at different stages of bioprospection, starting from directly capturing of bioactive compounds from natural product mixtures, further revealing the binding sites of these molecules in their pharmacological targets.

Keywords: *natural product bioprospection, LC-MS/MS untargeted metabolomics, high throughput protein crystallography, deep learning, drug discovery and development.*

References:

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*TOAD POISON: A RETROSPECTIVE OF FOURTEEN YEARS OF
RESEARCH - SECONDARY METABOLITES, BIOLOGICAL ACTIVITIES,
ENVIRONMENTAL INTERACTION, DEVELOPMENT METHODS AND
STRUCTURAL MODIFICATION*

Gerardo Magela Vieira Júnior

magela@ufpi.edu.br

*Laboratório de Produtos Naturais - Departamento de Química, Universidade Federal do Piauí, Piauí,
Brazil*

Toad poison is a fascinating source of bioactive secondary metabolites, such as alkaloids, arginine derivatives, biogenic amines, bufotoxins and bufadienolides, among others like peptides and proteins. Over fourteen years researching toad poison, our group has worked with toad species from Amazon, Cerrado and Caatinga Brazilian biomes. Anurans of the Bufonidae family have a pair of parotid glands, present in the dorsolateral region of the body, which store biological secretions of high toxicity and varied chemical composition, having the function of defense against infections, microorganisms, and predators. In my research, approximately 70 compounds were identified and/or isolated from toad poison species of Bufonidae family (*Rhinella marina*, *R. jimi*, *R. diptchya*, *R. granulosa*, *Rhaebo guttatus*), mainly bufadienolides and alkaloids. A large number of biological activities of extracts and/or isolated compounds were evaluated, such as cytotoxic, antiparasitic, antitumor, Na, K-ATPase inhibition, phytoalexin induction, antibacterial, antifungal, acetylcholinesterase inhibition and larvicidal, where the extracts and/or compounds presented promising potential in many of these activities. The metabolomic and ionic profiles of *Rhinella jimi* were investigated in different biomes in the state of Piauí - Brazil, where it was observed that PCA revealed that abiotic factors such as biome and seasonality influence in the ionome but did not show significantly differences in their secondary metabolites. A comprehensive approach combining analytical and chemometric techniques was developed to investigate the venom profile (peptides and proteins). Two quantification methods for bufadienolides were established: one using HPLC-UV for specific bufadienolides and another using UV-Vis for total bufadienolides found in toad poison. Currently, some bufadienolides are being submitted to reactions to obtain acylated and amino-ester derivatives, aiming to enhance their cytotoxic and antiparasitic activities.

Keywords: *Toad poison, secondary metabolites, biological activities, environmental interaction, development methods, structural modification*





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TOWARDS A GREENER NATURAL PRODUCTS CHEMISTRY

Cristiano Soleo Funari^{1*}, Daniel Rinaldo², Vanderlan da Silva Bolzani³, Robert Verpoorte⁴,
Leonardo de Oliveira Sartori¹, Lucas Apolinário Chibli¹, Bruna Ribeiro de Lima¹, Serhat
Sezai Cicek⁵, Verena Spiegler⁶

cristiano.funari@unesp.br

1-Green Biotech Network, School of Agricultural Sciences, São Paulo State University, Av. Universitária, 3780, Botucatu, SP, 18610-034, Brazil. 2-Green Biotech Network, School of Sciences, São Paulo State University, Bauru, SP, 17033-360, Brazil. 3- NuBBE, Institute of Chemistry, São Paulo State University, Araraquara, SP, 14800-900, Brazil. 4- Institute of Biology, Leiden University, Leiden, 2300RA, The Netherlands. 5- Hamburg University of Applied Sciences, Hamburg, 21033, Germany. 6- Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Münster, 48149, Germany.

This presentation will begin with an overview of how phytochemists have responded to the principles of green chemistry since 1990, the year the U.S. Environmental Protection Agency introduced the Pollution Prevention Act - a landmark initiative widely regarded as a catalyst for enhancing sustainability across various branches of chemistry. Particular emphasis will be placed on the role of solvents, which represent a major environmental concern in chemistry as a whole, and in natural products chemistry in particular. It will be shown that some advances in terms of sustainability have been observed in the extraction stage, but also that they are not yet broadly validated from a process perspective aiming to isolate natural products. In contrast, purification processes have seen little evolution, with hazardous solvents and suboptimal methodologies still commonly employed. The talk will then highlight some original contributions from the speaker's research group towards more sustainable natural products chemistry practices. Finally, six recommendations for performing natural products chemistry consistent with the guidelines of green chemistry will be proposed.

Keywords: green solvents, alkaloid extraction and pre-purification, bitter acids extraction



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UNCOVERING BIOACTIVE AGENTS FROM AMAZONIAN MYRTACEAE WITH ANTIDIABETIC AND ANTIVIRAL ACTIONS: A 15-YEAR RESEARCH OVERVIEW

Marcos B. Machado^{1*}, Andrezza S. Ramos¹, Kidney O.G. Neves¹, Edinilze S. C. Oliveira¹, Leonard D.R. Acho², Natasha M. Cassani³, Flávia L. D. Pontes⁴, Emerson S. Lima², Francinete R. Campos⁴, Francisco Celio M. Chaves⁵, Edgar A. Sanches⁶, Jaqueline de A. Bezerra⁷, Alan D. C. Santos^{1,8}, Ana Carolina G. Jardim³

marcosmachado@ufam.edu.br

1-NEQUIMA, Departamento de Química, ICE, UFAM, 69067-005, Manaus, AM, Brazil. 2- FCF, UFAM, 69067-005, Manaus, AM, Brazil. 3-Laboratório de Pesquisa Antiviral, UFU, 38405-302, Uberlândia MG, Brazil, 4- Departamento de Farmácia, UFPR, 80210-170, Curitiba, PR, Brazil, 5- Embrapa Amazônia Ocidental, 69010-970, Manaus-AM, Brazil, 6-Laboratorio de Polimeros Nanoestruturados, ICE, UFAM, 69067-005, Manaus, AM, Brazil, 7- IFAM, 69020-120, Manaus, AM, Brazil, 8- Núcleo de Pesquisa de Produtos Naturais, UFSM, 97105-900, Santa Maria, RS, Brazil

The Amazon biome, which covers nearly half of Brazil's territory and represents 25 % of the world's remaining forests, has long been the focus of multidisciplinary research. Biologists, pharmacologists, chemists, and other specialists have identified metabolites with significant potential for the pharmaceutical, agrochemical, cosmetic, and food industries. However, achieving the sustainable use of this biodiversity has posed a challenge for Brazilian governments over the last 60 years. Production, quality control of natural resources, and logistics have been the main bottlenecks to the region's sustainable development. In this context, the NEQUIMA (Núcleo de Estudos Químicos de Micromoléculas da Amazônia) research group, in partnership with the UFAM NMR Laboratory and partner institutions, is dedicated to identifying compounds with antiglycation, antiviral, and nutraceutical potential in Amazonian matrices, employing NMR and MS as its principal analytical tools. Furthermore, NEQUIMA develops encapsulated bioproducts and NMR-based analytical methods to quantify active ingredients, while also contributing to the discovery of new antiglycation and antiviral compounds. Through these activities, NEQUIMA contributes to the training of human resources (undergraduate, master's, and doctoral levels in Chemistry), to the publication of scientific articles, and to the valorization and sustainable development of the Amazon biome.

Keywords: Amazon, ¹H NMR-based metabolomics, qNMR, antiglycan, antiviral, chemometrics

Acknowledgements: FAPEAM, CNPq, CAPES, and FINEP agencies.





***ANIMAL NATURAL PRODUCTS: IDENTIFICATION AND/BY SYNTHESIS OF
NOVEL STRUCTURES FROM SPRINGTAILS AND FROGS***

Stefan Schulz*

Stefan.schulz@tu-braunschweig.de

Institute of Organic Chemistry, Technische Universität Braunschweig, Braunschweig, Germany.

Compared to plants, microorganisms, or fungi, secondary metabolites of terrestrial animals have been less often investigated, except perhaps for insects. One of those neglected groups are Collembola, important soil-dwelling arthropods often occurring in large numbers. They constitute a sister lineage to the Insecta, but the common precursor dates back to more than 450 mya. This long time leads to surprising differences in the secondary metabolites of these lineages that will be discussed. We focused our studies on three aspects, which are important in Chemical Ecology: epicuticular lipids, defense compounds, and volatile signals. Several difficulties must be overcome when working with these animals, namely their small size, difficult and slow rearing, and often uniform appearance. However, with trace analytical techniques and chemical synthesis, we could show that springtails often rely on the terpenoid biosynthetic pathway for both epicuticular lipids and signals. For defense, compound classes are produced that are not known from other genera.

While the defense chemistry of certain frog lineages is well explored, their chemical communication systems are rarely investigated. Certain groups developed gular or femoral glands that are likely used in chemical communication. Our results show that batrachopolyenes, unusual hydrocarbon steroids with a *nor*-A-ring, are found in several distinct lineages, suggesting a common precursor. In contrast, highly diversified macrocyclic lactones are used mainly within the Mantellinae and seem to represent a derived compound class. Related lactones occur in various sources, such as insects, bacteria, or mammals, indicating a preferred structural motif that was introduced several times independently during evolution.

We report here on the identification of these compounds, which proved quite difficult due to the small amounts of material available or conservation restrictions. Therefore, GC/MS, GC/IR, and various other methods were used for structure confirmation, including total synthesis, because NMR analysis was only possible in some cases.

Keywords: *Steroids, macrocyclic lactones, GC/MS, terpenoids, total synthesis*





FROM SILENCE TO SOLUTIONS: THE HIDDEN LANGUAGE OF PLANTS AND INSECTS IN PEST MANAGEMENT.

Maria Carolina Blassioli Moraes¹, Miguel Borges¹, Raul A Laumann¹, Mirian F.F. Micheref¹

carolina.blassioli@embrapa.br

1. Laboratório de Semioquímicos- Embrapa Recursos Genéticos e Biotecnologia, Brasília-DF

Plants and insects communicate mainly through volatile molecules known as semiochemicals. These compounds, when released by plants in response to herbivore injury, are called herbivory-induced plant volatiles (HIPVs) and serve as cues for natural enemies, helping them locate their prey or hosts. Herbivores also rely on these volatiles to obtain critical information about the plant's condition, for instance, whether it is already colonized by conspecifics or other herbivores, or if it is infected by pathogens. The production and composition of these volatile blends are influenced by several factors, including the developmental stage of the plant, herbivore density, and the identity of the herbivore species. As a result, plant volatile profiles are often species-specific and can even vary among different plant genotypes. Insects depend on efficient chemical communication for survival. Through chemical cues emitted by other insects or plants, they can recognize mates, avoid enemies, and select suitable oviposition or feeding sites. Pheromones play a vital role in mating and survival strategies. In this Conference, we will present studies that demonstrate the influence of plant volatiles on both natural enemies and herbivores in different agricultural systems, cotton, maize, and soybean, and the potential of using the HIPVs for pest control. Furthermore, research conducted over the past 25 years in Brazil has led to the identification of pheromones from several key neotropical insect species, such as *Diatraea saccharalis* (a major pest of sugarcane) and *Euschistus heros* (a primary pest of soybean). These discoveries provide a strong foundation for the development of innovative and sustainable pest control strategies based on semiochemicals.

Keywords:





ROUND TABLE LECTURES

**BIOMES AT RISK: THE IMPACT OF
ENVIRONMENTAL POLICIES ON
BRAZILIAN BIODIVERSITY**

4-7 November 2025, Belo Horizonte, MG, Brazil

**ARTIFICIAL INTELLIGENCE AND BIOMES: BIOINFORMATICS AND
CHEMINFORMATICS IN SUPPORT OF BIODIVERSITY CONSERVATION AND
SUSTAINABLE USE**

Raquel Cardoso de Melo Minardi^{1*}

raquelminardi@gmail.com

*1-Departamento de Ciência da Computação, ICEx, Universidade Federal de Minas Gerais,
MG, Brazil.*

The advance of climate change and inadequate environmental policies has put the rich biodiversity of Brazilian biomes at risk. In this context, the integration of data science, artificial intelligence (AI), and bioinformatics can offer innovative and sustainable solutions. This presentation will discuss how AI methods — with an emphasis on deep neural networks, structural bioinformatics, and cheminformatics — have been applied to the discovery, screening, and prediction of natural products with pharmacological and agricultural potential derived from Brazilian biodiversity. I will present computational approaches that integrate molecular, structural, and functional data, aiming not only to accelerate the identification of bioactive compounds but also to prioritize species and ecosystems of biotechnological interest, contributing to conservation strategies driven by the bioeconomy. By exploring the chemical potential of biomes through digital tools, it is possible to support the formulation of evidence-based public policies that combine environmental protection with sustainable development, especially in regions of high vulnerability and biological richness.

Keywords: *Artificial intelligence, machine learning, bioinformatics.*





10th Brazilian Conference on Natural Products

XXXVI RESEM

4-7 November 2025, Belo Horizonte, MG, Brazil

***SUSTAINABLE USE OF MEDICINAL PLANTS IN TIMES OF CLIMATE CHANGE:
AN URGENT CALL FOR NEW RESEARCH STRATEGIES***

Javier Echeverría^{1*}

javier.echeverriam@usach.cl

1-Departamento de Ciencias del Ambiente, Facultad de Química y Biología, Universidad de Santiago de Chile, Santiago, Chile.

Climate change and human activities severely threaten the viability of plants and ecosystems, endangering the environment, biodiversity, and the sustainable development of plant-based products. Biotic and abiotic (ecosystem) factors influence species distribution and long-term survival, which in turn affect the quality of plants used as herbal medicines and other high-value products. In recent decades, various human impacts have significantly compromised these quality aspects. Climate change, overharvesting, habitat destruction, species vulnerability, and other factors have negatively affected the growth, reproduction, and adaptation of species populations, as well as the quality and quantity of primary plant materials supplied to pharmaceutical markets. Despite these increasing challenges, little is known about effective strategies to prevent or lessen these impacts, especially for vulnerable species collected from the wild or harvested from traditional production systems. Therefore, urgent strategies to conserve and augment plant populations are needed. This study introduces a new framework that incorporates the main sustainability factors to better understand and address species' vulnerability, helping to reduce the effects of climate change. The framework's usefulness was tested through seven case studies of vulnerable species (i.e., *Aquilaria malaccensis* Lam., *Boswellia sacra* Flück., *Crocus sativus* L., *Panax quinquefolius* L., *Pilocarpus microphyllus* Stapf ex Wardlew., *Rhodiola rosea* L., and *Warburgia salutaris* (G.Bertol.) Chiov.) from major biogeographic regions, all widely used as medicinal plants. These species present various challenges to their sustainability, impacting their current and future status both locally and globally. Their economic significance, combined with growing demand and risks of overexploitation, is also a critical concern. The proposed framework for the sustainability of medicinal and other high-value plant-based products in the phytopharmaceutical industry highlights strategies that promote conservation and sustainable resource use. It can also be adapted for other vulnerable species that require immediate attention.

Keywords: *climate change, conservation strategies, ecosystem factors, endangered medicinal plants, ethnopharmacology, key sustainability indicators, sustainable practices, traditional medicine.*



Sociedade Brasileira de Química
Divisão de Produtos Naturais



SPATIAL INTELLIGENCE FOR NATIONAL-SCALE RESTORATION: A LINEAR-PROGRAMMING FRAMEWORK TO PRIORITIZE AREAS FOR NATIVE VEGETATION RECOVERY ACROSS BRAZILIAN BIOMES

Renata de Toledo Capellão*, Luiz Gustavo Oliveira, Diogo Rocha, Clarice Braúna Mendes, Viviane Dib, Mariana Iguatemy, Helena Alves

r.capellao@iis-rio.org

Instituto Internacional para Sustentabilidade - IIS, Rua João Borges, 215 - Gávea, 22451-100, Rio de Janeiro/ RJ, Brazil.

Large-scale ecological restoration is a cross-cutting pathway to deliver benefits for biodiversity, climate, and water security. Brazil's updated National Plan for Native Vegetation Recovery (Planaveg 2025–2028) adopts spatial intelligence to guide restoration towards areas of highest impact, while halving associated costs. Here, we present the methodological framework and preliminary results of a nationwide prioritization that integrates ecological and socio-economic criteria, along with feasibility and cost factors, to rank all restoration-eligible areas across Brazilian biomes at 1 km resolution. Input data include multiple spatially explicit layers representing the relative contribution of restoration to biodiversity gains, climate change mitigation, water resources improvement, and socio-economic returns, in addition to the implementation and opportunity costs associated with restoration process. Prioritizations were conducted independently for each biome, with model parameters and benefit weights adjusted according to expert recommendations gathered in technical workshops. For each biome, two sets of scenarios are reported: (i) *Maximum Benefits Scenario*, pointing areas targeting optimal return for benefit criteria and (ii) *Cost-effective Scenario*, that identifies areas that present higher cost-benefit relationship. For each scenario, the framework delivers a restoration-priority ranking map by ordering all planning units until 100% of restorable areas are classified, yielding a biome-level priority gradient in 5%-point steps (20 classes). Additionally, optional spatial constraints by state and Otto level-2 basins were analyzed to ensure territorial representation. This cumulative ranking allows us to quantify stepwise gains as a function of total area restored and to assess the incremental ecological return of alternative strategies. Results deliver a transparent, reproducible decision surface that identifies where restoration can most efficiently improve biodiversity and ecosystems benefits while revealing trade-offs once implementation and opportunity costs are considered.

Keywords: *linear programming; spatial prioritization, ecosystem restoration*

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10th Brazilian Conference on Natural Products
XXXVI RESEM

ORAL SESSION ABSTRACT



CHEMICAL CHARACTERIZATION OF *LYCHNOPHORA PIRANIANA*: A NEW SPECIES NAMED IN HONOR OF PROFESSOR JOSÉ RUBENS PIRANI

Manuela Pezzato Toledo Prado^{1*}, Marília Ellias Galon¹, Marcelo Monge^{1,2}, Norberto Peporine Lopes¹.

manuela.pezzato@usp.br

1-Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Núcleo de Pesquisa em Produtos Naturais e Sintéticos - Universidade de São Paulo (USP), Avenida do Café, s/n, CEP 14040-903, Ribeirão Preto, SP, Brasil. 2-Plant Biology Graduate Program, Institute of Biology, Federal University of Uberlândia, Av. Ceará, 1188 - Umuarama, CEP 38405-240, Uberlândia, MG, Brasil.

The genus *Lychnophora* (Asteraceae) comprises approximately 30 species endemic to Brazil, primarily distributed in the rupestrian fields of the *Cerrado* and *Serra do Espinhaço*. Popularly known as 'arnicas', these plants are traditionally used in folk medicine for their anti-inflammatory and analgesic properties in the alternative treatment of muscle pain, contusions, and inflammations. Studies have demonstrated that *Lychnophora* species are rich in specialized metabolites such as flavonoids, diterpenes, and sesquiterpene lactones, which are frequently associated with various pharmacological activities, including anti-inflammatory and antioxidant effects. Beyond their ethnobotanical significance, *Lychnophora* species also hold economic relevance, particularly in the production of cosmetics and phytotherapeutics like anti-inflammatory creams and essential oils. Recently, novel species have been described to the genus, enriching taxonomic knowledge and expanding the possibilities for discovering bioactive compounds with the potential for developing new therapies.

This project aimed to perform the chemical characterization of *Lychnophora piraniana*, a new *Lychnophora* species named in honor of botanist José Rubens Pirani, whose contributions to the Brazilian flora are significant to the genus. Using liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) followed by data mining techniques, 230 metabolites were detected. Among these, several phenolic compounds, including flavonoids and hydrocinnamic acid derivatives, and sesquiterpene lactones were annotated. The detailed characterization of these compounds can reveal novel substances, contributing to the development of innovative therapeutic products and highlighting Brazilian biodiversity.

Keywords: *Lychnophora piraniana*, Metabolomics, Mass Spectrometry (LC-MS/MS), Natural Products and Asteraceae





QUALITY BY DESIGN APPLIED TO THE PRODUCTION OF THE HERBAL MEDICINE FROM *Monteverdia ilicifolia* (Mart. ex Reiss.) Biral

Alberto Araujo de Caux^{1*}, Rodney Alexandre Ferreira Rodrigues¹

aaraujodecaux@gmail.com

- 1- Centro Pluridisciplinar de Pesquisas Químicas, Biológicas e Agrícolas - CPQBA UNICAMP, Av. Alexandre Cazellato, 999, Betel, Paulínia/SP 13148-218;

With the advancement of quality tools, new opportunities have emerged to study and optimize processes that were previously not systematically controlled. In this context, Quality by Design (QbD) stands out as a strategic approach to ensure the efficacy, safety, and quality of herbal medicines, such as those derived from *Monteverdia ilicifolia* (Mart. ex Reiss.) Biral, commonly known as "Espinheira Santa", which is recognized for its antidyspeptic, antacid, and gastric mucosa-protective properties ⁽¹⁾. This study aimed to evaluate the extraction and spray-drying processes for obtaining an Espinheira Santa herbal medicine using QbD principles. Through process mapping and risk assessment, potentially critical factors were identified and subsequently challenged by means of Design of Experiments (DoE). For the extraction step, a 12-run Plackett–Burman design (8 factors) was conducted; for scaling-up, a Central Composite Design (CCD) with 7 runs (2 factors) was applied; and for the spray-drying step, a Rotational Central Composite Design (RCCD) with 17 runs (3 factors) was carried out. The response variables studied in each design were those related to Critical Quality Attributes (CQAs), that is, attributes that impact efficacy and safety ⁽²⁾. The effects (linear, quadratic, and interaction) were estimated, and the models were evaluated by ANOVA using the statistical software RStudio Version 4.4.0. Factors showing significant effects (p-value < 0.1) were identified as critical ⁽³⁾. In the extraction step, the following factors were significant for at least one CQA: “extraction type” (decoction or infusion), “drug-to-extract ratio” (1% to 6%), “herbal drug form” (cut or powdered), “vessel type” (glass or metal), “water quality” (purified or distilled), “exposure” (open or closed), “boiling time” (2 or 5 min), “stirring” (0 to 600 rpm), and “extraction time” (10 to 30 min). In the spray-drying step, maltodextrin addition (0 to 60%), feed rate (3.5 to 7.5 mL/min), and inlet temperature (120 to 200 °C) were significant for at least one CQA. In conclusion, the QbD approach enabled the identification of critical factors associated with the extraction and spray-drying processes of Espinheira Santa, ensuring process capability.

Keywords: Espinheira Santa, Extraction, Design of Experiments, Scaling-up, Spray drying.

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Acknowledgments: CNPq, COCEN.





SPATIAL METABOLOMICS REVEALS THE ROLE OF PENICILLIC ACID IN CHEESE RIND MICROBIOME DISRUPTION BY A SPOILAGE FUNGUS

Carlismari Oliveira Grundmann^{1*}, Christopher Tomo², Julia Hershelman², Benjamin Wolfe², Laura Sanchez¹

cgrundma@ucsc.edu

1- Department of Chemistry and Biochemistry - University of California Santa Cruz, UCSC, 1156 High Street, Santa Cruz, CA, USA. 2- Department of Biology, Tufts University, 200 College Avenue, Medford, MA, USA.

Microbial interactions in cheese rinds influence community structure, fermentation, and the development of sensory properties such as flavor, aroma, and texture^{1,2}. However, the chemical mechanisms mediating these interactions in cheeses and other fermented foods remain poorly understood. Here, we investigated how the spoilage mold *Aspergillus westerdijkiae* chemically inhibits beneficial cheese-rind bacteria using microbial community assays, transcriptomics, MALDI-MSI, LC-MS/MS, and genome mining. In cheese rind community and co-culture experiments, *A. westerdijkiae* strongly inhibited bacterial growth, with pronounced effects on *Staphylococcus equorum* and *Brachy bacterium alimentarium*. In co-culture with *S. equorum*, transcriptomic profiling revealed broad changes, including upregulation of a putative *bceAB* gene associated with resistance to antimicrobial compounds. The integration of MALDI-MSI, fungal genome mining, and LC-MS/MS revealed spatially localized production of bioactive metabolites at the fungal–bacterial interface, such as notoamides and circumdatins. Additionally, the mycotoxins penicillic acid and ochratoxin B showed broader spatial diffusion compared to the other metabolites, suggesting their primary role in community disruption. The presence of these mycotoxins was confirmed by LC-MS/MS comparison with commercial standards, with penicillic acid concentrations increasing 2.5-fold in co-culture with *B. alimentarium* compared to monoculture. In contrast, interactions with *S. equorum* did not show the same increase but triggered production of distinct metabolites, such as notoamides, underscoring a partner-specific metabolic response. To validate ecological function, purified penicillic acid was tested in cheese curd agar bioassays. After 10 days of exposure, increasing concentrations (10, 100, 1000 µM) produced progressively stronger inhibition of *B. alimentarium*, with only minor effects on *S. equorum* at these concentrations. These results show that *A. westerdijkiae* deploys a context-dependent arsenal of mycotoxins and indole alkaloids, with responses varying by bacterial partner, suggesting species-specific chemical strategies. Together, our findings show that fungal chemical mechanisms disrupt cheese-rind communities by inhibiting beneficial bacteria, leading to likely negative sensory outcomes with implications for microbial ecology and food safety.

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Keywords: natural rind cheese, fungal-bacterial interaction, mycotoxins, imaging mass spectrometry





ANALYSIS OF THE CHEMICAL, ANTIOXIDANT AND ANTI-INFLAMMATORY PROPERTIES OF *Swinglea glutinosa* (Bl.) Merr.

Christian Fernando Lizalda-Aponte¹, Valentina Castaño Mosquera¹, Luz Angela Veloza¹, Juan Carlos Sepúlveda Arias², Monica Cala³, Francisco Javier Jiménez-González^{1*}

jjimenez@utp.edu.co

1-Grupo Polifenoles, Facultad de Tecnología, Universidad Tecnológica de Pereira, Pereira, Colombia. 2-Grupo Infección e Inmunidad, Facultad de Ciencias de la Salud, Universidad Tecnológica de Pereira, Pereira, Colombia. 3-MetCore, Vicerrectoría de Investigación e Innovación, Universidad de los Andes, Bogotá, Colombia.

Swinglea glutinosa (Bl.) Merr. (Rutaceae) is a shrub native to the Philippines. In traditional medicine, it has been used to treat skin conditions and hemorrhages, while in Colombia it is used for joint inflammation. Despite its ethnobotanical use, the information on its chemical composition and biological properties is limited, which motivated the present study. The research focused on the characterization of polar metabolites from the pulp, peel, and leaves of *S. glutinosa*, as well as the evaluation of its antioxidant and anti-inflammatory potential *in vitro*. Extracts were obtained from the fruits and leaves using butanol and water. These extracts were characterized by RP-LC-ESI/MS-QTOF, and their metabolites were annotated using bioinformatics tools such as MS-DIAL, SIRIUS, and GNPS molecular network. The antioxidant activity was determined through Folin-Ciocalteu, DPPH, and ORAC assays. The anti-inflammatory activity was evaluated in LPS-stimulated RAW264.7 murine macrophages. The levels of inflammatory mediators such as PGE2, NO, IL-1 β , IL-6, IL-10, and TNF- α were measured using specific kits and reagents. The results of the molecular characterization of the *S. glutinosa* extracts showed the presence of glycosylated flavonoids, alkaloids, and hydroxycarboxylic acids, with a particular abundance of apigenin and its isomers. The total phenol content in the pulp and peel extracts was 31,3 and 9,3 mg EAG/g Extract, respectively. Regarding antioxidant activity, the pulp and peel extracts inhibited the DPPH radical by 22,9% and 19,5% (at 150 μ g/mL). The ORAC method highlighted the pulp and leaf extracts, with values of 2410,16 and 2802,9 μ molTE/g. In the evaluation of anti-inflammatory activity, the butanolic fruit extracts inhibited the biosynthesis of PGE2, IL-1 β , and IL-6 by more than 50% after 24 h. Additionally, it was observed that the extracts modulated the mRNA expression of target genes such as iNOS, IL-1 β , and IL-6. Preliminary cytotoxicity assay results, in normal cells Hek-293 using the MTT method, indicate that the extracts do not contain lethal compounds.

Keywords: *Swinglea glutinosa*, LC-MS, anti-inflammatory mediators, ROS, phytochemistry, *In silico*.





ANTARCTIC LICHENS AS A PLATFORM TO DISCOVER BIOACTIVE MOLECULES WITH NEUROPROTECTIVE AND ANTI-INFLAMMATORY POTENTIAL

Cristian Cordero¹, Gerald Zapata ², Karem Henriquez ³, Iván Opazo-Aballay¹, Mario Aranda⁴

cristiancordero07@gmail.com

1 Laboratorio de Investigación de Alimentos y Medicamentos (LIFA). Facultad de Química y Farmacia. Pontificia Universidad Católica de Chile. Santiago, Chile. 2 Molecular Graphics Suite, Facultad de Ciencias Químicas y Farmacéuticas, Universidad de Chile, Santiago, Chile. 3 Laboratorio de Biotecnología y Genética de Alimentos (BGA), Facultad de Ciencias, Universidad del Bío-Bío. Chillán, Chile.

Antarctic lichens endure extreme cold, intense UV radiation, strong winds, and chronic nutrient scarcity—pressures that drive distinctive secondary metabolism. We investigated eight Antarctic lichens as a source of bioactive molecules with neuroprotective and anti-inflammatory potential. To link chemistry with function, we applied an **effect-directed analysis (EDA)** integrating **HPTLC bioassays**, **LC-MS profiling**, and **molecular docking**, enabling the pinpointing and characterization of **COX-2** and **acetylcholinesterase (AChE)** inhibitors. Chemical profiling revealed a landscape dominated by depsides, depsidones, dibenzofurans (notably usnic acid), naphthoquinones, and fatty acids. Functional assays demonstrated COX-2 inhibition, AChE inhibition, and antioxidant activity, consistent with mechanisms relevant to neuroinflammation and oxidative stress. Docking supported plausible binding of representative metabolites within the catalytic sites of COX-2 and AChE, indicating concordance between structure and mechanism. A salient observation was **polypharmacology**. Several metabolites were active across more than one readout: **usnic acid** and **sphaerophorin** consistently exhibited dual antioxidant and enzyme-inhibitory behavior. In addition, an **unusual fatty acid**, **pentahydroxyoxoheptacosanoate**, detected in multiple species, showed **remarkable anti-inflammatory activity**, highlighting underappreciated lipophilic contributors to lichen bioactivity. Collectively, these findings expand the chemical and functional map of Antarctic lichen chemodiversity and underscore their value as reservoirs of drug-like natural products. The integrated **EDA–HPTLC/LC-MS–docking** strategy provides a rapid, efficient route to identify mechanism-anchored leads from complex matrices and prioritizes candidates for cell-based validation in **neuroprotection** and **inflammation** research.

Keywords: lichen, bioactive molecules, neuroprotection, inflammation, COX-2, acetylcholinesterase (AChE)





***CABREUVANOLS A-C, THREE NEW CASSANE-DERIVED DITERPENES FROM
Myrocarpus frondosus AND THEIR ANTI-INFLAMMATORY EFFECTS***

Ana Caroline da Silva^{1*}, Eduardo M. Dalmarco², Beatriz Garcia Mendes Borba²,
Louis P. Sandjo¹

ana.caroline.s@posgrad.ufsc.br

1-LQPN, Department of Chemistry, CFM, UFSC, Campus Universitário Trindade, 88040-900,
Florianópolis, SC, Brazil. 2- Department of Clinical Analysis, CCS, UFSC, Campus Universitário
Trindade, 88040-970 Florianópolis, SC, Brazil

Myrocarpus frondosus (Fabaceae) is a species native to South America, popularly known as Cabreúva, and has been traditionally used for its medicinal properties, especially anti-inflammatory properties [1]. This study aimed to isolate and characterize new metabolites from the bark of this plant, in addition to evaluate their biological activity. Thus, seven compounds were obtained by using successive chromatographic techniques. Three were new cassane diterpenes, trivially named Cabreuvanols A, B, and C (2–4), while the four known compounds were ayapin (1), afromosin 7-O- β -D-apiofuranosyl-(1 $\rightarrow$ 2)-glucopyranoside (5), tyrsifloside (6), and afromosin 7-O- β -D-glucopyranoside (7). Their structure was assigned by the mean of 1D/2D NMR and HR-MS data, while the absolute configuration of cabreuvanol A (2) was confirmed by X-ray crystallography. The crude extract, the fractions, and compounds 1-3 were evaluated for their cytotoxicity against mouse J774 macrophages and for their anti-inflammatory effects through inhibition of nitric oxide (NOx) production [2,3]. The crude extract and fractions showed low cytotoxicity and high capacity to inhibit NOx production, with a significance of 70% inhibition at the tested concentrations, for ethyl acetate (EAF) and dichloromethane (DCMF) fractions. The extract and these two fractions were more potent than the reference drug, dexamethasone, at a dose of 2.75 μ g/mL (20.65 $\pm$ 0.87 μ g/mL). The new compounds, cabreuvanols A and B also showed inhibitory effects. Compound 3 was more cytotoxic than others. Furthermore, anti-inflammatory activity was demonstrated in a murine model of acute lung inflammation (ALI) caused by LPS. In this model, the crude extract and fractions significantly reduced NOx levels, while compounds 1 and 2 moderately reduced NOx by 58.6 $\pm$ 4.7% and 23.4 $\pm$ 8.8%, myeloperoxidase (MPO) activity, exudation, and cell migration in bronchoalveolar lavage fluid, confirming the anti-inflammatory effect in vivo. The results indicate that Cabreúva is a source of bioactive diterpenoids with potential application in the development of anti-inflammatory agents.

The authors would like to thank the institutions, CAPES and FAPESC for its funding support.

Keywords: *Myrocarpus frondosus*, Structure elucidation, Diterpenes, Anti-inflammatory activity

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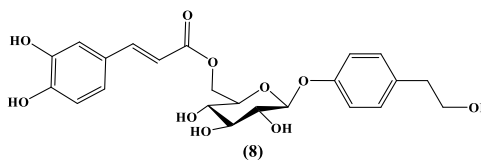
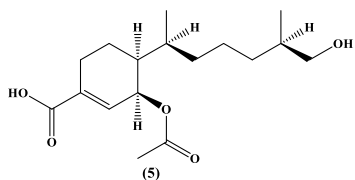
PHYTOCHEMISTRY OF *MOQUINIASTRUM SORDIDUM*: GNPS-GUIDED DEREPLICATION, TWO NEW METABOLITES, AND STEREOCHEMICAL ELUCIDATION USING IPAP/PIP-HSQMBC

Tamires Cordeiro^{1*}, **Francielli Alana Pereira Valeze¹**, Bianca D. B. Sahm², Fernanda F. Dourado¹, Marta R. B. do Carmo³, Letícia Costa Lotufo², Ernani A. Basso¹, Maria Helena Sarragiotto², Debora Cristina Baldoqui¹

alanafranhp@gmail.com

1- Departamento de Química, Universidade Estadual de Maringá, Av. Colombo, 5790, Maringá, PR, Brazil. 2-Instituto de Ciências Biomédicas, Universidade de São Paulo, Av. Prof. Lineu Prestes, 1524, São Paulo, SP, Brazil. 3- Departamento de Biologia Geral, Universidade Estadual de Ponta Grossa, Av. Carlos Cavalcanti, 4748, Ponta Grossa, PR, Brazil.

Recent taxonomic revisions based on molecular phylogenetics transferred species from *Gochnatia* to *Moquiniastrium*, which now includes 22 species, 19 in Brazil's Cerrado and Atlantic Forest. Here, we report a phytochemical study of *Moquiniastrium sordidum*. The plant was extracted with ethanol, yielding a crude extract partitioned into hexane, dichloromethane, ethyl acetate, and hydromethanolic fractions. Dereplication was performed using UHPLC-HRMS with molecular networking. Chromatographic separation afforded nine compounds, including two new metabolites: a sesquiterpene (**5**) and a phenolic glycoside (**8**). Known compounds identified were simiarenol (**1**), oleanolic acid (**2**), hispidulin (**3**), tyrosol (**4**), genkwanin (**6**), and apigenin (**7**). The relative configuration of compound **5** was established using *pip*-HSQMBC-IPAP NMR, which afforded accurate long-range ^{2,3}J_{CH} coupling constants. With four stereogenic centers, conformational searches (CREST) followed by DFT calculations (ORCA) were performed. Comparison between Boltzmann weighted theoretical parameters and experimental data enabled assignment of the absolute configuration as 1*R*, 6*S*, 7*S*, 11*R*. Dereplication enabled the putative identification of 45 metabolites: 12 flavonoids, 10 chlorogenic acid derivatives, 5 hydroxycinnamic acid derivatives, 9 terpenes, and 9 others. Manual inspection of fragmentation patterns, supported by GNPS2 tools, facilitated recognition of structural families within the molecular network. Preliminary cytotoxic screening against HCT-116 cells showed that the dichloromethane fraction inhibited proliferation by 92% at 50 µg/mL, while activity dropped below 50% at 5 µg/mL.



Keywords: *Moquiniastrium sordidum*, *Gochnatia sordida*, dereplication, diagnostic fragment ions.





New insights into cichorine biosynthesis in *Aspergillus nidulans* through bioinformatic and metabolomic analyses

Lucas Penha Dutra¹, Terumi Mascarenhas², Jakob Blæsbjerg Hoof², Uffe Hasbro Mortensen², Diogo Montes Vidal¹, Thomas Ostenfeld Larsen^{2*}

lucaspdutra98@gmail.com

1-Neplam, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 2-DTU Bioengineering, Department of Biotechnology and biomedicine, DTU, Søtofts Plads, 221, Kongens Lyngby, Denmark.

Cichorine is an isoindolinone alkaloid mainly produced by fungi such as *Aspergillus nidulans*. Its derivatives have been reported to display diverse biological activities, including antioxidant, antimicrobial, cytotoxic, and antiproliferative effects against several cancer cell lines¹. Cichorine originates from 3-methylorsellinic acid (3-MOA), and although its biosynthetic gene cluster (BGC) has been described in *A. nidulans*², the functional roles of several genes remain only partially understood, particularly those involved in nitrogen incorporation and oxidation steps. In this work, it was combined bioinformatic with metabolomic analyses of *A. nidulans* mutant strains to further characterize the cichorine biosynthetic pathway. The *A. nidulans* genome (NCBI accession: GCA_000011425.1) was screened with antiSMASH, and Cic BGC protein sequences were analyzed by BLASTp and InterPro. In earlier studies, the Cic BGC was overexpressed, yielding strain NID792, which served as the background for constructing targeted gene deletions. Mutant strains included NID952 (Δ AN6444), NID954 (Δ AN6449), NID956 (Δ AN6447), NID1012 (Δ AN6448), and NID1010 (Δ AN6445). Extracts from these strains were subjected to UHPLC-ESI-HRMS/MS analyses in both positive and negative ionization modes. AntiSMASH predicted 18 genes in the Cic BGC. However, comparative sequence analysis indicated that only five genes are directly involved in cichorine biosynthesis: AN6448 (polyketide synthase), AN6447 (*O*-methyltransferase), AN6445 (GMC oxidoreductase, 49% identity to PatE), AN6449 (CYP450 monooxygenase), and AN6444 (nonribosomal peptide synthase-like – NRPS-like, 40% identity to StbB). The function of AN6448, AN6447, AN6445, and AN6449 had been previously confirmed through metabolomic analyses of mutants² and corroborates with bioinformatic and metabolomic results obtained here. Additionally, it was proposed that the uncharacterized AN6444 Cic gene is involved in the conversion of 3-MOA to its corresponding aldehyde in early steps of cichorine biosynthesis.

Keywords: Cichorine biosynthesis, CRISPR/Cas, HPLC-MS/MS metabolomics.

References: ¹Bailly. *Eur. J. Med. Chem. Rep.*, 9, 100112, 2023.; ²Sanchez et al. *Med. Chem. Comm.*, 3, 997, 2012.

Acknowledgements: UFMG, DTU, CAPES.





MYRICITRIN ACYLATED DERIVATIVES: ENZYMATIC SYNTHESIS, ADMET PROPERTIES, AND DOCKING STUDIES

Natalie Giovanna da Rocha Ximenes^{1,4*}, Nátalie Tavares Delgado¹, João Pedro Neves de Mello², Paula Alvarez Abreu², Marcelo Mignoni³, Shaft Corrêa Pinto⁴, Michelle Frazão Muzitano⁴, Ivana Correa Ramos Leal¹

natalieximenes@gmail.com

1 - Laboratório de Produtos Naturais e Ensaios Biológicos (LaProNEB), Departamento de Produtos Naturais e Alimentos, Centro de Ciências da Saúde, UFRJ. Avenida Carlos Chagas Filho, 373, Rio de Janeiro, RJ, 21941-599, Brazil. 2 - Laboratório de Modelagem Molecular e Pesquisa em Ciências Farmacêuticas. UFRJ- Campus Macaé, Av. São José do Barreto 764, São José do Barreto, Macaé, RJ, Brazil. 3 - URI, Av. Sete de Setembro, 1621 - Fátima, Erechim - RS, 99709-910, Brazil 4 - Instituto de Ciências Farmacêuticas, Centro Multidisciplinar UFRJ Macaé, Av. Aluizio da Silva Gomes, 50, RJ, 27933-378 - Brasil.

Flavonoids constitute one of the largest classes of secondary metabolites and are notable for their pharmacological properties. However, their applicability is limited due to their hydrophilic nature. The use of lipases for enzymatic acylation of these compounds has resulted in greater stability and solubility. This study aims to perform transesterification reactions using nine vinyl esters with Novozyme®435 followed by the isolation of the products. It also aims to perform their ADMET properties and docking evaluation. Each reaction mixture consisted of 22.5 mg of myricitrin, 4.5 - 11.25 mg of the enzyme (Novozyme® 435 lipase (1531 U/g) (from *Pseudozyma antarctica*) (20-50% relative to the amount of flavonoid), and 1.5 mL of the vinyl ester. Exceptionally, the reaction with vinyl benzoate (40 MI) was carried out for 288 h and 29.93 mg of enzyme. For propionate and pivalate reactions, isopropanol (0.5 mL) was used as solvent. The ionic liquid [C₄mim][BF₄] was used alternatively. The reactions were monitored by TLC and the kinetics were established through the obtained relative area percentages by UHPLC-DAD. The highest conversion percentages to monoesters were reached after 144 h, except for the reaction with vinyl propionate, in which the maximum peak was achieved at 72 h. The products furnished isolated yields of 20.20%, 47.91% and 9.8% for myricitrin benzoate, butyrate, and pivalate, respectively; 27.06%, 47% and 30.2% for myricitrin cinnamate, laurate, and neodecanoate, respectively; and 23.1%, 62.7% and 32.8% for myricitrin decanoate, propionate, and stearate, respectively. The structures of the products were elucidated by NMR and Mass Spectrometry, and their ADMET properties were evaluated using ADMETlab 3.0 and VegaHub softwares. Myricitrin propionate and benzoate showed the highest drug score and drug likeness values, and predicted low toxicity in mammalian cells. Docking studies with the enzyme myeloperoxidase — a target of great biological relevance — are currently in progress, as well as their *in vitro* evaluation. The authors would like to acknowledge CAPES, CNPq, and FAPERJ.

Keywords: ADMET, docking, ionic liquids, lipase, myeloperoxidase





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POSTER SESSION ABSTRACT



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Session
Biosynthesis and
Molecular Biology of NP



**DECODING THE *PENICILLIUM ITALICUM*-CITRUS INTERACTION:
FUNCTIONAL INSIGHTS INTO NRPS-DERIVED CYCLIC PEPTIDES IN CITRUS
INFECTION**

Evandro Silva^{1,2*}, Julio César Barbosa¹, Adrián González García³, Roberto G. S. Berlinck²,
Ana-Rosa Ballester³, Luis González-Candelas³, and Taicia Fill¹.

evandroas20@gmail.com

1-Universidade Estadual de Campinas, Instituto de Química, IQ-UNICAMP Rua Josué de Castro, s/n, Campinas - SP, 13083-970, Brazil. 2-Univrsidade de São Paulo, Campos de São Carlos, Av. Trab. São Carlense, 400, São Carlos - SP, 13566-590, Brazil. 3-Instituto de Agroquímica y Tecnología de Alimentos, IATA-CSIC, 46980 Paterna, Valencia, Spain

Penicillium italicum is a postharvest pathogen responsible for the blue mold disease in citrus fruits, particularly under cold and dry storage conditions¹. Despite its relevance, the molecular determinants of *P. italicum* virulence remain poorly understood². In this study, we uncover a direct link between the fungus's secondary metabolism and its pathogenicity by integrating untargeted metabolomics, gene deletion, and functional assays. LC-HRMS analysis of infected citrus tissues revealed the active and stage-specific production of cyclic peptides, including fungisporin and structurally related tetrapeptides, during host colonization. These compounds are functionally characterized for the first time as secondary metabolites of *P. italicum*. Genome mining identified the *hcpA* gene (PITC_041250) as a candidate NRPS responsible for their biosynthesis. Using the wild-type strain PHI-1 (access number: GCA_002116305.1), we constructed a $\Delta hcpA$ mutant through homologous recombination by *Agrobacterium tumefaciens*-mediated transformation. Deletion of *hcpA* abolished production of the identified peptides, confirming their biosynthetic origin. Phenotypic analysis showed no defects in growth or sporulation under standard conditions, but the mutant displayed increased sensitivity to osmotic stress. Pathogenicity assays on citrus fruits demonstrated significantly smaller lesions and reduced infection incidence compared to the wild-type, indicating that *hcpA*-dependent peptides are critical for full virulence. This work provides the first functional evidence linking a biosynthetic gene cluster to virulence in *P. italicum*, expanding current knowledge of its secondary metabolism. The findings highlight cyclic tetrapeptides as previously unrecognized virulence factors and potential molecular targets for innovative postharvest control strategies in citrus production. The authors acknowledge the FAPESP: 2022/03594-8, 2023/03831-2, 2022/02992-0. Work at IATA-CSIC was funded by PID2021-126005OBI00, AGROALNEXT/2022/028, PIE 202270I070, and the Severo Ochoa Center of Excellence program CEX2021-001189-S.

Keywords: *Penicillium italicum*, citrus blue mold, NRPS, cyclic peptides, gene deletion, metabolomics.

¹ Silva E et al, (2024). Molecular Omics, 20:154-168, ² Kanashiro A. M. et al, (2020). Frontiers in Microbiology, 11:606852.





INFLUENCE OF ABIOTIC FACTORS ON PIGMENT BIOSYNTHESIS BY *Aspergillus* sp. USING PLACKETT-BURMAN DESIGN

Enzo Mendes Leão^{1*}, Mariana Ramos de Almeida¹, Jacqueline Aparecida Takahashi¹

emleaoufmg@gmail.com

1- Department of Chemistry, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

There is growing interest in natural products that can replace synthetic dyes, due to the negative impacts of the latter on human health and the environment¹. Fungi of the genus *Aspergillus* stand out for their production of natural and non-toxic pigments, such as asperversin (yellow), aspergilline (black), and auroglaucine (orange-red), representing a safe, renewable, and sustainable alternative¹. In this context, this study aims to develop natural colorants from filamentous fungi and sought to identify the abiotic factors that influence the production of intracellular and extracellular pigments by *Aspergillus* sp., using the Plackett–Burman experimental design. The effects of carbon and nitrogen sources (sucrose, glucose, meat extract, yeast extract, and urea), the influence of the presence of copper and glycine, as well as the incubation time and the role of agitation in the fermentation process were evaluated. After 21 and 33 days, the media were vacuum filtered to separate the biomass from the fermented broth, in which the production of extracellular pigments was quantified by UV/VIS spectrophotometry (395 nm). To evaluate intracellular pigment production, the biomass was treated with absolute ethanol (0.2 g/mL), stirred for 48 h, and the resulting extract was analyzed by spectrophotometry under the same conditions, with all readings taken in triplicate. In extracellular production, the most relevant factors were incubation time (−0.0183) and glycine (−0.0040), both with a negative effect, indicating that prolonged cultivation periods together with addition of this amino acid reduces pigment biosynthesis in the liquid medium. In contrast, for intracellular production, incubation time (0.3894) on a fermentation containing yeast extract as nitrogen source (0.1081) stood out, both with positive effect, suggesting that longer incubation periods and the addition of yeast extract favors the accumulation of pigments in the biomass. These results provided relevant insights for optimizing the fermentation process and scaling up the production of natural pigments from the fungal species studied, with the aim of developing alternative colorants for the food industry, in line with demands for safer, more sustainable, and environmentally viable products for food industry. The authors acknowledge the financial support provided by CNPq.

Keywords: *Pigment biosynthesis; Experimental designs; Plackett–Burman; Aspergillus sp.*

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DEREPLICATION AND ISOLATION OF SECONDARY METABOLITES FROM *Protium warmingianum* TWIG EXTRACTS

***Igor Alencar Sales da Silva*^{1*}, Fernando Cotinguiba da Silva¹**

alencariss@ufrj.br

1- IPPN-UFRJ, Instituto de Pesquisa de Produtos Naturais Walter Morz - Universidade Federal do Rio de Janeiro. Av. Carlos Chagas Filho, 373 - Centro de Ciências da Saúde - CCS - Cidade Universitária, Rio de Janeiro - RJ, 21941-599. Brasil.

The genus *Protium* (family Burseraceae) stands out for its wide distribution and for being home to 84 of the 175 globally recognized species in Brazil, primarily in the Amazon. These species are known for producing aromatic resins with potential applications in the pharmaceutical and cosmetic industries. Despite the genus' relevance, the species *Protium warmingianum*, the target of this work and endemic to Rio de Janeiro, remained chemically unexplored. This study aimed to identify, isolate, and characterize the secondary metabolites of *P. warmingianum*. Leaf and twig samples were subjected to maceration with methanol, generating crude extracts. Preliminary analysis by LC-MS/MS and data processing on the MZMine and GNPS platforms allowed the annotation of dozens of natural products, including flavonoids, lignans, coumarins, and terpenoids, classes of compounds known for their biological activities. For structural confirmation, the dichloromethane partition of the branches was fractionated by chromatography on a flash silica column. The fractions obtained were analyzed by ¹H NMR and ¹³C NMR, which enabled the identification of classes such as triterpenes and phenylpropanoids, establishing, for the first time, the chemical profile of this species. Regarding the biological evaluation, the partitions and fractions were subjected to preliminary antimicrobial tests, which, however, did not demonstrate positive results. Future investigations are planned to explore other biological activities, such as antioxidant, anti-inflammatory, and cytotoxic, based on the profile of the identified compounds. Currently, the process of identifying and annotating the substances is ongoing, and their complete characterization will contribute to a more comprehensive understanding of the secondary metabolism of the species *P. warmingianum* and the genus *Protium*.

Keywords: *Dereplication, Protium warmingianum, flavonoid, coumarin, phytochemistry, secondary metabolism.*





**VOLATILE PROFILE AND MOLECULAR CHARACTERIZATION OF *Piper*
(PIPERACEAE) SPECIES OCCURRING IN THE AMAZON**

Bruna de Araújo Guimarães^{1*}, Pablo Luis Baia Figueiredo², Christina Cleo Vinson
Williams¹, Joyce Kelly R. da Silva¹

brunadearaujo.guimaraes@gmail.com

1- LABITPNA, Laboratório de Bioprospecção e Inovação Tecnológica de Produtos Naturais da
Amazônia, ICB, UFPA, R. Augusto Corrêa, 01, Belém, PA, Brazil.

2- Programa de Pós-Graduação em Ciências Ambientais, Universidade do Estado do Pará, Tv.
Enéias Pinheiro, n° 2626, Belém, PA, Brazil

Studies on the chemical variability and molecular characterization of the genus *Piper* are essential to understand the range of traits expressed within and among species. This study aimed to characterize different chemotypes of *Piper* species occurring in the state of Pará, Brazil, and to evaluate their genetic diversity. Twenty-three samples were collected in Altamira, Bagre, Bragança and Metropolitan Region of Belém. Essential oils were obtained by hydrodistillation (3 h) and analyzed by gas chromatography–mass spectrometry (GC-MS). The most abundant compounds detected were dillapiole (0–93.4%), *E*-nerolidol (0–30.6%), eugenol (0–26.3%), methyl eugenol (0–23.0%), limonene (0–19.6%), *E*-caryophyllene (0.2–19.0%) and α -pinene (0–15.5%). Principal component analysis of the chemical profiles grouped the samples into five chemotypes characterized mainly by: Group I was differentiated by the highest percentage of compounds belonging to classes of Alkanes, Aldehydes, Alcohols, Ketones and Esters (14.7%), although the major ones were Oxygenated Sesquiterpenes (OS, 25.4%) followed by Monoterpene Hydrocarbons (MH, 23.0%); Group II was distinguished by the presence of Diterpenes (DT, 9.8%) and high values of Monoterpene Hydrocarbons (MH, 20.6%) and OS (20.0%); Group III was characterized by the highest levels of Phenylpropanoids (PP, 60.4–66.4%) followed by SH (12.9–29.4%); Group IV grouped the samples with the highest levels of HM (34.8–59.8%) and high OS levels (11.4–27.3%); finally, Group V presented the highest SH (27.9–70.2%) and OS levels (10.9–50.4%). Molecular characterization was performed from the sequencing of the ITS region and revealed 14 haplotypes among 20 individuals, with haplotype diversity ($H_d = 0.963$) and nucleotide diversity ($\pi = 0.06745$), indicating high variability. Besides, the ITS sequences presented 82 parsimony informative sites and 100 polymorphic sites, totaling 127 mutations, indicating the potential of the ITS gene to be used as barcode for *Piper* genus. Overall, the *Piper* species from Pará exhibited marked chemical heterogeneity and haplotype diversity, contributing to the understanding and documentation of their chemical and molecular characterization and potential for applied uses. The authors thank the support CAPES and CNPq.

Keywords: DNA barcode, essential oil, plant barcoding, sesquiterpenes





**CHEMICAL EPIGENETIC MODULATION AS A STRATEGY FOR TRIGGERS
METABOLITE IN UNCARIA TOMENTOSA (WILLD. EX SCHULT.) DC.**

Marilia Fontes Barbosa^{1*}, Mario Machado Martins², Adriana Aparecida Lopes¹, Ana Maria Soares Pereira¹

mari_fbs@outlook.com

1-Unidade de Biotecnologia Vegetal, Universidade de Ribeirão Preto (Unaerp), Av. Costábile Romano, 2201, Ribeirânia, Ribeirão Preto, SP, 14096-900, Brazil. 2-Laboratório de Nanobiotecnologia Dr. Luiz Ricardo Goulart, Universidade Federal de Uberlândia (UFU), Rua Acre, Umuarama, Uberlândia, MG, 38408-100, Brazil.

Nature, through its medicinal plants, has contributed significantly to the development of new drugs. Among these plants, *Uncaria tomentosa* (cat's claw) is of particular interest, being a species native to the Amazon region that has been used in traditional medicine due to its anti-inflammatory action and chemical diversity, which includes alkaloids, polyphenols, and quinovic acid derivatives. However, it is important to note that plants are conditioned to physiological interactions and generally produce these compounds in low concentrations. In this context, *in vitro* cultivation emerges as a promising strategy, demonstrating the optimization of the production of specialized metabolites through specific pathways that are regulated by epigenetic mechanisms. These mechanisms modulate gene expression through activation or silencing under various conditions, reflecting the variation in the chemical composition and concentration of metabolites. The process of epigenetic modulation is mediated by mechanisms such as histone modifications, occurring without any alteration of the genetic code. The present study was conducted to evaluate the effect of sodium butyrate (NaBut), a histone deacetylase inhibitor, on the chemical profile biosynthesis of specialized metabolites in *U. tomentosa* adventitious roots by LC-MS. The adventitious roots were treated with NaBut for a period of 60 days, and then the methanolic extracts obtained were purified by solid phase extraction on a C18 cartridge and semi-preparative HPLC-DAD. Spectrometric analyses were performed on an Agilent Infinity 1260 HPLC system coupled to a high-resolution QTOF mass spectrometer with electrospray ionization. The data obtained by HPLC-DAD and LC-MS showed variations in the concentrations of specialized metabolites at lower treatment doses of NaBut treatment and biosynthesis of azelaic acid was observed, a compound not previously reported in the species. These present results represent the first record of the use of epigenetic strategy chemical in *U. tomentosa* adventitious roots, and thus demonstrate the potential of NaBut in the production of metabolites through the activation of silenced biosynthetic pathways. The authors are grateful for the support of their institutions and financial support from CNPQ.

Keywords: histone deacetylase, biosynthesis, LC-MS, Rubiaceae, cat's claw





VOLATILE SECONDARY METABOLITES IN POSTHARVEST CITRUS FUNGAL INFECTIONS: FROM PATHOGEN-HOST INTERACTION TO TERPENE BIOSYNTHESIS

Júlio César J. Barbosa^{1*}, Gabriela Bassi da Silva², Anna Clara Couto³, Maria Clara Santana Aguiar¹, Túlio Ramos Zauza¹, Leandro Wang Hantao³, André Ricardo de Lima Damasio², Taicia Pacheco Fill^{1,*}

barbosa.jcj3@gmail.com, taicia@unicamp.br

1-LaBioQuiMi, Institute of Chemistry, UNICAMP, Brazil; 2-LEBIMO, Institute of Biology, UNICAMP, Brazil; 3-LCGC, Institute of Chemistry, UNICAMP, Brazil;

Brazil is the world's largest producer of oranges and one of the main exporters of citrus juice, making citriculture a strategic sector for the global economy. However, postharvest fungal pathogens such as *Penicillium digitatum*, *Penicillium italicum*, and *Geotrichum candidum* cause significant losses due to rapid enzymatic degradation of the pulp and dissemination through wounds. These pathogens produce a variety of secondary metabolites (SMs) with cytotoxic, enzymatic, and phytotoxic functions essential for host colonization. Among these, volatile organic compounds (VOCs) are also known to play central roles in e.g. plant–insect, plant–microbe and microbe–microbe interactions. To better understand these interactions and characterize the volatile profile involved, we analyzed VOC emissions using the solid-phase microextraction (SPME) technique. In order to monitor the VOCs produced during the interaction between these pathogens and the citrus host, analyses using SPME, associated with two-dimensional gas chromatography (GC×GC-TOFMS), were performed on healthy fruits and fruits after 7 days of infection. A total of 240 compounds were identified, including esters, biotransformed monoterpenoids (e.g., carvone, carveol, α -terpineol), and sesquiterpenes such as himachoulene and β -caryophyllene. Biotransformation assays with limonene and terpineol confirmed the conversion of these volatiles by the pathogens, reinforcing their adaptive role in response to citrus defense. *P. italicum*, in particular, produced triquinane-type tricyclic sesquiterpenes both *in vitro* and during host infection. Genome mining revealed 53 biosynthetic gene clusters (BGCs), of which 24.53% were associated with terpene biosynthesis. Within BGC of the *P. italicum* PHI genome, we identified a putative Presilphiperfolan-8- β -ol synthase, an enzyme related to sesquiterpenoids biosynthesis. This enzyme was heterologously expressed in *Escherichia coli* ArcticExpress (DE3), purified — with an approximate size of 60 kDa — and incubated *in vitro* with the natural substrate (2E,6E)-FPP in order to correlate the sesquiterpenoids produced under this condition with those identified during the interaction between *P. italicum* strain PHI and the citrus host. The integration of VOC analysis provided new insights into the chemical mechanism of infection by different phytopathogens through the identification of characteristic biomarkers of each pathogen. In addition, this study delves into the investigation of the biosynthetic machinery employed by *P. italicum* strain PHI in terpene production.

Keywords: Chemistry Ecology, *Penicillium italicum*, VOCs, pathogen–host interaction, genome mining, biotransformation





New insights into cichorine biosynthesis in *Aspergillus nidulans* through bioinformatic and metabolomic analyses

Lucas Penha Dutra¹, Terumi Mascarenhas², Jakob Blæsbjerg Hoof², Uffe Hasbro Mortensen², Diogo Montes Vidal¹, Thomas Ostenfeld Larsen^{2*}

lucaspdutra98@gmail.com

1-Neplam, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 2-DTU Bioengineering, Department of Biotechnology and biomedicine, DTU, Søtofts Plads, 221, Kongens Lyngby, Denmark.

Cichorine is an isoindolinone alkaloid mainly produced by fungi such as *Aspergillus nidulans*. Its derivatives have been reported to display diverse biological activities, including antioxidant, antimicrobial, cytotoxic, and antiproliferative effects against several cancer cell lines¹. Cichorine originates from 3-methylorsellinic acid (3-MOA), and although its biosynthetic gene cluster (BGC) has been described in *A. nidulans*², the functional roles of several genes remain only partially understood, particularly those involved in nitrogen incorporation and oxidation steps. In this work, it was combined bioinformatic with metabolomic analyses of *A. nidulans* mutant strains to further characterize the cichorine biosynthetic pathway. The *A. nidulans* genome (NCBI accession: GCA_000011425.1) was screened with antiSMASH, and Cic BGC protein sequences were analyzed by BLASTp and InterPro. In earlier studies, the Cic BGC was overexpressed, yielding strain NID792, which served as the background for constructing targeted gene deletions. Mutant strains included NID952 (Δ AN6444), NID954 (Δ AN6449), NID956 (Δ AN6447), NID1012 (Δ AN6448), and NID1010 (Δ AN6445). Extracts from these strains were subjected to UHPLC-ESI-HRMS/MS analyses in both positive and negative ionization modes. AntiSMASH predicted 18 genes in the Cic BGC. However, comparative sequence analysis indicated that only five genes are directly involved in cichorine biosynthesis: AN6448 (polyketide synthase), AN6447 (*O*-methyltransferase), AN6445 (GMC oxidoreductase, 49% identity to PatE), AN6449 (CYP450 monooxygenase), and AN6444 (nonribosomal peptide synthase-like – NRPS-like, 40% identity to StbB). The function of AN6448, AN6447, AN6445, and AN6449 had been previously confirmed through metabolomic analyses of mutants² and corroborates with bioinformatic and metabolomic results obtained here. Additionally, it was proposed that the uncharacterized AN6444 Cic gene is involved in the conversion of 3-MOA to its corresponding aldehyde in early steps of cichorine biosynthesis.

Keywords: Cichorine biosynthesis, CRISPR/Cas, HPLC-MS/MS metabolomics.

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Acknowledgements: UFMG, DTU, CAPES.





METABOLIC PROFILING OF ECLIPTA PROSTRATA CALLUS CULTURE UNDER EPIGENETIC MODULATION

Bruna Gomes Bitar¹, Daniel Yuri Akiyama², Ana Maria Soares Pereira¹, Taicia Pacheco Fill², Adriana Aparecida Lopes^{1*}

adrianalps@gmail.com

1-Biotechnology Unit, University of Ribeirão Preto (UNAERP), Av. Costabile Romano, 2201, Ribeirão Preto-SP, 14096-900, Brazil. 2-Institute of Chemistry, University of Campinas (UNICAMP), Rua Josué de Castro, s/n - Cidade Universitária, Campinas-SP, 13083-970, Brazil

Eclipta prostrata (L.) L., a medicinal species of the Asteraceae family, is native to Brazil. It is imperative to note that, given the medicinal importance of the species in question, strategies based on *in vitro* plant cell cultures have been explored. The synthesis of berberine by *Coptis japonica*, paclitaxel by *Taxus* species, shikonin by *Lithospermum erythrorhizon* cell cultures and ginsenosides by *Panax ginseng* cell cultures exemplifies the efficacy of medicinal compound production through plant cell cultures. In this study, we present a series of epigenetic control experiments employing the histone deacetylase inhibitor sodium butyrate (1 mM) in *E. prostrata* callus culture. Following a three-week period of incubation, the methanolic extract was prepared from the callus culture. The analysis of crude extracts was conducted by liquid chromatography and high-resolution mass spectrometry, resulting in the generation of a molecular network. This network was constructed employing the Ion Identity Molecular Networking (IIMN) workflow on GNPS, alongside *in silico* prediction of molecular structural features using SIRIUS 4 with standard parameters for the Orbitrap mass analyser. The results of the study indicated the presence of six novel compounds that were produced during epigenetic modulation experiments using *E. prostrata* callus culture. The molecular ions of 3,4-dimethylbenzoic acid (m/z 133.0648), cinnamic acid glycosylated (m/z 309.0969), lupeone (m/z 425.3776), ursolic acid (m/z 439.3568), syringin (m/z 390.1760) and monolinolenin (m/z 353.2682) were identified. The compound monolinolenin is a common constituent found in either GNPS or SIRIUS 4. The present study reports the results of a metabolic profiling of *E. prostate* callus culture following epigenetic modulation. The *in-silico* prediction showed that all compounds are not found in the genus *Eclipta* but in other plants from Asteraceae family. The present study establishes a novel connection between these compounds in this species, thereby paving the way for potential biotechnological exploitation.

Keywords: Micropropagation, medicinal plant, callus culture, GNPS.





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Session
Biodiversity & Natural Products



MULTIVARIATE ANALYSIS APPLIED TO CAFFEINE EXTRACTION USING CHOLINE BASED NADES

Maria Vitoria Tosta Reis Grise^{1*}, Jorge Mauricio David², Amenson Trindade Gomes³
Rodrigo De Paula^{1,3}

maria.g1240@ufob.edu.br

1- Federal University of Western Bahia (UFOB), POSQUIPA, Barreiras/BA, Brazil. 2- Federal University of Bahia (UFBA), Institute of Chemistry, Salvador, BA, Brazil. 3- Federal University of Recôncavo da Bahia (UFRB), Center for Teacher Education, Amargosa, BA, Brazil.

Coffee, a raw material rich in bioactive molecules, has a long-standing history of consumption in Brazil and worldwide. Among these molecules, caffeine (1,3,7-trimethylxanthine) stands out due to its stimulant, anti-inflammatory, and diuretic properties. With the growing interest in environmentally sustainable practices, several programs have been developed to encourage the adoption of less environmentally harmful extraction processes. Over the past decade, Deep Eutectic Solvents (DES) and their natural counterparts (Natural Deep Eutectic Solvents – NADES) have gained increasing prominence. These solvents are biodegradable, biocompatible, exhibit low flammability, high dissolution capacity, and are cost-effective. In the search for optimal extraction conditions using DES or NADES, mathematical modeling has been successfully employed to optimize the overall process. In this context, the present study aimed to optimize caffeine extraction from roasted and ground coffee powder, evaluating which choline-based NADES formulation (Choline Chloride:Lactic Acid – ChCl:LA, Choline Chloride:Oxalic Acid – ChCl:OA, Choline Chloride:Citric Acid – ChCl:CA, Choline Chloride:Urea – ChCl:U, or Choline Chloride:Tartaric Acid – ChCl:TA) yielded the best caffeine extraction using the water bath extraction method. Furthermore, the study evaluated which variables (extraction time, temperature, water volume, and NADES mass) exerted the greatest influence on the extraction efficiency. Caffeine quantification was performed using the standard addition method. Based on previously developed studies (Grise et al., 2025), multivariate analysis revealed that the use of ChCl:LA in a 1:1.5 molar ratio resulted in the extraction of 56.1 mg/g of caffeine under optimized extraction conditions (15 minutes, 90 °C, 5 mL of water, and 10 g of NADES). The most influential variables identified were the amount of NADES and the extraction temperature. Regarding the analysis of the most effective extracting solvent, the following combinations were identified as the most efficient (in descending order): ChCl:OA, ChCl:LA, and ChCl:U. Moreover, ATR-FT-IR spectroscopy enabled the identification of bonds and interactions among the constituents of the selected NADES. Further studies focusing on optimizing caffeine extraction using ChCl:OA, as well as the development and optimization of a ternary system, are currently underway. The author (M.V.T.R. Grise) is grateful to CAPES for the fellowship.

Keywords: Caffeine, Natural Deep Eutectic Solvents, Sustainable extraction. Grise, M. V. T. R.; Gomes, A. T.; Da Silva, E. P.; David, J. M.; De Paula, R. Multivariate analysis caffeine extraction from roasted and ground coffee powder using eutectic mixtures as a sustainable system. (Submitted manuscript)





CHEMICAL STUDY AND ANTIOXIDANT ACTIVITY EVALUATION OF EXTRACTS AND FRACTIONS FROM *Miconia nervosa*

Yasmin Loureiro Shiray^{1*}, Diego Godina Prado¹, Tarcisio Paiva Mendonça², Cecília Silva Pereira², Tiara da Costa Silva³, Mário Machado Martins⁴, Raquel M. F. Sousa¹, Foued Salmen Espíndola², Alberto de Oliveira¹

yasmin.shiray@gmail.com

1-NuPPeN, Instituto de Química, UFU, Av. João Naves de Ávila, 2121, Uberlândia, MG, 38408-100, Brazil. 2-LABIBI, Instituto de biotecnologia, UFU, Av. João Naves de Ávila, 2121, Uberlândia, MG, 38408-100, Brazil. 3 -ICENE, UFTM, Av. Randolfo Borges Júnior, Uberaba, MG, 38025-440, Brazil. 4 -LabNanos, Instituto de biotecnologia, UFU, Av. Pará, 1720, Uberlândia, MG, 38400-902, Brazil

The Brazilian Cerrado is one of the most biodiverse biomes in the world, and its flora has attracted significant scientific interest due to its wide range of chemical and biological properties, particularly in traditional medicine. *Miconia nervosa* was selected for study based on previous reports of biological activities within the same genus, including antimalarial, anti-inflammatory, analgesic, and antidiabetic effects. In this context, the present study aimed to investigate the antioxidant potential of leaf extracts and fractions from *Miconia nervosa* and annotate its specialized metabolites. Hexane (HE) and ethanol (EE) extracts were obtained sequentially by maceration, followed by liquid-liquid extraction of EE to yield dichloromethane (PD), ethyl acetate (PA), and aqueous (PAq) fractions. Antioxidant activity was assessed using DPPH radical scavenging and ferric reducing antioxidant power (FRAP) assays, and total phenolic content (TPC) was determined using the Folin-Ciocalteu method. The PA, PD, and PAq fractions exhibited the highest DPPH inhibition with values greater than 91%, comparable to the reference standard quercetin (94% antioxidant capacity). In the FRAP assay, PA showed the strongest activity, with 109 μmol Trolox equivalents per gram of extract. The highest TPC values were also found in PA (509 mg GAE/g) and PAq (829.3 mg GAE/g). The most active fraction (PA) was further analyzed by negative-mode ESI-HPLC-MS/MS, leading to the annotation of metabolites including gallic acid derivatives, flavonoids, and hydrolyzable tannins.

Acknowledgements: CAPES, CNPq, PROPP-UFU, FAPEMIG.

Keywords: Melastomataceae, Cerrado, (–)-ESI-HPLC-MS-MS, antidiabetic, antioxidant





EVALUATION OF ETHANOLIC EXTRACTS FROM *Lafoensia replicata* FOR PHOTOPROTECTIVE USE IN COSMETICS: A MULTIVARIATE CHEMICAL AND METABOLOMIC APPROACH

Débora Machado de Lima^{1*}, Tiara da Costa Silva^{2,3}, Mário Machado Martins², João Flávio da Silveira Petrucci¹, Raquel Maria Ferreira de Sousa¹

*deboramalima@gmail.com

1-Instituto de Química, UFU, CEP 38400-902, Uberlândia, MG, Brazil. 2-Instituto de Biotecnologia, UFU, 38405-319, Uberlândia, MG, Brazil. 3-Instituto de Ciências Exatas, Naturais e Educação, UFTM, 38025-440, Uberaba, MG, Brazil.

The demand for effective and safe natural ingredients for cosmetic formulations has encouraged the investigation of plants rich in bioactive metabolites. *Lafoensia replicata*, a native species of the Cerrado, has already demonstrated significant antioxidant and antimicrobial activities and is mainly composed of flavonoids, phenolic acids, and especially tannins. In this study, the potential of ethanolic extracts of *L. replicata* to be used as a photoprotective ingredient in cosmetic formulations was investigated. Five leaf extracts were prepared by maceration using ethanol/water mixtures at concentrations of 20, 40, 60, 80, and 96%. Six replicates of each extract were submitted to (i) chemical analysis, including total phenolic content, DPPH assay, flavonoid levels, condensed and hydrolysable tannins, (ii) spectrophotometric measurements for Sun Protective Factor (SPF) determination using the Mansur method; (iii) mass spectrometry experiments to assess chemical composition; and (iv) multivariate analysis. Principal Component Analysis (PCA), based on the chemical analysis and SPF data, showed that the extracts obtained with 20 and 96% of ethanol formed distinct clusters, while the other extracts (40, 60 and 80% ethanol) were grouped within the same cluster. Hydrolysable tannins appeared as the most important feature for the extract discrimination, with the highest level found in the 20% ethanolic extract. Additionally, an untargeted metabolomic analysis of the extracts was carried out using liquid chromatography/electrospray ionization time-of-flight mass spectrometry (LC-ESI-QTOF) and molecular feature extraction (MFE). Eight compounds with a high molecular mass and a structure compatible with tannins were identified. Cosmetic formulations were developed using 20% and 96% ethanolic extracts, and the SPF was evaluated. A commercial sunscreen was used as a positive control. All of the samples had an SPF of 30, and the *t*-test revealed no statistically significant differences between them (95% confidence interval). These findings reinforce the potential of *L. replicata* as a source of bioactive compounds for natural cosmetic formulations. Moreover, the results suggest that the photoprotective effect was not significantly affected by solvent concentration, indicating the feasibility of using lower concentrations of solvent - an important environmental advantage. Acknowledgments: FAPEMIG, CAPES and CNPq.

Keywords: tannins, natural cosmetics, protective factor





EVALUATION OF THE CHEMICAL COMPOSITION AND ACTIVITY OF THE ETHANOLIC EXTRACT FROM THE AERIAL PARTS OF *Mandevilla velame*

Raphael Ernane Matos Guimarães^{*1}, Débora Machado de Lima¹, Tiara da Costa Silva^{2,3}, Eber Moreira de Alcântara⁴, Mário Machado Martins², Raquel Maria Ferreira de Sousa¹

*raphaelernane@ufu.br

1-Instituto de Química, UFU, CEP 38400-902, Uberlândia, MG, Brasil. 2-Instituto de Biotecnologia, UFU, 38405-319, Uberlândia, MG, Brasil. 3-Instituto de Ciências Exatas, Naturais e Educação, UFTM, 38025-440, Uberaba, MG, Brasil. 4- Instituto de Ciências Agrárias, UFU, CEP 38500-000, Monte Carmelo, MG, Brasil.

Mandevilla velame, commonly known as "Velame Branco" is a plant native to the Cerrado, traditionally used for its roots, particularly due to their anti-inflammatory activity. However, the extraction of its underground parts results in the death of the plant, raising concerns about the sustainability of its use. In this context, the present study aimed to evaluate the chemical composition and biological activities of the ethanolic extract from the aerial parts of the plant as a viable and less impactful alternative. Leaves of *M. velame* were collected in Abadia dos Dourados, Minas Gerais, Brazil (herbarium voucher: HUFU 85230). After drying and grinding, the plant material was subjected to solvent maceration. Initially, hexane was used, and the resulting extract was filtered and removed using a rotary evaporator under vacuum after 48 hours (5 repetitions), yielding the hexane extract. Subsequently, the plant material from the hexane extraction was subjected to ethanolic maceration using the same procedure, yielding the ethanolic extract. Quantitative analyses of phenolic compounds revealed the following contents: total phenolics (155.9±1.1 mg gallic acid equivalents/g extract), total flavonoids (14.37±0.0 mg quercetin equivalents/g extract), and total proanthocyanidins (32,2±0.4 mg catechin equivalents/g extract). Antioxidant assays demonstrated significant activity, with DPPH (EC₅₀: 4.25±0.23 µg/mL) and FRAP (224,69±8,4 µmol Trolox equivalents/g sample) results indicating strong antioxidant potential. Chemical characterization by liquid chromatography/electrospray ionization time-of-flight mass spectrometry (LC-ESI-MS/MS-QTOF) indicated the presence of proanthocyanidins (such as proanthocyanidin A2), phenolic acids (caffeoylquinic acid and chlorogenic acid), and flavonoids (quercetin-3O-glucuronide). It is concluded that the ethanolic extract from the aerial parts of *M. velame* exhibits significant antioxidant activity, attributed to the presence of phenolic compounds, reinforcing its potential as a sustainable source for natural product chemistry. Acknowledgments: FAPEMIG, CAPES and CNPq.

Keywords: Antioxidant, proanthocyanidins, natural product, sustainability.





ELECTROCHEMICAL QUANTIFICATION OF TANNINS AND CATECHINS IN Syzygium cumini PHYTOTHERAPEUTICS AND Syzygium malaccense EXTRACTS USING 3D-PRINTED SENSORS

Dayane Vasconcelos Petine^{1*}, Diego Godina Prado¹, Mariana Cardoso Marra¹, Raquel Gomes da Rocha¹, Tiara da Costa Silva^{2,3}, Mário Machado Martins², Rodrigo Alejandro Abarza Muñoz¹, Raquel Maria Ferreira de Sousa¹

*dayane.petine@ufu.br

1-Instituto de Química, UFU, CEP 38400-902, Uberlândia, MG, Brazil. 2-Instituto de Biotecnologia, UFU, 38405-319, Uberlândia, MG, Brazil. 3-Instituto de Ciências Exatas, Naturais e Educação, UFTM, 38025-440, Uberaba, MG, Brazil.

Phytotherapeutics based on *Syzygium cumini*, a plant species included in the Brazilian Unified Health System (SUS) list, are widely used due to their antioxidant and hypoglycemic effects, attributed to phenolic compounds like catechins and tannins. Quantifying these classes of compounds is essential to ensure the safety and efficacy of herbal medicines. However, conventional analytical methods, such as high-performance liquid chromatography (HPLC), are expensive and require advanced infrastructure. In contrast, electroanalytical techniques offer low-cost and sensitive alternatives suitable for routine quality control applications. In addition to *S. cumini*, this study explores *Syzygium malaccense*, a species native to Southeast Asia and also cultivated in Brazil, commonly known as Red Jambo. It is used in folk medicine due to its anti-inflammatory and hypoglycemic properties and is rich in polyphenols, with a composition similar to that of *S. cumini*. This study aimed to develop and validate an electrochemical method using square wave voltammetry (SWV) for the quantification of catechins and tannins in commercial *S. cumini* phytotherapeutics and extracts from *S. malaccense* leaves and twigs. Extracts were obtained via sequential maceration with hexane and ethanol. All samples were characterized by total phenolics (Folin-Ciocalteu assay) and liquid chromatography/electrospray ionization time-of-flight mass spectrometry (LC-ESI-MS/MS-QTOF). Electrochemical measurements were performed using 3D-printed working electrodes made from carbon black–polylactic acid (CB-PLA) via fused deposition modeling (FDM). After electrochemical activation, analyses were conducted in 0.5 mol L⁻¹ H₂SO₄ containing 30% ethanol. Catechin was used as the analytical standard. Well-defined redox peaks were obtained, with detection limits in the 10⁻⁷ mol L⁻¹ range. *S. cumini* phytotherapeutics exhibited quantifiable levels of catechins, while *S. malaccense* extracts also showed significant concentrations. Results aligned with spectrophotometric and LC-MS data. These findings highlight the potential of 3D-printed electrochemical sensors as tools for phytochemical analysis. Acknowledgments: FAPEMIG, CAPES and CNPq.

Keywords: *Syzygium cumini*; catechin; tannins; voltammetry; 3D-printed sensors; *Syzygium malaccense*.





ANTIOXIDANT ACTIVITIES AND CHEMICAL STUDY OF *MICONIA AFFINIS* LEAF EXTRACTS AND FRACTIONS.

Sophia Cardoso Jabur^{1*}, Diego Godina Prado¹, Tiara da Costa Silva², Mário Machado Martins³, Raquel Maria Ferreira de Sousa¹, Alberto de Oliveira¹.

sophia.jabur@ufu.br

1-NuPPeN, Instituto de Química, UFU, Av. João Naves de Ávila, 2121, Uberlândia, MG, 38408-100, Brazil. 2-ICENE, UFTM, Av. Randolfo Borges Júnior, Uberaba, MG, 38025-440, Brazil 3 -LabNanos, Instituto de biotecnologia, UFU, Av. Pará, 1720, Uberlândia, MG, 38400-902, Brazil

The Cerrado biome harbors a rich diversity of plant species with notable potential for use in traditional medicine due to their bioactive properties. *Miconia affinis* (Melastomataceae) emerges as an up-and-coming candidate. This study aimed to evaluate the antioxidant activity of leaf extracts and fractions obtained from *M. affinis* and to annotate its major specialized metabolites. Ethanolic (EE) and hexanic (HE) extracts were obtained by maceration, followed by liquid-liquid extraction of EE to yield dichloromethane (DF), ethyl acetate (EAF), and aqueous (AqF) fractions. Antioxidant capacity was determined via DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging assay, with EAF displaying the highest activity ($EC_{50} = 2.75 \mu\text{g/mL}$). Phytochemical screening was performed using thin-layer chromatography (TLC) in ethyl acetate fraction, which revealed the presence of hydrolyzable tannins, indicated by a blue coloration upon reaction with iron(III) chloride. (–)-ESI-HPLC-MS/MS analysis of the most active fraction, the ethyl acetate fraction (EAF), confirmed the presence of pedunculagin, casuarinin, gallic acid derivatives (methyl gallate, ethyl gallate, methyl digallate), and quercetin galloyl hexoside, a flavonoid not detected by TLC due to the limitations of the reagents used (NP/PEG and aluminum chloride). These findings elucidate the bioactive chemical composition of *M. affinis* and highlight its potential for further pharmacological investigation.

Acknowledgements: CAPES, CNPq, PROPP-UFU, FAPEMIG.

Keywords: *Miconia affinis*, Melastomataceae, antioxidant, (–)-ESI-HPLC-MS-MS, Cerrado, flavonoid





ELECTROCHEMICAL CHARACTERIZATION OF ISO- α -ACIDS FROM *Humulus lupulus*

Karinne Teixeira Goncalves^{1*}, Marina Di-Oliveira¹, Rodrigo Alejandro Abarza Muñoz¹,
Raquel Maria Ferreira de Sousa¹

*karinne.teixeira@ufu.br

¹Instituto de Química, Universidade Federal de Uberlândia, Uberlândia - MG, 38400-902,
Brazil

Humulus lupulus, commonly known as hops, is a climbing plant belonging to the Cannabaceae family. Commercial interest focuses on the lupulin glands, which produce a soft resin in their inflorescences containing the plant's specialized metabolites. Hops are grown mainly for beer brewing due to the presence of α acids, which after a high-temperature isomerization reaction produce iso- α acids, which are a mixture of compounds responsible for the bitterness of beer. The efficiency of this isomerization can be evaluated using Nuclear Magnetic Resonance (¹³C-NMR), a technique used to confirm the success of the isomerization of α -acid mixtures. Although highly effective, NMR is an expensive technique for routine batch analysis and quality control of these compounds in hops and, potentially, in finished products such as beer. In this regard, electroanalytical techniques offer sensitive and low-cost alternatives suitable for routine quality control applications. With the aim of further studying α -iso acids, we proposed to analyze their electrochemical behavior using a screen-printed electrode. Initially, plant material from Sabro variety hop pellets was purchased and hot extraction with hexane was performed for two hours, with a yield of 21%. The extract was then subjected to α -acid separation using a 4% (w/v) methanolic solution of lead acetate, yielding 32% α -acids. After separation, the isomerization process was carried out under reflux with heating for 1 hour in an inert atmosphere, followed by pH adjustment (~1) and extraction with ethyl ether, resulting in a yield of 43% iso- α -acids. The device consists of a cell containing a working electrode, which is a graphite foil (GF), and an auxiliary electrode (Ag|AgCl) and a counter electrode (Platinum wire). With this arrangement, an anodic process is observed at around 1.2 V (vs. Ag|AgCl), referring to the oxidation of alpha iso-acids. In addition, characterization by ¹³C NMR showed chemical shifts at 87.6 and 90.6 ppm, attributed to the carbinolic carbon in the ring structure of the molecule, characteristic of alpha iso acids. The analytical parameters of the calibration curve constructed with GF revealed a linear range of 1.00 to 4.00 mg·L⁻¹ ($r^2 = 0.998$), sensitivity of 0.0523 $\mu\text{A}\cdot\text{L}\cdot\text{mg}^{-1}$, detection and quantification limits of 0.09 and 0.30 mg·L⁻¹, respectively. In summary, the results obtained were promising for future analyses, with the possibility of quantifying iso- α -acids in beer using the electroanalytical method. Acknowledgments: CAPES, CNPq, FAPEMIG.

Keywords: *Humulus lupulus*, ¹³C NMR characterization, GF electrode, beer.





**PRODUCTION AND CHARACTERIZATION OF PROTEASE INHIBITORS
OBTAINED FROM CALLUS CULTURE OF *Bauhinia holophylla***

Rodrigo Michelinini de Oliveira Thomasi^{1*}, José Antônio da Silva², Ana Hortência Fonsêca Castro¹

rodrigo.michelinini97@gmail.com

1- Laboratório de Farmacobotânica e Plantas Medicinais (LAFAB), UFSJ, Av. Sebastião Gonçalves Coelho, 400, Divinópolis, Mg. 2- Laboratório de Química de Proteínas (LABQPR), UFSJ, Av. Sebastião Gonçalves Coelho, 400, Divinópolis

Preservation processes are essential for the conservation of plant species. Among these preservation techniques, *in vitro* cell and tissue culture stands out, as it enables the production of significant amounts of bioactive compounds in a short period of time, avoiding impacts of plant extractivism. For instance, callus and cell suspension cultures can be employed to produce a wide variety of bioactive compounds, including flavonoids, cardenolides, lectins, and protease inhibitors (PIs). PIs are particularly sought after for their broad biological potential against bacteria, viruses, insects, and tumor cells. In legume seeds, these compounds are abundantly expressed, representing about 1–10% of the total soluble protein (TSP) content. *Bauhinia holophylla* (Fabaceae: Cercidoideae) is a native plant from Cerrado and to date, the *in vitro* production of PIs from this species has not been reported in the literature. Therefore, this project aimed to produce and characterize protease inhibitors from callus cultures of *B. holophylla*. Callus cultures from leaf explants were established using MS (Murashige & Skoog) and WPM (Wood Plant Medium) medium. The influence of the plant growth regulators 2,4-dichlorophenoxyacetic acid (2,4-D) and 6-benzylaminopurine (BAP), at different concentrations on callus induction, TSP and PI content were also assessed. The obtained inhibitors were purified by crude protein precipitation, followed by clarification and molecular exclusion chromatography (SEC). Protease inhibitory activity was evaluated using trypsin inhibition assay with the substrate BAPNA (α -N-benzoyl-DL-arginine-p-nitroanilide hydrochloride). The TSP content was determined using the Bradford method. For characterization, denaturing gel electrophoresis was performed using Biorad® system. In crude protein precipitate, Kunitz-type inhibitors (approximately 20-21 kDa) were identified. Combinations of 2,4-D and BAP in WPM medium appear to promote higher total soluble protein (TSP) content, more efficient callus induction, and increased production of protease inhibitors (PIs) in *B. holophylla* callus. The authors thank the support from UFSJ and FAPEMIG. This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001.

Keywords: Protease inhibitors, Callus culture, *Bauhinia holophylla*, *In vitro* plant preservation, Cerrado.





**CHEMICAL PROFILE AND DEREPLICATION OF METABOLITES FROM
Lasiodiplodia sp. USING DIFFERENTIAL ¹H NMR AND SIMILARITY
CALCULATION**

Lucas Silva Tironi^{1*}, Jan Schripsema², Jaine Honorata Hortolan Luiz¹

lucas.tironi@sou.unifal-mg.edu.br

1- Instituto de Química, Universidade Federal de Alfenas, R. Gabriel Monteiro da Silva, 700, Alfenas, MG, 37130-001, Brazil. 2- Grupo Metabolômica, Laboratório de Ciências Químicas, Universidade Estadual do Norte Fluminense, Av. Alberto Lamego, 2000, Campos dos Goytacazes, RJ, 28013-602, Brazil.

Endophytic fungi are recognized for producing a wide variety of specialized metabolites, often with complex and diverse chemical structures. In this study, the chemical profile of organic extracts obtained from the fermentation of *Lasiodiplodia* sp., an endophyte isolated from *Handroanthus impetiginosus*, was investigated. The extracts were analyzed by ¹H NMR, and their spectra were processed using SIMBA software (Schripsema, 2019) to assess similarities and differences throughout the cultivation period. Spectral comparison enabled a comprehensive analysis of the biosynthetic profile of this fungus. Furthermore, detailed 1D and 2D NMR analysis of extract POLd-14 led to the identification of two known compounds: 3-carboxy-2-methylene-4-heptanolide and decumbic acid. All NMR spectra were acquired using a Bruker 400 MHz spectrometer and processed with TopSpin 4.1.4 software. These findings highlight the potential of *Lasiodiplodia* sp. as a promising source of bioactive compounds and reinforce the relevance of NMR as a dereplication tool in complex mixtures. The authors acknowledge the financial support provided by FAPEMIG.

Keywords: *Lasiodiplodia*, similarity and differential ¹H NMR, dereplication, specialized metabolites





SYNTHESIS OF GOLD NANOPARTICLES USING MELALEUCA EXTRACT

Luane Silva Soares^{1*}, Lucas Henrique Faria Santos¹, Kennedy Batista Gonçalves², Fernanda Braz Aguiar¹, Tiago Silveira Gontijo¹, Lívia Siman Gomes², Juliana Cristina dos Santos Almeida¹, Rosimeire Coura Barcelos¹

luane1682@outlook.com

¹ Federal University of São João Del-rei (UFSJ), Campus Centro-Oeste Dona Lindu, Divinópolis/MG - Brazil – 35.501-296

² Nanomaterials and Graphene Technology Center (CTNANO), Federal University of Minas Gerais, BH/MG - Brazil – 31.310-260.

Nanotechnology is a broad area of constant growth in today's society. The properties of matter on a nanometric scale, in relation to conventional ones, have been driving advances in the field of research and innovation. *Callistemon viminalis* is a plant belonging to the Myrtaceae family, which has several properties, including antioxidant, antimicrobial, anti-inflammatory action, among others. In this context, the use of plant extracts for the synthesis of gold nanoparticles (AuNPs) provides advances in nanotechnology, since it uses more sustainable methodologies for synthesis. This approach replaces chemical compounds with natural extracts, making the process less aggressive to the environment. In addition to eliminating toxic agents, plant extracts confer therapeutic properties to nanoparticles, due to their rich phytochemical composition. [1] The removal of Melaleuca was done by maceration using a reflux system, weighing 10 g of dry and pulverized plant material and then adding 100 mL of water, with the previously ready solution, it was added over heating until it reached boiling and kept for 40 minutes at reflux. After this time elapsed, the solution was subjected to centrifugation for 5 minutes at 1.600 rpm, the supernatant was filtered. After the extract was ready, it was stored in a freezer -80 °C and lyophilized until the solvent was completely removed. The synthesis of AuNPs was carried out based on the methodology of ELIAS et al., 2024, first the gold solution was prepared using a stock solution (0.1 mol/L) and from it diluted to a concentration of 1mM. Afterwards, a solution with the 10mg/mL extract was prepared and filtered through a 0.22 µm nylon membrane. After the prepared solutions were received, the extract was added to the gold and stirred for 10 minutes, inspiring a change in color. It was then centrifuged at 5.000 rpm for 10 minutes and stored at 4°.[3] The methodology is demonstrated and researched in gold nanospheres with an absorption peak of approximately 520 nm. The project is still in progress, along with test results, such as for example an antioxidant using DPPH.

Keywords: Nanoparticulas, Melaleuca, Nanoesferas, sintese verde, extrato vegetal.

[1] LIU, Yun; DENG, Jie; HUANG, Hao; et al. A novel wound dressing based on a gold nanoparticle self-assembled hydrogel. *Materials Today Bio*, v. 22, 100817, 2024.

[2] ELIAS, Nurul Ashikin et al. Antibacterial properties of synthesized Melaleuca cajuputi-leaf gold nanoparticles. *Materials Letters*, v. 366, p. 136565, 2024.





KNOWLEDGE AND PERCEPTION OF RESIDENTS OF THE CORCOVADO COMMUNITY, MARAJÓ ARCHIPELAGO, ABOUT MEDICINAL PLANTS

Eduardo Antonio Abreu Pinheiro^{1*}, Benedita da Costa Gonçalves¹, Vitória Maigda Magno Gomes¹, Rayane Pereira Barreiros¹, Joelma Câmara da Silva e Silva¹, Elisângela Monteiro Cordeiro¹, Maylanne Batista do Nascimento¹

eduardo.pinheiro@ifpa.edu.br

1-Edital nº01/2025/PROPPG, Instituto Federal do Pará, IFPA- Campus Breves, Av. Antônio Fulgêncio, s/n, Breves, PA, Brazil.

Medicinal plants, as well as their uses and indications, are part of the daily lives of the marajoara population. This research aimed to investigate traditional knowledge and perceptions of 49 residents of the Corcovado Community and to carry out an ethnobotanical survey of medicinal plants located in this rural area of the municipality of Breves. Residents were given questionnaires regarding their knowledge, social representation, the most commonly used medicinal plants and the diseases most commonly treated with these plant species in the community. Residents pointed out that the most commonly used plants are bloodroot, cow's foot and pariri, and most said they learned how to use these botanical species from their parents. As for the most used part of the plant, the leaf had the highest percentage. As for the method of preparation, residents use teas and bottled drinks the most. The diseases most commonly treated with phytotherapy in the Corcovado Community are diabetes, hypertension and anemia. Regarding possible toxic effects, 92% reported that they never felt any adverse effects from the use of medicinal plants. After conducting semi-structured interviews with residents of the Corcovado Community, the guided tour technique was used to collect, identify and prepare exsiccates, resulting in 60 medicinal plants present in various backyards of the aforementioned location. This study demonstrates that the population of this marajoara community uses medicinal plants quite frequently, and there is a need for greater dissemination of this practice, since people in general have shown interest in phytotherapy as an alternative for the treatment of various conditions. Furthermore, this research enabled the perpetuation of traditional knowledge, contributing to further studies that can conduct bioprospecting and correctly indicate the use of medicinal plant species from the Amazon.

Keywords: *tradicional knowledge, medicinal plants, ethnobotanical survey, Corcovado Community, Marajó Archipelago, Amazon.*





Eco-friendly approaches to malaria and dengue control: larvicidal, antiparasitic and antiviral activities of *Piper alatipetiolatum* essential oil

André C. de Oliveira^{1*}, Ingrid Suellen C. Sá², Felipe Moura Araujo da Silva², Glenda Quaresma Ramos³, Rosemary Aparecida Roque¹, Renata Galvão de Azevedo⁴, Gemilson Soares Pontes⁴, Sergio Massayoshi Nunomura⁵, Rita de Cássia Saraiva Nunomura²

andrebiologo2011@gmail.com

1-Laboratório de Controle Biológico e Biotecnologia da Malária e da Dengue, Instituto Nacional de Pesquisas da Amazônia, 69067-375, Manaus, Amazonas, Brasil. 2-Central Analítica, Centro de Apoio Multidisciplinar, Universidade Federal do Amazonas, 69080-900, Manaus, Amazonas, Brasil. 3-Centro Multiusuário para Análise de Fenômenos Biomédicos, Universidade do Estado do Amazonas, 69065-001, Manaus, Amazonas, Brasil. 4-Laboratório de Virologia, Instituto Nacional de Pesquisas da Amazônia, Manaus, Amazonas, 69067-375, Manaus, Amazonas, Brasil. 5-Laboratório de Princípios Ativos da Amazônia, Instituto Nacional de Pesquisas da Amazônia, 69067-375, Manaus, Amazonas, Brasil

In Brazil, malaria and dengue are diseases caused by *Plasmodium* and DENV, respectively, and primarily transmitted by *Anopheles darlingi* and *Aedes aegypti* mosquitoes that have developed resistance to insecticides often toxic to non-target organisms. In May 2025, over 1,242,400 probable cases of dengue and 29,955 confirmed cases of malaria have been reported. In response, eco-friendly vector control strategies have increasingly focused on natural products from Amazonian plants, particularly *Piper* species. This study aimed to investigate the essential oil (EO) and its major compounds from *P. alatipetiolatum* as potential agents against mosquito vectors and the etiologic agents of malaria and dengue. The EOs were extracted by hydrodistillation and characterized using GC-based techniques. The major compounds were isolated by column chromatography and identified by HRMS, GC-MS, GC-FID, and ¹H and ¹³C NMR. These products were evaluated against *An. darlingi* and *Ae. aegypti* larvae, *P. vivax*, and DENV. Toxicity was also assessed in non-target aquatic organisms, including *Hemiptera*, *Coleoptera*, and *Diptera*. For the first time, the sesquiterpene 6-ishwarone was isolated from essential oil, as well as ishwarol B and ishwarane. The EO and the compounds 6-ishwarone, ishwarol, and ishwarane showed larvicidal activity (LC₅₀ from 29.31 to 40.76 µg/mL), with cellular damage and changes in antioxidant enzymes such as SOD, CAT, GST, and α- and β-esterases. Antiparasitic (IC₅₀ from 3.7 to 11.2 µg/mL) and antiviral (IC₅₀ from 5.8 to 13.24 µg/mL) activities were also observed, with no cytotoxicity to VERO or PBMC cells. These products showed toxicity to non-target organisms only at high concentrations (LC₅₀ from 2,098.80 to 7,707.13 µg/mL), indicating environmental safety. Thus, EOs and compounds from *P. alatipetiolatum* and *P. purusanum* may serve as eco-friendly alternatives for controlling mosquito vectors and the pathogens of malaria and dengue.

Keywords: *Piper*, sesquiterpenes, mosquitoes, ¹³C NMR, dengue, malaria.





COMPARISON BY GC-MS OF *Bixa orellana* L. (BIXACEAE) SEED OILS OBTAINED BY DIFFERENT EXTRACTION METHODS

Ister Cordeiro Mariotini*, Mariana Santos Pinheiro, Claudia Mashouah Jamal.

ister.mariotini@edu.ufes.br

Department of Pharmaceutical Sciences, Health Sciences Center, Federal University of Espírito Santo, Vitória, ES, 29040-091, Brazil

Bixa orellana L. (Bixaceae), commonly known as annatto, is a plant native to tropical America and part of Brazil's biodiversity. Previous studies have identified several bioactive compounds in this species, including flavonoids and carotenoids, which confer a variety of pharmacological properties such as anti-inflammatory, antimicrobial, insect-repellent, antileishmanial, antioxidant, and antihyperlipidemic activities. In Brazil, the seeds of *B. orellana* are primarily used as a natural red food dye, largely due to the presence of the apocarotenoid bixin - comprising approximately 80% of the total carotenoids in the seeds - along with norbixin and other compounds. This study aimed to compare the extraction yield, phytochemical profile, and gas chromatography-mass spectrometry (GC-MS) results of oil extracted from *B. orellana* seeds with those of a commercially available oil. Seeds were collected in Itarana, Espírito Santo, Brazil, and fixed oil (FO) extraction was performed using the method described in the 7th edition of the Brazilian Pharmacopoeia. The process involved solvent extraction under reflux in a Soxhlet apparatus using petroleum ether at 35°C for 4 hours. For comparison, one commercial oil (CO), obtained by cold pressing, was purchased. Phytochemical screening revealed the presence of flavonoids, steroids, triterpenes, and coumarins in the FO, whereas only coumarins were detected in the commercial oil. GC-MS analysis identified linoleic, linolenic, oleic, and eicosanoic acids in both samples. However, the FO also contained a broader range of compounds, including terpenes such as β -selinene, (+)-aromadendrene, α -humulene, d-nerolidol, geranylgeratriene, farnesene, farnesol and farnesyl acetate. These results underscore the importance of selecting appropriate extraction methods and implementing quality control procedures to ensure the chemical integrity and potential efficacy of the final product.

Keywords: *Bixa orellana* L., extraction, phytochemical, CG-MS





***SUSTAINABLE USE OF AGRICULTURAL WASTE: GREEN EXTRACTION
METHODS FOR OBTAINING RESVERATROL FROM PEANUT***

Mirella Thaisa Ferreira Ranzeti^{*1,2}, Gabriela Cremasco², Daniel Rinaldo^{1,2}

mirella.ferreira@unesp.br

1- Instituto de Química, UNESP, Av. Prof. Francisco Degni, 55, Araraquara, SP, Brazil. 2- Green Biotech Network, Faculdade de Ciências, UNESP, Av. Eng. Luís Edmundo Carrijo Coube, 2085, Bauru, SP, Brazil.

Brazil ranks seventh in the world in peanut (*Arachis hypogaea*) production, with the state of São Paulo being the sixth-largest national producer – an activity that, like any agro-industrial chain, generates a significant amount of solid residues, including stems, shells, roots, and other by-products. These residues represent a promising source of bioactive compounds, with resveratrol, a stilbene classified as a secondary metabolite, standing out due to its well-documented anti-inflammatory, antioxidant, and anticancer properties, making it highly attractive to the pharmaceutical, cosmetic, and food industries. In this context, this aims of this study was to develop green and efficient methods for extracting resveratrol from peanut residues, using Natural Deep Eutectic Solvents (NADES) as a sustainable alternative to conventional organic solvents. Three extraction techniques are evaluated: Microwave-Assisted Extraction (MAE), Ultrasound-Assisted Extraction (UAE), and Dynamic Maceration Extraction (DME), each employing eight different NADES at a ratio of 1:20 (peanut residue powder: solvent, w/v). In the preliminary screening with MAE, UAE and DME techniques, the latic acid/glycerol-based NADES (1:1, mol/mol), with 20% water addition, showed the highest extraction efficiency for resveratrol. The most efficient NADES from each technique were compared with one another and with conventional extraction methods reported in the literature (using methanol and ethanol). The combination of latic acid/glycerol-based NADES with MAE exhibited the best performance, achieving an extraction efficiency 2 times higher than the NADES used in the other techniques and 2.7 times greater than the conventional solvent-based methods. The results obtained validate the proposed approach, demonstrating the potencial of strategies aligned with principles of Green Chemistry and the Circular Economy. The use of tailored NADES, combined with energy-assisted techniques such as MAE, represents a promising approach for the valorization of agro-industrial residues, contributing to value addition in the peanut production chain.

Keywords: *Micro-wave assisted extraction, ultrasound assisted extraction, dynamic maceration extraction, peanut waste, green solvents*





**SCREENING OF BRYOZOANS FROM SÃO SEBASTIÃO COASTLINE AND
ISOLATION OF NOVEL INDOLE ALKALOIDS FROM *Amathia brasiliensis***

Kleyton J. G. Morais^{1*}, Caue A. W. Zuccarino,¹ Rafael V. C. Guido², Antonio G. Ferreira³,
Leandro M. Vieira⁴, Roberto G. S. Berlick¹

kjmorais@usp.br

1 – Instituto de Química de São Carlos, USP, Av. Trabalhador Sancarlense, 400, São Carlos, SP, Brazil. 2 – CIBFar, Instituto de Física de São Carlos, USP, Av. Trabalhador Sancarlense, 400, São Carlos, SP, Brazil. 3 – LRMN, Universidade Federal de São Carlos, Avenida Biblioteca Comunitária, DQ, São Carlos, SP, Brazil. 4 – LAEBry, Departamento de Zoologia do centro de Biocincências, Universidade Federal de Pernambuco, Av. Prof. Moraes Rego, 1235, Recife, PE, Brazil

The marine biodiversity is an exceptional source of bioactive compounds with potential applications in biotechnology and medicine. Among marine invertebrates, bryozoans (phylum Bryozoa) stand out due to their production of structurally unique secondary metabolites, including indole alkaloids and macrolactones. This study aimed to perform a chemical screening of bryozoans collected at the São Sebastião coastline (SP). Fourteen samples representing nine bryozoan species were freeze-dried and extracted with MeOH. The extracts were partitioned into hexane, EtOAc, and H₂O. EtOAc fractions were pre-fractionated using solid-phase extraction with cyanopropyl-modified silica-gel columns, and the fractions obtained were analysed by HPLC-UV-MS. A dereplication step was carried out by comparing MS data with natural product databases. *Amathia brasiliensis* sample (SS23BRI-14) was selected for further investigation. Three fractions (BRI14A, BRI14B, and BRI14F) were submitted to biological assays. Fractions BRI14B and BRI14F displayed promising antiplasmodial activity, inhibiting the growth of *Plasmodium falciparum* at $95 \pm 1\%$ and $94 \pm 0\%$, respectively, at concentrations of 50 $\mu\text{g/mL}$. Fraction BRI14A was fractionated by HPLC, yielding three major compounds (BRI14A24, BRI14A28 and BRI14A10D). Structural elucidation was performed using 1D and 2D NMR (¹H, ¹³C, COSY, HSQC, HMBC), UPLC-QToF-MS/MS, and optical rotation. Three novel halogenated indole alkaloids were isolated and identified by analysis of spectroscopic data. Our findings indicate that the bryozoan *Amathia brasiliensis*, endemic of Brazil, is a source of unique secondary metabolites and reinforces the importance of investigating secondary metabolites from Brazilian marine invertebrates. The authors thank CAPES for the student research scholarship and FAPESP for financial support through the thematic project.

Keywords: Marine natural products, Bryozoa, alkaloids





PROSPECTING SECONDARY METABOLITES FROM GRAM-NEGATIVE BACTERIA ASSOCIATED WITH PROPOLIS

Evelyn Assis de Andrade^{1*}, Almir M. G. Júnior², Simone P. Lira², Roberto G. S. Berlinck¹

*evelyn.aandrade@usp.br

1- Chemistry Institute of São Carlos, University of São Paulo, São Carlos, SP, Brasil.

2 - Luiz de Queiroz College of Agriculture, University of São Paulo, Piracicaba, SP, Brasil.

Gram-negative bacteria are a largely underexplored source of secondary metabolites, despite their increasing importance in natural products research. The present study aims to evaluate the potential of Gram-Negative bacteria isolated from propolis samples to produce bioactive metabolites. Gram-Negative bacterial strains were isolated from three types of propolis collected from different Brazilian biomes: (a) Caatinga green propolis and *Mimosa tenuiflora* resin (Remanso, BA); (b) green propolis and *Baccharis dracunculifolia* resin (Garanésia, MG); and (c) red propolis and *Dalbergia ecastophyllum* resin (Marechal Deodoro, AL). Collected samples underwent serial dilutions, were inoculated on selective media, and incubated while closely monitoring bacterial growth. Colonies with Gram-negative morphology were isolated, purified, and cryopreserved in 20% glycerol. Strains were also grown on a 1-liter scale for the extraction of growth media. Extracts were prepared by liquid-liquid partitioning and solid-phase extraction. Selected extracts underwent LC-MS-based metabolite profiling to assess their chemical diversity and identify potential bioactive compounds. Preliminary results show a high taxonomic diversity among the Gram-negative isolates, encompassing 15 bacterial genera. Special focus was given to strains isolated solely from Caatinga green propolis, a biome that remains underexplored in natural product research and may harbor bacteria with unique metabolic profiles. These findings highlight the potential of Gram-negative bacteria as sources of structurally novel and pharmacologically significant bioactive compounds.

Keywords: Brazilian propolis, natural product screening, bioprospecting, bioactive compounds.





ANTI-PLASMODIAL BROMINATED METABOLITES FROM MARINE SPONGES OF THE BRAZILIAN COAST.

Caue A. W. Zuccarino^{1*}, Mariane M. Mendanha¹, Andrés F. T. Peña¹, Marcelo R. de Amorim¹, Rafael V. C. Guido², Antônio G. Ferreira³, Roberto G. S. Berlinck¹

cauezuccarino@gmail.com

1-IQSC, Instituto de Química de São Carlos, USP, Av. Trab. São Carlense 400, São Carlos, SP, Brazil. 2-IFSC, Instituto de Física de São Carlos, USP, Av. Trab. São Carlense 400, São Carlos, SP, Brazil. 3-Departamento de Química, UFSCAR, Rod. Washington Luís, São Carlos, SP, Brazil.

Malaria is an infectious disease caused by *Plasmodium* parasites. In 2023, an estimated 263 million confirmed cases were reported resulting in approximately 600.000 deaths across 83 malaria-endemic countries.¹ Marine sponges are known to be an outstanding source of biologically active natural products. In the present investigation we evaluated the biological and chemical profile of three marine Verongida sponges collected at the coast of Brazil. The biological material was freeze-dried, extracted with MeOH and partitioned into hexane, AcOEt and H₂O fractions. Fractionation of the extracts resulted in enriched fractions which were subjected to the anti-*Plasmodium* assay and HPLC-UV-MS analyses. *Aplysina alcicornis* fractions (AASP) and *Aiolochoiria crassa* (AiCr) were selected for further bioassay-guided investigation. Fractions AASP7, AASP12 and AiCr_F1 inhibited the growth of *Plasmodium falciparum* at $98 \pm 1\%$, $98 \pm 1\%$ and $95 \pm 1\%$, respectively, at concentrations of 50 $\mu\text{g/mL}$. Fractions were submitted to purification by HPLC-UV, resulting in six pure compounds (AASP7-pS7_p12C, AASP7-pS7_p12G, CSF3-T2, AASP7-pS7_p5, AASP7-pS7_p12, AASP12-pS7M). Structural elucidation was performed using spectroscopic and spectrometric analyses. Pure compounds were submitted to the antiplasmodial assay, compound CSF3-T2 displayed $94 \pm 1\%$ (IC₅₀ of 50 μM) and compound AASP12-pS7M displayed $99 \pm 1\%$ (IC₅₀ of 1.94 μM) of growth inhibition of *Plasmodium falciparum*. Our results demonstrate the importance of studying Brazilian marine invertebrates. The authors thank CNPq, CAPES for the student's scholarship as well as FAPESP for the financial support.

Keywords: Marine sponge, isolation, antiplasmodial, HPLC-UV-MS, NMR

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BIOACTIVE SECONDARY METABOLITES PRODUCED BY THE MARINE FUNGUS *Nigrograna* sp.

Andrés F. T. Peña^{1*}, Marcelo R. de Amorim¹, Rafael V. C. Guido², Antonio G. Ferreira³, Roberto G. S. Berlick¹

andres.torres@usp.br

1 – Instituto de Química de São Carlos, USP, Av. Trabalhador Sancarlense, 400, São Carlos, SP, Brazil. 2 – CIBFar, Instituto de Física de São Carlos, USP, Av. Trabalhador Sancarlense, 400, São Carlos, SP, Brazil. 3 – LRMN, Universidade Federal de São Carlos, Avenida Biblioteca Comunitária, DQ, São Carlos, SP, Brazil

Malaria is a potentially fatal disease caused by *Plasmodium falciparum*, with a high global incidence, particularly concentrated in Sub-Saharan Africa and, in Latin America, in countries such as Colombia, Ecuador and Brazil. In 2021, the World Health Organization reported 247 million cases and over 419,000 deaths resulting from this disease (MADHAV et al., 2023). Although artemisinin derivatives initially showed effectiveness in malaria treatment, the emergence of resistant strains of *P. falciparum* has compromised their therapeutic efficacy, highlighting the urgent need to identify new natural bioactive compounds with antimalarial potential (PENNA-COUTINHO et al., 2021) (KYEI-BAFFOUR et al., 2020).

In this study, secondary metabolites from aqueous, AcOEt, and mycelial extracts produced by the marine fungus *Nigrograna* sp. M13 have been isolated, identified and subjected to bioassays. Pre-purification of the extracts was performed using size-exclusion chromatography on Sephadex LH-20, and by solid-phase extraction. The resulting fractions were subjected to chemical and biological dereplication, prioritizing those that exhibited poorly investigated m/z ions in natural product databases, as well as those that demonstrated antiplasmodial activity $\geq 90\%$. Selected fractions were purified by HPLC-UV and identified. A series of aromatic polyketides and unusual nitrogenated metabolites have been isolated and identified, two of which displayed moderate antiplasmodial activity, with IC₅₀ values of $4.9 \pm 0.3 \mu\text{M}$ and $7.1 \pm 0.8 \mu\text{M}$, respectively.

Acknowledgments: The authors thank FAPESP, CNPq, and CAPES for financial support and fellowships granted.

Keywords: Marine natural products, Marine fungi, *Nigrograna* sp.

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BIOACTIVE SECONDARY METABOLITES FROM TWO SPECIES OF MARINE SPONGES OF THE GENUS *Aaptos*

Barbara Aliende Almeida^{1*}, Caue A. W. Zuccarino¹, Karina F. Baraco¹, Rafael V. C. Guido², Antônio G. Ferreira³, Roberto G. S. Berlinck¹

barbaraaliende14@usp.br

1-IQSC, Instituto de Química de São Carlos, USP, Av. Trab. São Carlense 400, São Carlos, SP, Brazil.

2-IFSC, Instituto de Física de São Carlos, USP, Av. Trab. São Carlense 400, São Carlos, SP, Brazil. 3-Departamento de Química, UFSCAR, Rod. Washington Luís, São Carlos, SP, Brazil.

Marine sponges are a prolific source of secondary metabolites. Marine sponges of the genus *Aaptos* are broadly distributed in the marine ecosystem, with approximately 20 species described. Since the beginning of the 1980s, many research groups worldwide have carried out chemical investigations on *Aaptos* species that culminate in the discovery of the representative 1*H*-benzo[d,e][1,6]-naphthyridine alkaloids, collectively known as aaptamines.¹ These alkaloids present several potent biological activities.

In this report we present the biological and chemical investigation of two marine sponges belonging to the genus *Aaptos* collected along the Bahia state coastline, Brazil. The two specimens of *Aaptos* sp. (BA07ES-60 and 100) were freeze-dried, extracted with MeOH, the extract evaporated and partitioned with hexane, and subsequently between AcOEt and H₂O. Fractionation of the organic fraction by size-exclusion chromatography and solid-phase extraction (SPE-C18 and SPE-CN) resulted in chemically enriched fractions which were subjected to HPLC-UV-MS analyses. The aqueous fractions obtained from the extracted material of BA07ES-100 were analysed by HPLC-UV-MS. Subfractions that possibly contain structurally correlated aaptamine derivatives are currently undergoing purification and isolation by HPLC-UV. Pure compounds will be subjected to the antiplasmodial assay to investigate their biological activity. Our results demonstrate the importance of studying the ecological diversity of the Tropical Southwestern Atlantic coast of Brazil. The authors thank CNPq, CAPES for the student's scholarship as well as FAPESP for the financial support.

Keywords: Marine sponge, isolation, antiplasmodial, HPLC-UV-MS, NMR

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EXTRACTION AND PHYTOCHEMICAL CHARACTERIZATION OF *COFFEA ARABICA* L. OIL FROM BAHIA

Jayne Ferreira da Silva Oliveira^{1*}, Paulinne Moreira Lima¹, Micaela Sousa Coutinho Silva¹, Isabela Dias dos Santos¹, Lara Beatriz de Andrade Silva¹, Maria Alice Sousa Marinho¹, Juliano Geraldo Amaral.¹

jayne.oliveira@ufba.br

1-Instituto Multidisciplinar em Saúde – Campus Anísio Teixeira / Universidade Federal da Bahia,
Rua Hormindo Barros, 58, Candeias, Vitória da Conquista, Bahia.

Vegetable oils are widely used in the pharmaceutical and cosmetic industries due to their therapeutic and bioactive properties, making them indispensable for promoting human health. In this context, coffee, one of the most widely consumed natural products worldwide, has attracted growing interest. Green seeds, especially from the species *Coffea arabica* L., enable the extraction of an oil rich in phenolic compounds and sterols. According with this, the present study aimed to characterize the physicochemical and phytochemical profile of the oil extracted from green seeds of *Coffea arabica* L. cultivated in the Southwestern region of Bahia, Brazil. For this purpose, 10 samples (SisGen A4142D9) were collected from different producers in the region for lipid extraction, followed by physicochemical analyses (pH, density, refractive index, and acid value) and phytochemical characterization by gas chromatography coupled to mass spectrometry (GC-MS), with the aid of the Global Natural Products Social Molecular Networking (GNPS) platform. The physicochemical results showed mean values of pH 5.6 (CV = 9%), density 0.9503 g/cm³ (CV = 3.09%), refractive index 1.475 (CV = 0.10%), and acid value 12.85 mg KOH/g (CV = 40%). The low coefficients of variation for density and refractive index indicate good stability among the samples and confirm characteristics consistent with high-quality vegetable oils. The slightly acidic pH is in agreement with the presence of phenolic compounds. However, the high acid value suggests possible lipid degradation, which may be associated with deficiencies in storage, seed maturation, or a lack of standardization in grain processing. This underscores the need for stricter control of processing conditions. Phytochemical analysis revealed the presence of unsaturated fatty acids, such as linoleic and oleic acids, as well as palmitic acid and compounds from the diterpene group. These components are known for their antioxidant, anti-inflammatory, and emollient properties, reinforcing the functional and therapeutic potential of the oil. Therefore, this study will serve as a basis for the use of green coffee oil in the cosmetics sector, while also providing data for the development of pharmaceutical products.

Keywords: Oil, GNPS, *Coffea arabica* L, Molecular networks.





DIVERSITY OF THE FUNGAL MICROBIOME ASSOCIATED WITH ECHINODERMS FROM SÃO SEBASTIÃO (SÃO PAULO), TOWARDS METABOLOMICS

Julia Farias Ikenaga^{1,2*}, Matheus Gotha², Cauê Arantes Wagner Zuccarino², Kleyton Junior Gomes de Moraes², Roberto Gomes de Souza Berlinck²

juliaikenaga@gmail.com

1-Department of Genetics and Evolution, Federal University of São Carlos, São Carlos 13565-905, Brazil 2- São Carlos Institute of Chemistry, University of São Paulo (USP), São Carlos 13566-590, Brazil

Marine organisms have acquired chemical adaptations that provide them protection against different predators, as well as chemical cues for environmental adaptation. These chemicals are secondary metabolites which are produced and/or accumulated when marine macroorganisms are exposed to stressful situations, and present an array of bioactivities. Frequently these compounds are produced by microorganisms associated to macroorganisms. Echinoderms (sea-stars, holothurians or sea cucumbers, and brittle stars) are marine invertebrates that participate directly in the marine nutrient cycling processes, and typically provide complex triterpene saponins as secondary metabolites. Much less investigated are fungi associated with echinoderms, in particular from echinoderms' viscera. The few studies developed have shown that secondary metabolites produced by fungi associated with echinoderms are remarkably unique both structurally and biologically. The present investigation aimed at the isolation identification of fungal strains associated with echinoderms' viscera collected on the coast of São Sebastião (SP, Brazil), as well as to evaluate their production of secondary metabolites under different culture conditions. Nineteen of such fungal strains were grown in different media, which were extracted with EtOAc, the extracts defatted and subjected to a solid-phase extraction pre-purification. Analysis of fractions was performed by HPLC-UV-MS, UPLC-HRMS and UPLC-MS/MS. Metabolomics analysis was performed using GNPS, MetaboAnalyst 6.0 and SIRIUS 4. Among the detected secondary metabolites, some were brominated, and the majority are assigned as polyketides, sesquiterpenes, and aromatic compounds. Results of this investigation will be presented and discussed.

Keywords: *marine biotechnology, microbial metabolism, marine diversity, fungi*

Acknowledgements: to FAPESP, CAPES and CNPq for the financial support.





UNTARGETED METABOLOMIC OF *Andira legalis* EXTRACTS FROM JURUBATIBA SANDBANK OF THE RIO DE JANEIRO STATE AND THEIR ANTIBACTERIAL AND ANTIBIOFILM POTENTIALS.

Carla Monteiro Leal^{1*}, Stella M. Castro¹, Gabrielle L. de Queiroz¹, Marilia dos R. N. Chen¹, Brenda C. M.¹, Diego Rodrigues², Anderson da R. Gripp², Rodrigo Lemes², Fernanda S. Cavalcante³, Henriette Uthe⁴, Jörg Ziegler⁴, Maria Isabel S. dos Santos¹, Ludger A. Wessjohann⁴, Ivana Correa Ramos Leal¹.

farmacarlaleal@gmail.com

1-LaProNEB, DPNA, UFRJ, Av. Carlos Chagas Filho, 373, RJ, Brazil. 2-NUPEM, Instituto de Biodiversidade e Sustentabilidade, UFRJ, Av. São José do Barreto, 764, RJ, Brazil. 3-LIH, Instituto de Microbiologia Paulo de Góes, UFRJ, Av. Carlos Chagas Filho, 373, RJ. 4- IPB, MetaCom, Weinberg 3 06120 Halle (Saale), Germany.

The National Park of Jurubatiba Sandbank is a Federal conservation unit, located along the north coast of the RJ State. Among the plants found in Restinga, *Andira legalis* (AL) is common in Clusia Open Shrub Formation (COSF) and Post-beach Formation (PBF). The aim of the study is to search for antibacterial and antibiofilm compounds of AL extracts. Leaves of AL (n= 20; COSF and PBF) was collected in the summer (-S) and autumn (-A) seasons, and was stored at -80°C. The dried and crushed material was extracted with MeOH:H₂O (8:2). The chemical analyses were performed in the Agilent 1290 infinity II HPLC system coupled to timsTOF Bruker®. Data processing was performed in MetaboScape® while the data analysis in the Sirius, Metlgel, GNPS2, and Metaboanalyst. The MIC (*solid medium*) of the extracts was measured using the *Steers* replicator inoculation method, at 128 to 512 µg/mL, in duplicate. There were tested 32 multidrug-resistant bacteria isolated from nasal colonization of neonates. The MBC and MIC (*liquid medium*) were also evaluated at concentrations varying from 16 to 512 µg/mL. The active extracts were further evaluated for their ability to prevent biofilm formation at sub-MIC concentrations (<256 µg/mL) against the bacterial strains that demonstrated higher susceptibility. Epigallocatechin, procyanidin A- and B-types, O- and C-glycoside flavonoids were annotated. AL specimens from COSF and PBF, collected in summer (-S) and autumn (-A), inhibited *S. haemolyticus* at 128 µg/mL. One specimen (COSF-S) inhibited *S. epidermidis* at 128 µg/mL, while one specimen COSF-A inhibited *S. aureus* at 128 µg/mL. By the MIC assay, in *liquid medium*, these same specimens inhibited *S. haemolyticus*, *S. epidermidis* and *S. aureus* at 32 µg/mL, 32 µg/mL and 128 µg/mL, respectively. In the antibiofilm activity evaluation, two AL specimens from COSF-S, showed 39% and 44% inhibition of *S. haemolyticus* at 256 µg/mL. In the future, LC-HRMS/MS data will be correlated with environmental conditions, such as soil mineral components, temperature, pH and humidity, by the use of local sensors.

Keywords: Healthcare-associated infections; metabolomics; bioinformatic tools; antimicrobial activity.





NADES AS A SUSTAINABLE ALTERNATIVE FOR ANTHOCYANIN EXTRACTION FROM AÇAÍ (*EUTERPE OLERACEA* MART.)

Rafael Pignoli Alvares^{1*}, Gabriela Cremasco¹, Mirella Thaisa Ferreira Ranzeti², **Daniel Rinaldo^{1,2}**

daniel.rinaldo@unesp.br

1-Green Biotech Network, School of Sciences (FC-UNESP - Bauru); 2-Institute of Chemistry (IQ-UNESP - Araraquara)

Brazil is the world's leading producer of açai (*Euterpe oleracea* Mart.), with approximately 93% of its annual production of 1.7 million tons concentrated in the state of Pará. Rich in anthocyanins and other antioxidant compounds, açai has gained prominence in the food, cosmetic, and pharmaceutical industries. However, the large-scale extraction of these compounds using conventional methods can generate substantial volumes of toxic waste, increase treatment costs, and lead to environmental impacts. As an alternative, nine Natural Deep Eutectic Solvents (NADES) were prepared and used as extraction media, applying a miniaturized Microwave-Assisted Extraction (MAE) technique. HPLC-DAD analyzed the extracts obtained, and extraction efficiency was evaluated based on the total integrated area of the chromatographic bands corresponding to anthocyanins. The larger the area, the higher the extraction efficiency. The most promising NADES (lactic acid: glycerol, 1:1 mol/mol) was optimized using a Central Composite Design (CCD), considering three independent variables: plant/solvent ratio (mass/mass), temperature (°C), and extraction time (min). Extractions were performed using an advanced microwave system (Ethos Easy), with the plant/solvent ratio being the only variable with a significant effect. The optimal conditions were a ratio of 1:25 (mass/mass), a temperature of 40 °C, and an extraction time of 65 min. The method was compared to two conventional ultrasound-assisted extraction (UAE) procedures: the first using 80% (v/v) methanol, ratio 1:5 (m/v), 45 °C, 25 min; the second using 75% (v/v) ethanol, ratio 1:7 (m/v), 40 °C, 50 min. The Analytical GREENness (AGREE) metric was used to assess the environmental performance of all methods. Results showed that the lactic acid:glycerol-based NADES achieved the highest extraction efficiency (1.4 times greater than the most efficient conventional solvent) and the best environmental profile. It is concluded that the combination of lactic acid: glycerol NADES (1:1 mol/mol) with MAE constitutes an effective and sustainable strategy for extracting anthocyanins from açai, promoting the valorization of plant by-products based on Green Chemistry principles and the United Nations Sustainable Development Goals. The authors gratefully acknowledge financial support from the CNPq, grant #303887/2024-9, and the FAPESP, grant # 2025/03036-3, Brazil.

Keywords: *Experimental Design, Green Extraction, Microwave-Assisted Extraction.*





INVESTIGATION OF ANTIFUNGICAL ACTIVITY AGAINST *Candida auris* FROM FRACTIONS OF *Siparuna glycyarpa* OBTAINED BY COUNTERCURRENT CROMATOGRAPHY

Nayara S. Ricardo^{1*}, Esthella A. S. Silva², Ana Beatriz S. Garcias², Diégina A. Fernandes², Simony C. Mendonça³, Daniel C. de Moraes⁴, Antonio F. Perreira⁴, Suzana G. Leitão³; Gilda G. Leitão^{1*}

*nayara.sales0217@gmail.com

¹Programa de Pós-Graduação em Ciências Farmacêuticas (PPGCF/FF/UFRJ); ²Instituto de Pesquisa de Produtos Naturais (IPPN/UFRJ); ³Faculdade de Farmácia (FF/UFRJ); ⁴Departamento de Microbiologia Geral, Instituto de Microbiologia Paulo de Góes (UFRJ)

Candida auris has emerged as a multidrug-resistant fungal pathogen of global concern, associated with severe invasive infections and high mortality rates. Azoles remain the primary class of antifungal drugs used for candidiasis; however, resistance in *C. auris* poses a significant challenge to current therapeutic strategies. *Siparuna glycyarpa* (Siparunaceae), native to the Brazilian Amazon, recognized for its rich and diverse chemical composition, including alkaloids, chalcones, and both free and glycosylated flavonoids. The present study aims to evaluate fractions from *S. glycyarpa* with potential antifungal activity against *C. auris*, focusing on their ability to inhibit efflux pumps, either alone or in combination with fluconazole. A portion of the SGD extract underwent initial clean-up by liquid–liquid extraction using hexane–ethyl acetate–methanol–water (HEMWat, 1:1:1:1, v/v). The upper phase (SGDU) was subsequently fractionated by high-speed countercurrent chromatography (HSCCC) on an HTPrep apparatus equipped with a 112 mL column (2.0 mm i.d.) operated at a flow rate of 2.5 mL/min, using HEMWat 7:3:6:4 as the solvent system. A total of 140 fractions (2 mL each) were collected, 80 during the elution phase and 60 during the extrusion phase. Based on thin-layer chromatography (TLC) profiles, these fractions were combined into 23 subfractions, which were then evaluated *in vitro* against *C. auris*. Of these, seven fractions, in which chalcones (2',6'-di-hidroxi-4,4'-dimetoxi-di-hidrochalcona and 2',6'-di-hidroxi-4'-metoxi-di-hidrochalcona) identified by NMR, demonstrated significant efflux pump inhibitory activity when combined with fluconazole at a concentration of 100 µg/mL. This finding suggests possible synergistic interaction between the compounds present in the fractions and fluconazole, potentially restoring the drug's effectiveness against resistant *C. auris* strains.

Keywords: Siparunaceae, Countercurrent Chromatography, Antifungal Activity

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COMPARATIVE ANALYSIS OF THE PHYTOCHEMICAL PROFILE AND ANTI-SARS-COV-2 POTENTIAL OF *Siparuna bifida* LEAF EXTRACTS FROM THE AMAZON AND ATLANTIC FOREST BIOMES

Edilaine Santos Sant'ana Moraes¹, **Diégina Araújo Fernandes^{1*}**, Simony Carvalho Mendonça², Gilda Guimarães Leitão¹
*diegina@ufrj.br

¹Laboratório de Fitoquímica e Cromatografia contracorrente – IPPN/UFRJ - 21491-599, Brazil.

²Departamento de Produtos Naturais e Alimentos – FF/UFRJ - 21941-902, Brazil.

The genus *Siparuna* (Siparunaceae), widely distributed across the tropical Americas, includes aromatic species traditionally used in Brazilian folk medicine to treat colds and flu. Several species have demonstrated antiviral activity, attributed mainly to alkaloids and flavonoids, reinforcing the therapeutic relevance of this genus. Despite this, *Siparuna bifida* (Poepp. & Endl.) A.DC. remains poorly studied in terms of its chemical composition and biological properties. This study aimed to investigate the phytochemical profile and antiviral potential of *S. bifida* leaf extracts, focusing on the inhibition of the SARS-CoV-2 papain-like protease (PL_{pro}), a key enzyme involved in viral replication and immune evasion. Specimens were collected from two ecologically distinct Brazilian biomes—the Amazon Rainforest and the Atlantic Forest—to evaluate the influence of environmental factors on metabolite composition and bioactivity. Dried leaves were exhaustively macerated in ethanol, and the crude extract was subjected to liquid–liquid partitioning with solvents of increasing polarity (hexane, dichloromethane, ethyl acetate, and n-butanol), yielding four extracts. These were analyzed by UHPLC-DAD-MS/MS, and data processing using MZmine enabled metabolite annotation. Antiviral activity was assessed through a FRET-based enzymatic assay targeting PL_{pro}, and Feature-Based Molecular Networking (FBMN) was applied to visualize metabolite clustering based on MS/MS fragmentation patterns. The hexane extracts of Atlantic Forest and Amazon exhibited the most pronounced inhibitory effect, with 87% and 58.2% inhibition at 100 µg/mL, respectively, suggesting a correlation between low-polarity constituents and antiviral activity. This enhanced activity may be related to the higher relative abundance of annotated compounds in hexane and dichloromethane extracts from Atlantic Forest biome. Chemical analysis led to the annotation of eleven isoquinoline alkaloids, including reticuline and its derivatives. These compounds formed a distinct molecular network in FBMN analysis, allowing a clear association between chemical structure and biological activity. The results underscore the potential of *S. bifida* as a source of bioactive alkaloids with antiviral properties and demonstrate the effectiveness of molecular networking as a tool for the targeted screening of complex natural matrices.

Keywords: Brazilian biomes; Siparunaceae; Benzyltetrahydroisoquinoline alkaloids; FRET; SARS-CoV-2.

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EVALUATION OF NATURAL PIGMENTS EXTRACTED FROM JARACATIÁ (*Jacaratia spinosa*) PEEL USING INFRARED SPECTROSCOPY

Lucas Santos de Jesus^{1*}, Luana Vitória Pereira dos Santos¹, Miguel Gustavo Beilner de Oliveira², Anahí Tamara Rauh³, Idemir Citadin⁴, Sirlei Dias Teixeira⁵, Edimir Andrade Pereira⁵

jesus.2002@alunos.utfpr.edu.br

1- Student of the Chemistry Course, UTFPR, PB, Via do Conhecimento, Pato Branco, s/n, PR, Brazil.
2- Student of the Agronomy Course UTFPR, PB, Via do Conhecimento, Pato Branco, s/n, PR, Brazil.
3- Student of the Interinstitutional Master's Program in Agronomy (MINTER-CAPES), Rua Nacional 12, Miguel Lanús, Posadas, Misiones, Argentina. 4- Professor/Researcher at the Department of Agronomy UTFPR, PB, Via do Conhecimento, Pato Branco, s/n, PR, Brazil. 5- Professor/Researcher at the Department of Chemistry UTFPR, PB, Via do Conhecimento, Pato Branco, s/n, PR, Brazil.

Jaracatiá (*Jacaratia spinosa*) is an unconventional food plant (panc), popularly called *mamoeiro-bravo* or *mamãozinho*, it is native from the Atlantic Forest and found in regions of Brazil, Argentina, and Paraguay. It belongs to the Caricaceae family and can be used in the food industry, especially as a source of natural dyes. In recent decades, there has been a great scientific interest in this panc, which was widely used by the rural population of southern Brazil, by its fruit and branches. This work aimed to extract and characterize natural pigments from the peels of ripe fruits of *J. spinosa* by Fourier-transform infrared spectroscopy (FTIR). The fruits were collected in different locations in the province of Misiones, Argentina. Extractions were performed with ethanol-water in a 70:30 ratio, and six samples of different genotypes were evaluated. The obtained extracts, with yellow coloration, were analyzed by FTIR to identify functional groups related to bioactive compounds, possibly carotenoids and flavonoids present in the jaracatiá peel. Two samples were selected: sample 6 (highest pigment yield) and sample 8 (most intense yellow color), whose spectra showed absorptions in the region of 2,900 to 2,800 cm⁻¹, which correspond to symmetric and asymmetric vibrations of C-H groups, methyl and methylene, attributed to carotenoids (yellow dyes). The absorption at wavelengths of 1,717 cm⁻¹ can be related to the carbonyl group of a cyclic ketone, which, associated with the bands observed at 3,600 to 3,000 cm⁻¹ representing OH groups (water, alcohol, and phenol), may indicate the presence of flavonoids such as flavones and flavonols. Thus, through FTIR analyses, it could be inferred that the jaracatiá peel contains phenolic pigments with antioxidant potential. The applied methodology allows rapid and efficient characterization of natural dyes, reinforcing the value of jaracatiá as a functional and promising resource for applications in food industry, and also representing a key tool for future analyses aimed at characterizing the fruit pulp.

Keywords: natural dyes, FTIR, flavonoids, carotenoids.





**CHEMICAL CHARACTERIZATION AND PHYTOTOXIC POTENTIAL OF
PYROLIGNONEOUS ACID**

Larissa Abatti^{1*}, Ana Paula Palaro Klein Hendges¹, Gabriela Pilatti², Marcus André Cardoso de Araújo², Michelangelo Muzell Trezzi², Sirlei Dias Teixeira¹

larissaabatti@alunos.utfpr.edu.br

1-Departamento de Química, PPGTP, UTFPR, Via do conhecimento, km 1, Pato Branco, PR, Brazil.

2-Departamento de Agronomia, UTFPR, Via do conhecimento, km 1, Pato Branco, PR, Brazil

Pyroligneous Acid (PA) is a liquid obtained from the pyrolysis of wood, a process in which charcoal is produced and condensed smoke is collected simultaneously. PA has a reddish-brown color and may contain more than 200 compounds. The quantity and diversity of these compounds vary according to the plant species used and the collection temperature. Some plants produce compounds, called allelochemicals, that can interfere with the growth and development of other plants and can act as bioherbicides if their effectiveness is properly demonstrated. In this context, researchers have investigated PA for its properties as an herbicide derived from natural products. Therefore, the work aimed to chemically characterize the PA obtained from *Eucalyptus grandis*, and to evaluate its inhibitory potential through phytotoxic tests: mean emergence time (MET) and emergence speed index (ESI) of the target plants. PA was subjected to partition liquid-liquid with *n*-hexane and chloroform, called PAHex and PACHlorof, which were chemically characterized by GC-MS and subsequently analyzed via PCA. The correlation between GC-MS and the analysis of PCA loadings made it possible to verify that toluene, ethylbenzene, 3,5-dimethoxy-4-hydroxy-toluene, and *o*-xylene were only identified in PAHex, and 2-methoxy-phenol, 2-methoxy-4-methyl-phenol, 4-ethyl-2-methoxy-phenol, and 5-*tert*-butylpyrogallol are in greater quantities in PAHex when compared to the PACHlorof. The compound 2,6-dimethoxyphenol was the majority in both PAHex (21.98%) and PACHlorof (48.43%). The phytotoxicity tests were conducted at concentrations of 10%, 25%, 40%, 55%, 70%, 85%, and 100% of PA, formulated with 0.5% adjuvant mixture (1 SP80:9 TW20), applied in *Phaseolus vulgaris*, *Eragrostis plana* Nees, and *Euphorbia heterophylla*. The results demonstrated a consistent pattern in response to increasing allelochemical concentration, characterized by an increase in MET and a reduction in ESI, observed in all target plants, corroborating Pesenti (2021). This behavior suggests that the compounds present in PA significantly interfere with the initiation of seed germination, acting as inhibitors. These results reinforce PA's potential as a bioherbicide. Acknowledgments: UTFPR - Pato Branco, LAPNEQ-UFPR, and CAPES.

Keywords: allelochemical, bioherbicide, gas chromatography, natural products, wood vinegar.

Pesenti, M. C. Chemical Characterization of Pyroligneous Extract Obtained from *Eucalyptus grandis* and Allelopathic Tests of the Distilled Fraction. UTFPR, Pato Branco, 2021.





IDENTIFICATION AND BIOSYNTHESIS OF PEPTAIBOLS TRICHOKONINS VI AND VIII WITH ANTIPLASMODIAL ACTIVITY

Matheus Gotha^{1*}, Ariane F. Bertonha², David E. Williams³, Karen J. Nicacio⁴, Marcelo R. de Amorim¹, Cauê A. W. Zuccarino¹, Sydney M. Schoellhorn⁵, Anna Caroline C. Aguiar⁶, Lamonielli F. Michaliski¹, Lara D. Sette⁷, Antônio G. Ferreira⁸, Raymond J. Andersen³, Rafael V. C. Guido⁹, Roberto G. S. Berlinck¹

matheusgotha@alumni.usp.br, rgsberlinck@iqsc.usp.br

1-São Carlos Institute of Chemistry, University of São Paulo, 13560-970, São Carlos, Brazil. 2-LNBio, Brazilian Center for Research in Energy and Materials, 13083-970, Campinas, Brazil. 3-Departments of Chemistry and EOAS, UBC, 2036 Main Mall, Vancouver, Canada. 4-UFMT, 78060-900, Cuiabá, MT, Brazil. 5-Department of Chemistry and BioDiscovery Institute, UNT, Denton, TX, 76203, USA. 6-DMIP, Unifesp, 04023-062, São Paulo, SP, Brazil. 7-Departamento de Biologia Geral e Aplicada, UNESP, IB, Rio Claro, Brazil. 8-Departamento de Química, UFSCar, 13565-905, São Carlos, SP, Brazil. 9-São Carlos Institute of Physics, USP, 13566-590, São Carlos, SP, Brazil.

The fungus genus *Trichoderma* is found in a wide range of habitats, with more than 200 described species.¹ Secondary metabolites produced by *Trichoderma* spp. have mainly been used commercially in biocontrol.² Modified peptides known as peptaibols are commonly produced by *Trichoderma* species. Typical features of peptaibols include an acyl fragment connected at the N-terminal, incorporation of α -aminoisobutyric (Aib) residues, amino alcohol of the reduced amino acid at C-terminal, and presence of other non-proteinogenic amino acids. *Trichoderma* sp. L2-2 strain was obtained from a lichen sample collected at Admiralty Bay in Antarctica. Cultures of *Trichoderma* sp. L2-2 yielded trichokonins VI and VIII after several separation steps. Both peptaibols presented 20 amino acid residues and were completely identified by NMR, HRMS, MS/MS and dichroism circular spectra analyses. The full genome sequencing and analysis of *Trichoderma* sp. L2-2 enabled the identification of a peptaibol biosynthetic gene cluster and the proposal for a biosynthetic assembly of trichokonins VI and VIII. Trichokonins VI and VIII also exhibited antiplasmodial activities at the sub-micromolar range against *Plasmodium falciparum*.

1- Dou, K. *et al.* Appl Environ Microbiol, 86 (18), 2020.

2- Pedrero-Méndez, A. *et al.* Microbiol. Res. 2025, 296, 128153.

Keywords: Trichokonin VI and VIII, Peptaibols, ¹H and ¹³C NMR analyzes, Secondary metabolite, Antiplasmodial





EVALUATION OF THE CHEMICAL COMPOSITION OF ANNONA SQUAMOSA L. SEED OIL FOR APPLICATION AS A NATURAL PESTICIDE

Sylvia Helena Meireles da Silva^{1*}, Eduardo Silva Correia¹, Wellington Correa da Silva¹, Marivaldo José Costa Correa², Lourivaldo da Silva Santos², Haroldo da Silva Ripardo Filho¹

ripardo.filho@ifap.edu.br

1- Instituto Federal do Amapá, Rodovia BR-210, Bairro Brasil Novo, Macapá, AP, Brasil. CEP: 68909-398. 2- Universidade Federal do Pará, Campus Belém, Rua Augusto Corrêa, 01, Bairro Guamá, Belém, PA, Brasil. CEP: 66075-110

The search for ecological alternatives to synthetic pesticides has intensified due to environmental impacts and concerns about effects on human health. In this context, *Annona squamosa*, commonly known in Brazil as ata, pinha or fruta-do-conde, native to tropical regions, stands out as a promising plant due to its bioactive compounds. Among these compounds, acetogenins have been widely reported for their insecticidal potential, which is strongly associated with the characteristic biological activity of the Annonaceae family (Crisafulli, 2007; Paes et al., 2019). In this context, this study investigates the insecticidal activity of oil extracted from *A. squamosa* seeds against the leaf-cutting ant *Acromyrmex balzani*, an agricultural pest of economic relevance. To obtain the oil, seeds were removed from ripe fruits, separated from the pulp, and washed. They were then oven-dried, ground in a mill, and macerated in hexane for seven days. The solvent was removed by simple distillation, and the chemical composition of the oil was determined by GC-MS. GC-MS analysis identified high concentrations of oleic acid (77%), palmitic acid (10.87%), and stearic acid (10.71%). These long-chain fatty acids participate in the polyketide pathway, in which they can be converted by specific enzymes into more complex structures, such as acetogenins. The presence of these precursors suggests that the fruit seeds contain the necessary elements for the biosynthesis of acetogenins (Colin-Oviedo et al., 2022; Gallimore, 2009). Understanding the chemical profile of this oil is essential for elucidating its relationship with insecticidal activity. In subsequent stages, the insecticidal activity of the obtained oil will be evaluated against leaf-cutting ants, and other parts of the plant will be investigated to further expand knowledge on the species' insecticidal properties.

Keywords: *Annona squamosa*, acetogenins, insecticide, oil, seeds, *Acromyrmex balzani*, GC-MS, long-chain fatty acids.





DEVELOPING A CHROMATOGRAPHIC METHOD FOR THE ISOLATION AND EVALUATION OF THE IN VITRO ANTI-SARS-COV-2 ACTIVITY OF LISBOAEFLAVANONOL A

João Pedro Lima Sampaio^{1,2*}, Sarah Larissa Gomes Flores¹, Kidney de Oliveira Gomes Neves², Victória Riquena Grosche³, Mark Harris⁴, Ana Carolina Gomes Jardim³, Anderson Cavalcante Guimarães¹, Marcos Batista Machado^{1,2}

Joao.sampaio@ufam.edu.br

1- UFAM, Department of Chemistry, ICE - Coroadó, 69067-005, Manaus - AM, Brazil. 2-UFAM, Analytical Center, NMRLab - Coroadó, 69067-005, Manaus - AM, Brazil., 3. Laboratory of Antiviral Research, Federal University of Uberlândia, Uberlândia 38405-302, MG, Brazil, 4 - University of Leeds, Woodhouse Lane, Leeds, LS2 9JT, UK

The genus *Eugenia*, part of the Myrtaceae family, is abundant in the Amazon with around 100 species, but remains chemically underexplored. This study focuses on lisboae flavanone A, a glycosylated flavonoid from *Eugenia lisboae* leaves, previously identified by Neves *et al.* (2021) as a potential SARS-CoV-2 inhibitor in *in silico* assays targeting the 3CLpro and RdRp proteins. This work had two primary goals: to optimize the isolation method of this flavonoid and to confirm its *in vitro* antiviral activity against SARS-CoV-2. Researchers applied advanced chromatographic methods (HPLC and CCC) to the methanolic leaf extract. The HPLC proved highly effective, boosting the isolation yield of lisboae flavanone A to 2.25%, a nearly tenfold increase compared to the previous 0.27% yield. This significant methodological improvement allows to produce larger quantities of the compound for future biological studies. The organic structure was characterized using NMR and MS data. For the antiviral assessment, the isolated flavonoid was tested *in vitro* at concentrations of 50, 10, and 2.0 µg. mL⁻¹ against the original SARS-CoV-2 strain (Wuhan-Hu-1) and the Delta and Omicron variants. The results confirmed its antiviral potential, showing a reduction in viral infectivity by 7.5% (at 50 µg. mL⁻¹), 22.1% (at 10 µg. mL⁻¹), and 27.5% (at 2.0 µg. mL⁻¹). Therefore, this study successfully established a more efficient isolation method for lisboae flavanone A and provided crucial experimental validation of its anti-SARS-CoV-2 activity, contributing to the potential development of a natural antiviral drug.

Keywords: Antiviral; *Eugenia lisboae*; HPLC; SARS-CoV-2.

Reference:

1. Neves, K.O., et al., *Lisboae flavanone A: A new flavonoid glycoside obtained from Amazonian Eugenia lisboae*. Phytochemistry Letters, 2021. **43**: p. 65-69.





BIOACTIVE NATURAL PRODUCTS FROM A *Melipona quadrifasciata* ASSOCIATED *Streptomyces* sp.

Rafael Gonçalves Padilha^{1*}, Claudia C. de Macedo¹, Amanda S. Hirata², Letícia N. de Campos³,
Letícia V. Costa-Lotufo², Ilana L. B. C. Camargo³, Mônica T. Pupo¹

rafael_padilha@usp.br

¹ School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, Brazil.

² Institute of Biomedical Sciences, University of São Paulo, São Paulo, Brazil.

³ São Carlos Institute of Physics, University of São Paulo, São Carlos, Brazil.

Microorganisms associated with social insects are valuable sources of bioactive natural products, particularly actinobacteria engaged in defensive mutualistic symbioses. Despite their ecological importance as pollinators, the microbiomes and symbiotic interactions of stingless bees remain underexplored, especially in *Melipona quadrifasciata*. This study aimed to characterize the metabolites produced by *Streptomyces* sp. MQFBRP26, isolated from forager bees, and assess its bioactive potential. The strain was cultivated on solid ISP2 medium and subjected to overlay soft-agar antagonism assays against entomopathogens (*Beauveria bassiana*, *Metarhizium anisopliae*, *Paenibacillus larvae*) and human pathogens (*Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Candida albicans*), showing activity against *S. aureus* and *P. larvae*. For large-scale cultivation (350 Petri dishes, 90 mm), the culture was extracted with ethyl acetate and fractionated using C18 SPE cartridges with a solvent gradient of H₂O, MeOH/H₂O mixtures (25%, 50%, 75%, 100%), and acetone. The fractions were evaluated for antimicrobial activity and cytotoxicity against tumor cell lines. Active fractions were chemically profiled using HPLC-DAD-ELSD and HPLC-MS/MS, and dereplication employed GNPS and the Dictionary of Natural Products and Natural Products Atlas databases. The fractions showed significant cytotoxicity against HCT-116, SK-MEL-28, and MCF-7 cell lines (IC₅₀ 0.014–0.045 µg/mL) and antimicrobial activity against seven bacterial strains, including *Staphylococcus epidermidis*, *Staphylococcus aureus* (two strains), *Enterococcus faecalis*, *Enterococcus faecium*, *Escherichia coli*, and *Acinetobacter baumannii* (MICs 8–512 µg/mL). Dereplication of the MeOH 75% and 100% fractions revealed quinoxalines, including annotations of quinomycins A, B, C, E, G, triostin C, and depsipechinoserin, as well as ions consistent with putative novel analogs. The MeOH 100% fraction was selected for isolation, yielding six compounds, two identified as quinomycins A and C, supporting the dereplication data. Additional chromatographic bands exhibited UV-Vis spectra similar to quinomycins A and C, but at low concentrations. The OSMAC strategy will be applied to modulate culture conditions and optimize metabolite production. These results highlight *Streptomyces* sp. MQFBRP26 as a promising source of bioactive quinoxalines with potential antimicrobial and anticancer applications, while improving understanding of defensive symbioses in *M. quadrifasciata*. The authors thank their institutions and acknowledge financial support from CNPq (grant 141619/2023-6), CAPES (Finance code 001) and FAPESP (grants 2013/07600-3; 2025/10223-4).

Keywords: *Streptomyces*, *Melipona quadrifasciata*, quinoxalines, natural products, symbiosis, cytotoxicity





INCORPORATION OF NATURAL PRODUCTS INTO AN ANTI-AGING COSMETIC FORMULATION

Fernanda Caroline Knob^{1*}, Tatiane Luiza Cadorin Oldoni¹, Karin Carla dos Santos Schmidt¹, Suelen dos Santos²

fernandaknob@alunos.utfpr.edu.br

1- Department of Chemistry, Federal University of Technology - Paraná, 85503-390, Pato Branco, Paraná, Brazil; 2- Department of Chemistry, State University of the Midwest (UNICENTRO) – CEDETEG, 85040-167, Guarapuava, Paraná, Brazil

The leaves of *Syzygium malaccense* (Red Jambo) are a rich source of phenolic compounds with antioxidant potential, contributing to the prevention of premature skin aging. This study aimed to incorporate both the crude extract and a purified fraction obtained from the leaves into a cosmetic formulation with antioxidant properties. The hydroalcoholic extract (HE) was prepared using 40% ethanol via exhaustive solid-liquid extraction, with solvent renewal every 24 h for six days, and subsequently purified through solvent partitioning with hexane, dichloromethane, ethyl acetate, and acetone, yielding an acetone fraction (Fr-Ace) with the highest concentration of bioactive compounds. Antioxidant activity of HE and Fr-Ace was evaluated by DPPH and ABTS radical scavenging assays, ferric reducing antioxidant power (FRAP), and the Folin-Ciocalteu method (RFC), while phenolic composition was determined by high-performance liquid chromatography. Both samples were incorporated into cosmetic formulations at 0.5% (w/w) and subjected to centrifuge stability testing (6,000 rpm for 20 min) and antioxidant activity analysis (DPPH assay). HE and Fr-Ace exhibited high antioxidant activity, with IC₅₀ values for DPPH scavenging of 27.82 mg L⁻¹ and 18.51 mg L⁻¹, 349.34 and 316.90 mg GAE g⁻¹ for RFC, 3892 and 3204 μmol TE g⁻¹ for ABTS, 8509 and 6261 μmol FeSO₄ g⁻¹ for FRAP, respectively, values of likely due to the presence of phenolic compounds such as myricitrin and mearnsitrin, chemical markers of the species and more abundant in Fr-Ace. The formulation containing HE showed particle sedimentation after centrifugation, suggesting incomplete solubilization of the extract, whereas the Fr-Ace formulation remained stable and exhibited antioxidant activity with an IC₅₀ of 8562 mg L⁻¹. These results demonstrate that incorporating *S. malaccense* extracts enables the development of antioxidant-rich cosmetic products, with the purified fraction showing superior antioxidant activity, higher phenolic content, and greater solubility within the formulation, confirming the efficiency of the purification process and its potential for applying plant-derived matrices in the development of bioactive-rich products. The authors acknowledge UTFPR, the Central Analysis Laboratory, and CNPq (304982/2024-5).

Keywords: Antioxidant Activity, Cosmetic formulation, Flavonoids, Phenolic compounds





TWO NOVEL UNUSUAL DITERPENES AND OTHER TERPENES FROM THE BARK OF *XYLOPIA CALOPHYLLA* (ANNONACEAE)

Liciane Assis Pinheiro^{1*}, Valdenizia Rodrigues Silva², Luciano de Souza Santos², Milena Botelho Pereira Soares², Daniel Pereira Bezerra², Emmanoel Vilaça Costa¹

liciane.assis15@gmail.com

1. GEQBiom, Programa de Pós-Graduação em Química, ICE, Universidade Federal do Amazonas, Av. General Rodrigo Octavio Jordão, 6200, Manaus, AM, Brazil. 2. Instituto Gonçalo Moniz-Fiocruz-BA (IGM/FIOCRUZ-BA), Rua Waldemar Falcão, 121, Salvador, BA, Brazil.

Xylopia calophylla R. E. Fries is a species of the genus *Xylopia*, the second largest in the Annonaceae family, still scarcely studied in the literature. Known as “envira-vassourinha”, it occurs in igapó, várzea, and terra firme areas of the Brazilian Amazon. The hexane extract from the bark, obtained by maceration, was subjected to classical chromatographic techniques (CC, CCDA, and CCDP), resulting in the isolation of 12 terpenoid compounds, including two new diterpenes uncommon in Annonaceae. Structural elucidation was carried out by 1D/2D NMR experiments and mass spectrometry (MS), supported by literature data. The compounds were identified as terpenoids: three steroids (β -sitosterol, stigmasterol, and campesterol); three ketosteroids (stigmast-4-en-3-one or β -sitostenone, stigmast-4,22-dien-3-one, and campest-4-en-3-one); one oxygenated sesquiterpene (spathulenol); and five kaurane-type diterpenes, three known (kaurenoic acid, *ent*-15-oxokaur-16-en-19-oic acid, and xylopinic acid) and two new, named calophyllin A and calophyllin B, differing by the presence of an acetyl group ($-\text{COCH}_3$). The isolated compounds were evaluated against four human tumor cell lines (H1299, HepG2, MDA-MB-231, and SCC9) and one normal cell line (MRC-5). Only *ent*-15-oxokaur-16-en-19-oic acid and calophyllin B exhibited relevant activity, with IC_{50} values below 20 $\mu\text{g/mL}$ in all tumor cell lines. The most notable was *ent*-15-oxokaur-16-en-19-oic acid, which showed strong and promising activity against HepG2 ($\text{IC}_{50} = 5.63 \mu\text{g/mL}$) and H1299 ($\text{IC}_{50} = 9.55 \mu\text{g/mL}$). These findings, described for the first time for *X. calophylla*, demonstrate the potential of the new diterpenes as prototypes for antitumor agents and justify the continuation of phytochemical and biological studies, as well as expanding the chemosystematic knowledge of the species and the genus.

Keywords: *Xylopia calophylla*; diterpenes; terpenes; cytotoxic activity.

Acknowledgments: CAPES, CNPq, FAPEAM, Rede de Pesquisa FitoAmazônia (Pró-Amazônia/CNPq, grant n° 445615/2024-9), UFAM, and CA/CAM/UFAM.





NEW INSIGHTS INTO THE CHEMICAL CONSTITUENTS OF THE BARK OF *GUATTERIA MEGALOPHYLLA* (ANNONACEAE)

Victória Brandão Nardelli^{*,1}, Josean Fachine Tavares², **Emmanoel Vilça Costa^{*,1}**

^{*}nardellibvic@gmail.com; ^{evc@ufam.edu.br}

1. GEQBiom, Programa de Pós-Graduação em Química, ICE, Universidade Federal do Amazonas (UFAM), Av. General Rodrigo Octavio Jordão, 6200, Manaus, AM, Brazil; 2. Departamento de Ciências Farmacêuticas, Universidade Federal da Paraíba (UFPB), João Pessoa, PB, Brazil.

Guatteria megalophylla Diels (Annonaceae) is a tree species distributed in Colombia, Ecuador, Peru, Guyana, and Brazil, with records from the states of Acre, Amazonas, Pará, and Rondônia. Previous studies have reported the presence of alkaloids in the stem, such as *O*,*O*-dimethylcurine, 12'-*O*-methylcurine, and isocondodendrine, as well as antioxidant activity in ethanolic extracts of the stem and leaves. The chemical composition of the leaf essential oil has also been investigated, along with its *in vitro* and *in vivo* antileukemic potential against HL-60 cells [1]. This study represents the first phytochemical investigation focused specifically on the bark of this species. The hexane and methanolic extracts of the bark were prepared by maceration, and the alkaloid fraction was obtained from the methanolic extract through acid–base treatment. These analyses led to the isolation of 13 compounds, identified by 1D/2D ¹H and ¹³C NMR spectroscopy and gas chromatography–mass spectrometry (GC–MS). The hexane extract was fractionated by classical chromatography, using open-column chromatography and preparative thin-layer chromatography (PTLC), yielding the steroids campesterol, stigmasterol, β-sitosterol; the ketosteroids stigmast-4-en-3-one or β-sitostenone, stigmast-4,22-dien-3-one, and campest-4-en-3-one; and the oxygenated sesquiterpenes 1,10-*epi*-cubenol and caryophyllene oxide (8). The alkaloid fraction was further separated by high-performance liquid chromatography (HPLC), leading to the isolation of the alkaloids 9-hydroxyguatterfiesine, (–)-pallidine, melosmine, liriodenine, and the oxygenated sesquiterpene oxyphyllenodiol A. The hexane and methanolic extracts, as well as the neutral and alkaloid fractions, were evaluated for *in vitro* cytotoxic activity against HepG2 (human hepatocellular carcinoma) and HCT116 (human colon carcinoma) cell lines. Although none of the extracts or fractions exhibited strong cytotoxicity, the alkaloid fraction showed the highest inhibition (49.7% and 32.97% against HepG2 and HCT116, respectively), compared with the methanolic extract (19.64% and 3.71%). The discovery of these compounds in *G. megalophylla* not only provides the first chemical characterization of its bark but also strengthens the phytochemical framework of the genus *Guatteria*, underscoring its pharmacological potential.

Keywords: *Guatteria megalophylla*; alkaloids; sesquiterpenes; steroids and ketosteroids.

Acknowledgements: FAPEAM, CAPES, CNPq, UFAM, LMCA, and FINEP.

References: [1] COSTA, R. G.A., *et al.* *In vitro* and *in vivo* growth inhibition of human acute promyelocytic leukemia HL-60 cells by *Guatteria megalophylla* Diels (Annonaceae) leaf essential oil. **Biomedicine & Pharmacotherapy**, 122, 2020.





ISOLATION OF GLYCOSYLATED FLAVONIDS FROM THE ETHYL ACETATE LEAF EXTRACT OF *Siparuna cymosa* Tolm. BY COUNTERCURRENT CHROMATHOGRAPHY

Adérito José Cavele¹, Diégina Fernandes Araújo¹, Gilda Guimarães Leitão^{1*}

ajcavele2@gmail.com; *ggleitao@ippn.ufrj.br

¹ Laboratório de Fitoquímica e Cromatografia contracorrente – Instituto de Pesquisa de Produtos Naturais – Universidade Federal do Rio de Janeiro - 21491 599, Brazil.

Countercurrent chromatography (CCC) is a liquid–liquid separation technique based on the partitioning of solutes between two immiscible liquid phases, one of which is retained as the stationary phase within the column, while the other is used as the mobile phase during the chromatographic process. This technique has proven to be highly effective for the isolation of secondary metabolites from complex matrices. In this context, *Siparuna cymosa* Tolm., an endemic Brazilian species from the Siparunaceae family, also popularly known as *erva-do-rato*, has been extensively studied in the field of natural products due to its rich diversity of secondary metabolites, particularly alkaloids and flavonoids. Previous studies have demonstrated that extracts of this species, especially the ethyl acetate extract (SCA), exhibit a broad range of pharmacological activities, including antiviral effects against influenza virus (H1N1) and SARS-CoV-2, potential antivenom activity against *Bothrops jararaca*, and antitumor activity against myeloid cell lines. Given this therapeutic potential, the present study aimed to isolate secondary metabolites from the SCA by CCC fractionation. The fractionation was carried out using the biphasic solvent systems HEMWat (hexane-ethyl acetate-methanol-water, 3:6:3:6, v/v) and EBUWat (ethyl acetate-butanol-water, 8:2:10, v/v), employing high-speed countercurrent chromatography (HSCCC) on an HTPrep apparatus equipped with a 120 mL column (2.0 mm i.d.), operated in normal mode (head-to-tail). The mobile phase was delivered at a flow rate of 2.0 mL/min. A total of 60 fractions were collected - 30 during the elution phase and 30 during the extrusion phase - with each fraction having a volume of 4 mL. The collected fractions were monitored by thin-layer chromatography (TLC), grouped according to chromatographic similarities, and analyzed by nuclear magnetic resonance (NMR) spectroscopy. The findings, supported by comparison with reported chemical shifts in the literature, suggest the presence of glycosylated flavonoids in the analyzed fractions. The purified compounds are currently being analyzed by liquid chromatography coupled with mass spectrometry (LC-MS), as well as by ¹³C-NMR and 2D NMR techniques (COSY, HSQC, HMBC) for full structural elucidation. Ongoing studies aim to further characterize the isolated substances and evaluate their biological activities.

Keywords: *Siparunaceae, Countercurrent chromatography, Bioactivity compounds, Flavonoids.*





EXPANSION OF THE ANNOTATION OF SECONDARY METABOLITES OF PASSIFLORA SPP. BY MASS SPECTROMETRY, MOLECULAR NETWORKS AND IN-SILICO TOOLS

Yolanda Trindade de Oliveira^{1*}, Laryana borges Garcia¹, Paulinne Moreira Lima¹, Catarina Silva Guimarães¹, Teonildes Sacramento Nunes², Danielle Rocha Pinho³, Norberto Peporine Lopes³, Gabriel Azevedo de Brito Damasceno¹, Angélica Ferraz Gomes¹, Juliano Geraldo Amaral¹

yolanda_7412@hotmail.com

- 1- Instituto Multidisciplinar em Saúde, Campus Anísio Teixeira, Universidade Federal da Bahia, Vitória da Conquista, Bahia, 45029-094, Brazil. 2- Universidade Estadual de Feira de Santana, Departamento de Ciências Biológicas, Feira de Santana, Bahia, 44036-900, Brazil. 3- Núcleo de Pesquisa em Produtos Naturais e Sintéticos (NPPNS), Departamento de Ciências Biomoleculares, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Ribeirão Preto, São Paulo, 14040- 903, Brazil.

The genus *Passiflora* L. is characterized by having edible fruits, with important chemical constituents that exert therapeutic benefits, such as anxiolytics activity, and the presence of flavonoids in most species. Brazil is one of the countries with the largest comprehensiveness of species, although they are still little investigated, which makes it difficult to truly understand the pharmacological potential of this genus. Thus, the objective of this study was the metabolomic analysis of Brazilian *Passifloras* with few reported phytochemical studies, using spectrometric techniques associated with molecular networks and in silico tools for expanding metabolic annotations. Exsiccates of 58 species of *Passiflora* were selected, deposited by the Herbarium of the State University of Feira de Santana (HUEFS), registered in SISGEN AB0AE7A. Spectral data were obtained by high-performance liquid chromatography (HPLC) coupled to a mass/mass spectrometer (MS/MS) with an electrospray ionization (ESI) source and a Q-Tof analyzer. The analysis was carried out using the Global Natural Products Social Molecular Networking (GNPS) platform, aided by in silico tools, such as Network Annotation Propagation (NAP), unsupervised substructure annotation technique (MS2LDA), and integrated by MolnetEnhancer to complementation of the results. The applied methods expanded the chemical annotations, which vary by levels of description on a large spectral scale, and in 8 species, chemical components were noted not yet documented in the literature were annotated. The in silico tools expanded the GNPS annotations by 30%, thus enabling chemical comparison with other more studied species with already recognized medicinal activities, being able revealing the pharmacological potential of these *Passifloras*, and enable the insertion of new products aimed at human well-being.

Keywords: CLAE-DAD-EM/EM; *Passiflora* spp.; MolnetEnhancer; Electrospray; Molecular Networking





DESIGN OF EXPERIMENT APLIED TO OPTIMIZATION OF BIOACTIVE EXTRACTION FROM SPONDIAS TUBEROSA RESIDUE

Bruna Santana Neves^{2*}, Amanda Vitoria Pereira Teles¹, Júlia Victoria Vieira de Castro¹,
Letícia Meira da Silva Queiroz¹, Juliano Geraldo Amaral^{1,2}, Gabriel Azevedo de Brito
Damasceno^{1,2}

brunasn@ufba.br

1-Instituto Multidisciplinar em Saúde – Campus Anísio Teixeira / Universidade Federal da Bahia,
Rua Hormindo Barros, 58, Candeias, Vitória da Conquista, Bahia.

2- Programa de Pós Graduação de Biociências – Campus Anísio Teixeira / Universidade Federal da
Bahia, Rua Hormindo Barros, 58, Candeias, Vitória da Conquista, Bahia

Spondias tuberosa, commonly known as umbu, is a native species of the Caatinga biome. The processing of umbu for food purposes generates a significant amount of waste, accounting for approximately 60% of its fresh mass, mainly composed of fruit peel and pulp. These residues exhibit a high concentration of secondary metabolites, including flavonoids, tannins, and anthocyanins, which are known for their antioxidant activity and potential as cosmetic raw materials. This study aimed to optimize the extraction of these compounds from umbu residues using a Design of Experiment (DOE). A 2⁴ factorial design was applied, assessing the independent variables: extraction method (turbulysis or ultrasound), solvent (water or 50% v/v ethanol), residue type (fresh or dried), and extraction time (5 or 15 minutes). The response variables included extraction yield, antioxidant activity determined by the DPPH assay, and flavonoid quantification (FQ), evaluated during both screening and optimization stages. The results indicated that dried residue and 50% ethanol were superior across all assays, while turbulysis was identified as the most efficient extraction method. The outcomes ranged as follows: extraction yield from 0 to 23.8 mg/mL, antioxidant capacity from 14% to 90%, and FQ from 1.10 to 23.50 µg QE/mg. Overall, the findings highlight the potential of *Spondias tuberosa* residues as a valuable source of bioactive compounds for cosmetic formulations, contributing to the valorization of by-products and the advancement of sustainable practices within the production chain.

Keywords: Extraction, Residue, *Spondias tuberosa*





2-ALKYL-4-QUINOLONES PRODUCED BY *Burkholderia* sp. C5.4, ENDOYPHITIC BACTERIA OF *Piper nigrum* L.

Willibrodus Usfinit¹*, Luana Cardoso de Oliveira², Eliane da Silva Santos¹, Sandra Valéria Dias Cardoso¹, Andrey Moacir do Rosario Marinho¹, Patrícia Santana Barbosa Marinho¹.

*w.b.u.talikakum@gmail.com

¹Universidade Federal do Pará; ²Universidade Federal do Sul e Sudeste do Pará.

Endophytic bacteria of the genus *Burkholderia* are species with high versatility and genetic adaptability, and can live in different environments. This genus has received increasing attention in research due to its ability to produce various secondary metabolites, including many compounds with antibacterial, antifungal, insecticidal, or herbicidal properties. The objective of this study was to isolate and characterize the secondary metabolites produced by the endophytic bacterium *Burkholderia* sp. C5.4, associated with black pepper (*Piper nigrum* L.). In the study, the bacterial pre-inoculum was prepared by culturing in culture medium 523 at 28 °C for 24 hours, and fermentation was carried out in Nutrient Broth (NB) and Pigment Production Medium (PPM) at 28 °C for two days in an orbital shaker. After the fermentation period, the cells were separated by centrifugation, macerated with acetone, and the solutions were filtered and concentrated to obtain the NB and PPM extracts. The extracts were solubilized in acetonitrile (1 mg/mL) and analyzed by HPLC-PDA using a C-18 5 µm (4.6 x 5 mm) analytical column, step elution with water/acetonitrile (80:20-40:60) for 20 min, flow rate of 1.0 mL/min, and column oven at 40 °C. The substances were isolated by semi-preparative HPLC using a semi-preparative C-18 5 µm column (19 x 150 mm), the same method as the analytical run for 24 min and flow rate of 17 mL/min. Both extracts showed the same chemical profile by HPLC-PDA with the presence of four chromatographic peaks (t_R = 7.5; 8.2; 10.3 and 11.9 minutes), which in the UV spectra showed four bands with λ_{max} of 212.6; 240.9; 320.0, and 334.8 nm, characteristic of 2-alkyl-4-quinolone alkaloids. Based on ¹H and ¹³C NMR and MS analyses, the substances were identified as PSC-B ((*E*)-2-(hept-2-en-1-yl)-3-methylquinolin-4(1*H*)-one), PSC-C (2-heptyl-3-methylquinolin-4(1*H*)-one), PSC-D ((*E*)-3-methyl-2-(non-2-en-1-yl)quinolin-4(1*H*)-one), and PSC-E (3-methyl-2-nonylquinolin-4(1*H*)-one), with m/z of 254.15 [M+H]⁺, 256.17 [M+H]⁺, 282.18 [M+H]⁺ and 284.19 [M+H]⁺, respectively. The results obtained confirm that bacteria of the genus *Burkholderia* are producers of secondary metabolites that may have potential in biotechnological applications. Future investigations will focus on evaluating activities aimed at developing bioproducts that can minimize phytosanitary problems in agriculture.

Keywords: Alkaloids, *Burkholderia*, bioproducts.





CHEMICAL INVESTIGATION OF *Dolichandra unguis-cati* CRUDE EXTRACT AND ANTIFUNGICAL ACTIVITY EVALUATION.

***Carolayne Cavalcante Brasil*^{1*}**, Viviani Motta¹, Valéria Maria Melleiro Gimenez², Jaqueline Stabile Gouveia¹, Regina Helena Pires¹, Patrícia Mendonça Pauletti¹

carolayne-cb@hotmail.com

1-University of Franca, UNIFRAN, Franca, Brazil, 14404-600

2-Faculdade de Zootecnia e Engenharia de Alimentos, FZEA, USP, Pirassununga, 13635-900.

Dolichandra unguis-cati or *Macfadyena unguis-cati* (Bignoniaceae) is a climbing species found in the Americas. Also known as “cat’s claw,” “bat’s claw,” “bat vine,” and “golden vine,” it is used in folk medicine for the treatment of hepatitis, venereal diseases, snake bites, malaria, dysentery, rheumatism, and inflammatory conditions. Studies have indicated the presence of saponins, flavonoids, triterpenes, lignans, and phenylethyl glycosides. The chemical investigation of Brazilian medicinal plants is relevant for drug discovery, biodiversity conservation, and sustainable development, aligning with the United Nations Sustainable Development Goals (SDGs), particularly those related to health, innovation, and ecosystem preservation. This study aimed to investigate the chemical composition of *D. unguis-cati* leaf extract, isolate pure compounds, and evaluate their antifungal activity. The methods employed included standard phytochemical techniques and analysis by Ultra-Performance Liquid Chromatography coupled with High-Resolution Mass Spectrometry (UPLC-HRMS/MS). The ions obtained were analyzed through Global Natural Products Social Molecular Networking (GNPS), which, based on fragmentation patterns, enabled the annotation of the following compounds: quinic acid, verbascoside, isoverbascoside, baicalin, and oroxylin glucuronide. Among these compounds, verbascoside had already been previously reported in this species. Subsequently, the *n*-butanol fraction allowed the isolation of this phenylethyl glycoside by preparative HPLC, and its chemical structure was identified by NMR analysis. The subfractions and the crude extract were also tested for sensitivity assays against *Candida albicans* ATCC 10231, *C. glabrata* (*Nakoseomyces glabratus*) ATCC 15126, *C. krusei* (*Issatchenkia orientalis*) ATCC 14243, *C. metapsilosis* ATCC 96143, *C. orthopsilosis* ATCC 96141, *C. parapsilosis* ATCC 90018, *C. rugosa* ATCC 40285, and *C. tropicalis* ATCC 13803. The best MIC (Minimum Inhibitory Concentration) values were obtained for the *n*-butanol and ethyl acetate subfractions. This investigation and the study of medicinal plants highlight the importance of dereplication in metabolomics to optimize the identification of already annotated compounds.

Keywords: Chemical composition, biodiversity, antifungal, molecular network, dereplication





SPATIAL DISTRIBUTION AND COMPARTMENTALIZATION OF CYCLOPEPTIDES AND 4-QUINOLONE ALKALOIDS IN WALTHERIA INDICA REVEALED BY MALDI-MSI

Raquel de Medeiros Silva^{*1}, Fernando Cotinguiba¹

raquel_demedeiros@hotmail.com

¹Instituto de Pesquisas de Produtos Naturais Walter Mors (IPPN) – UFRJ. Av. Carlos Chagas Filho, 373, Centro de Ciências da Saúde, Bloco H. Cidade Universitária, Ilha do Fundão, Rio de Janeiro, RJ. CEP: 21.941-902, Brazil

Waltheria indica L. (Malvaceae) is a pantropical shrub (“broom”) distributed throughout the Americas (Mexico-Brazil), West Africa, Southeast Asia, and Australia, frequently cited as an invasive species. In this study, we investigated the spatial distribution of 4-quinolone and cyclopeptide alkaloids in stems, leaves, and roots using MALDI–Mass Spectrometry Imaging (MALDI-MSI), a technique that enables direct metabolite mapping within tissues while requiring minimal biomass. Plant sections (50 µm) were prepared, coated with 2,5-dihydroxybenzoic acid (DHB), and analyzed in positive mode (MALDI-TOF/TOF, Bruker). In stems, 4-quinolones predominated in the xylem, including 2-hydroxymethyl-waltherione C or 10-hydroxy-waltherione C (m/z 364.1544), 8-hydroxy-waltherione M + Na⁺ or waltherione O + Na⁺ (m/z 378.204), 11-hydroxy-waltherione F + Na⁺ (m/z 370.1989), waltherione P + Na⁺ (m/z 376.1883), waltherione V or 11-dehydroxy-waltherione A (m/z 378.1700), walindicaone E (m/z 380.186), waltherione A or waltherione B (m/z 394.1577), melovininone (m/z 396.499), waltherione A + Na⁺ (m/z 416.1468), waltherione H + Na⁺ (m/z 422.2302), and waltherione D (m/z 512.1921). Most showed higher intensity in the xylem, with additional signals in the phloem and cortex. In leaves, no alkaloids were detected in the blade, but lateral sections revealed waltherione P + Na⁺ throughout the lamina but absent from the central region. Cyclopeptides, including adouetine Y’ or waltherine A (m/z 535.3200), appeared in scattered foci. In roots, alkaloids concentrated mainly in the cortex and endodermis: 10-hydroxy-waltherione C or 2-hydroxymethyl-waltherione C, waltherione V or 11-dehydroxy-waltherione A, 8-hydroxy-waltherione M + Na⁺ or waltherione O + Na⁺, and waltherione A or waltherione B. Waltherione P + Na⁺ was also detected across vascular tissues, while waltherione U + Na⁺ (m/z 414.1676) was distributed throughout the root, with highest abundance in the cortex. Overall, MALDI-MSI revealed tissue-specific localization and compartmentalization of alkaloids in *W. indica*, highlighting differences among organs and metabolite classes. These findings provide insights into the biosynthesis and ecological functions of these compounds, particularly their potential roles in chemical defense, intercellular signaling, and storage. This study contributes to sustainable use and understanding of plant chemical diversity, supporting Sustainable Development Goals (SDG) 3 (Good Health and Well-Being) and 15 (Life on Land).

Keywords: *Waltheria indica*; MALDI-MSI; 4-quinolone alkaloids; cyclopeptide alkaloids; SDG 15





LC/HRMS ANALYSIS AND ANTIBACTERIAL ACTIVITY FROM EXTRACTS OF *Baccharis punctulata* (Asteraceae)

Jociani Ascari^{1*}, Christiano Cattani Belini¹, Erika Izumi¹, Rute Cristina Bach, Edicléia Aparecida Bonini e Silva¹, Rosana Casoti², Lorena de Mendonça Lucena²

*jascari@utfpr.edu.br

1- Coordenação de Licenciatura em Ciências Biológicas, Universidade Tecnológica Federal do Paraná, 85892-000 Santa Helena –PR, Brasil. 2 -Departamento de Antibióticos-LAPRONAM, Universidade Federal de Pernambuco, 50670-901, Recife -PE, Brazil

Baccharis punctulata DC., popularly known as "Chilka saru saru", is used by rural communities in Bolivia for treatment of luxations, contusions and asthma. This species is widely distributed in South America, particularly in Brazil, in the Southeast and the South, Cerrado, Atlantic Forest and Pampa biome. Aerial parts of *B. punctulata* were collected in Itapejara D'Oeste Town, Paraná, Brazil in February 2024. Leaves were separated and dried for 3 hours in a recirculating oven under controlled temperature and subjected to hydrodistillation for 2.5 h. The essential oil was collected and stored under refrigeration. The aqueous extract obtained was then filtered and partitioned by clorofórmio, ethyl acetate at pH 8 and ethyl acetate at pH 4 (EBP). Chemical composition of extract EBP was evaluated using Liquid chromatography coupled to high-resolution mass spectrometry (LC/ESI/HRMS) and results revealed that EBP extract contain mainly phenolic acids such as caffeoylquinic acids, feruloylquinic acids, caffeoylshikimic acid and its derivatives. Were also observed as minorities classes of secondary metabolites flavonoids, coumarins and iridoids. The antibacterial activity of EBP was evaluated using the broth microdilution assay, standardized by the Institute for Clinical and Laboratory Standards. The microorganisms used in the study were *Staphylococcus aureus* N315 (MRSA), *Staphylococcus aureus* BEC9393 (MRSA), *Bacillus subtilis* INCQS 00002, *Escherichia coli* ATCC 25922 e *Salmonella entérica* ATCC13076. EBP extract was solubilized in DMSO and then diluted in an appropriate culture medium, added to a microplate at a maximum concentration of 5000 µg/mL, followed by serial dilutions to approximately 70 µg/mL. EBP showed more significant antibacterial activity with a minimum inhibitory concentration (MIC) of 1250 µg/mL against *B. subtilis* INCQS 00002, 2500 µg/mL against *S. aureus* BEC9393 (MRSA), and 5000 µg/mL against *S. aureus* N315 (MRSA). In conclusion, the data presented in this study showed, for the first time in the literature, the antibacterial activity from leaf extracts of *Baccharis punctulata* (Asteraceae) collected in Brazil.

Keywords: *Baccharis punctulata*, LS/MS, phenolic compounds, extracts





**IDENTIFICATION OF PHENOLIC COMPOUNDS BY HPLC-ESI-MS AND
DETERMINATION OF ANTIOXIDANT ACTIVITY OF SPECIES OF THE
ASTERACEAE FAMILY**

Eliane Cristina Costa^{1*}, Alexandre Milanez Brandão¹, Fernanda Rodrigues de Souza¹,
Michele Conceição Miranda¹, Lavínia Mota Cristianismo Silva¹, Abraão José Silva Viana²,
José Milton Leão Junior³, Carlos Victor Mendonça Filho⁴, Roqueline Rodrigues Silva¹

eliane.costa@ufvjm.edu.br

1-Departamento de Química, Universidade Federal dos Vales do Jequitinhonha e Mucuri-UFVJM,
Rodovia MGT 367, Diamantina, MG, 39100-000 Brazil, 2-Laboratório Integrado de Pesquisas
Multiusuário, UFVJM, Rodovia MGT 367, Diamantina, MG, 39100-000 Brazil, 3- Departamento de
Engenharia Florestal, UFVJM, Rodovia MGT 367, Diamantina, MG, 39100-000 Brazil, 4-
Departamento de Ciências Biológicas, UFVJM, Rodovia MGT 367, Diamantina, MG, 39100-000
Brazil

The Asteraceae family is known for its vast number of species and the pharmacological activities its of many plants. However, some species remain understudied, including *Lucilia lycopodioides*, *Lessingianthus* cf. *adenophyllus*, and *Richterago discoidea*. Therefore, this study aimed to identify phenolic compounds in acetone extracts using high-performance liquid chromatography-mass spectrometry (HPLC-ESI-MS) and to determine the antioxidant activity of these three species. The Folin-Ciocalteu reagent was used to determine the phenolic compounds, while DPPH was used for the antioxidant activity. HPLC-ESI-MS analyses were performed on a Thermo Scientific Ultimate 3000 liquid chromatograph operating in negative mode with gradient programming. The fragmentation study was performed using a parallel reaction monitoring (PRM) experiment. All three species described showed a high potential for antioxidant activity, with *Lucilia lycopodioides* presenting the highest total phenolic content (357.45 mg/g) in comparison to *Lessingianthus* cf. *adenophyllus* (351.21 mg/g) and *Richterago discoidea* (205.01 mg/g), as well as the result for free radical scavenging activity using DPPH with values of 91.46% at 500 ppm, for *Lucilia lycopodioides*; 88.82% at 500 ppm, for *Lessingianthus* cf. *adenophyllus* and 66.14% at 500 ppm, for *Richterago discoidea*, with the first species reaching values very close to the gallic acid standard (95.85% at 500 ppm). Using HPLC-ESI-MS, by comparison with phenolic compound standards, it was possible to identify the following compounds in the three species: protocatechuic acid; *p*-coumaric acid; caffeic acid; luteolin and chlorogenic acid. Furthermore, it was possible to identify rutin in *Lessingianthus* cf. *adenophyllus*. The conclusion is that all three species under study presented good results in antioxidant activity, with *Lucilia lycopodioides* being the most promising, indicating greater pharmacological potential against pathologies caused by oxidative stress.

Keywords: *Lucilia lycopodioides*, *Lessingianthus* cf. *adenophyllus*, *Richterago discoidea*, antioxidant activity

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PENTACYCLIC TRITERPENES FROM *Maytenus quadrangulata* (CELASTRACEAE): ISOLATION, SEMISYNTHESIS, AND CYTOTOXIC ACTIVITY

Mariana G. Aguilar^{1*}, Sandy F. M. Quintão¹, Túlio R. Freitas², Adriano P. Sabino², Grasiely F. Sousa^{1*}, Lucienir P. Duarte¹

*marianag.a9@gmail.com, grasielysousa@ufmg.br

1- Departamento de Química, UFMG; 2- Departamento de Análises Clínicas e Toxicológicas, Faculdade de Farmácia, UFMG.

The genus *Maytenus*, one of the largest within the Celastraceae family, is widely recognized for its pharmacological potential, exhibiting diverse biological activities such as anti-inflammatory, antiulcerogenic, antioxidant, antibacterial, and analgesic effects.^{1,2} *Maytenus quadrangulata*, a Brazilian species popularly known as “espinho-de-deus”, has been previously studied for its hexane leaf extract, which demonstrated significant cytotoxic effects from isolated triterpenes.³ In this context, the present study aims, for the first time, to perform a detailed analysis of the compounds present in the chloroform extract of *M. quadrangulata* leaves. The chloroform extract was subjected to successive column chromatography (CC), leading to the isolation of the triterpene friedelane-3 α ,25-diol (**1**) and a mixture of hydroxylated triterpenes (**M1**). To separate the constituents of mixture **M1**, an acetylation reaction was performed, followed by CC purification. This process yielded five new semisynthetic triterpenes: friedelane-3 α ,29-yl diacetate (**2**), friedelane-3 α ,11 β -yl diacetate (**3**), friedelane-3 α ,25-yl diacetate (**4**), 3 β -hydroxyfriedelane-24-yl acetate (**5**), and 11 β -hydroxyfriedelane-3 α -yl acetate (**6**), along with two previously reported triterpenes: friedelane-3 α -yl acetate (**7**) and 3 β ,24-yl diacetate (**8**). Furthermore, the triterpene friedelane-3 β ,24-diol (**9**) was obtained by hydrolysis of compound **5**. Compounds **1–3**, **5–7**, and **9** were evaluated for their cytotoxic activity against leukemia cell lines (K-562, THP-1) and healthy lung fibroblast cells (WI-26VA4). The IC₅₀ values of the tested compounds ranged from 28.9 μ M to over 300 μ M for THP-1 and K-562 cells, with selectivity indices between 0.3 and 3.3. The compounds showed low to moderate cytotoxicity relative to the positive controls (etoposide and cytarabine).

Figure 1: Chemical structure of compounds 1–9

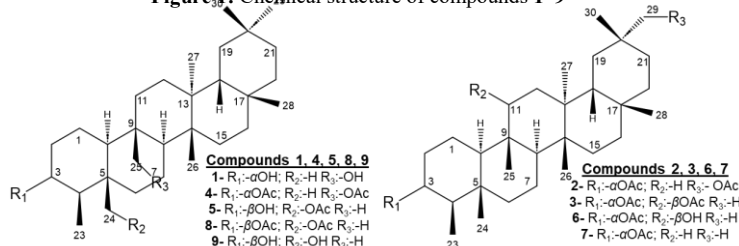


Table 1: IC₅₀ values and selectivity index of the tested compounds

Compounds	THP-1	SI	K562	SI	WI-26VA4
1	245.6 $\pm$ 12.5	0.3	45.9 $\pm$ 4.8	1.5	70.9 $\pm$ 5.6
2	210.5 $\pm$ 8.9	ND	66.5 $\pm$ 5.4	ND	> 300
3	230.4 $\pm$ 9.1	1.0	74.2 $\pm$ 6.3	3.3	244.5 $\pm$ 10.8
5	81.3 $\pm$ 8.8	1.3	58.9 $\pm$ 4.5	1.8	105.5 $\pm$ 10.3
6	120.8 $\pm$ 7.1	0.7	28.9 $\pm$ 3.6	3.1	88.9 $\pm$ 6.0
7	> 300	ND	> 300	ND	> 300
9	> 300	ND	35.4 $\pm$ 5.6	ND	> 300
Etoposide	ND	ND	34.6 $\pm$ 4.2	ND	ND
Cytarabine	40.7 $\pm$ 4.4	ND	ND	ND	ND
Doxorubicin	ND	ND	ND	ND	1.9 $\pm$ 0.9

Keywords: Triterpenes, Celastraceae, Cytotoxic activity, *Maytenus quadrangulata* *ND = not determined

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Acknowledgments: CAPES, CNPQ, FAPEMIG.





**OPTIMIZATION OF ULTRASOUND EXTRACTION OF BIOACTIVE COMPOUNDS
FROM THE SPECIES *Hancornia speciosa***

Juliana Panato Didonet¹, Feliciano Da Silva Neto¹, Nathália A. A. Nunes¹, Aline Biggi
Maciel Del Conte², Elisandra Scapin^{1,2*}

scapin@uft.edu.br

1-Curso de Engenharia Ambiental, Universidade Federal do Tocantins, Palmas, Tocantins, CEP 77001-090, Brazil. 2 -Programa de Pós-graduação em Biodiversidade e Biotecnologia - BIONORTE, Universidade Federal do Tocantins, Palmas, Tocantins, CEP 77001-090, Brazil.

The Brazilian Cerrado, the most biodiverse savanna worldwide, harbors species of high medicinal and economic relevance, such as *Hancornia speciosa* (mangaba). This species is recognized for producing secondary metabolites with antioxidant, anti-inflammatory, and wound-healing activities. This study aimed to optimize the ultrasound-assisted extraction (UAE) of bioactive compounds from *H. speciosa* leaves and to chemically characterize the extracts, increasing scientific knowledge about the biodiversity of the Tocantinense cerrado. A Central Composite Design (CCD) was employed, testing extraction times (30, 90, and 120 minutes) and ethanol concentrations (30%, 50%, and 70%) as independent variables. Leaves collected in Palmas-TO, Brazil (10°18'00" S, 48°31'41" W), were identified at the UNITINS herbarium (voucher HUTO 7278), dried, powdered, and extracted in an ultrasonic bath (200 W, 40 kHz). Extracts were evaluated for yield, total phenolic content (Folin–Ciocalteu method, mg GAE/g), and flavonoid content (quercetin method, mg QE/g). The maximum extraction yield was 41.53%, obtained at 90 min/50% ethanol, while the highest phenolic content occurred under the same condition (242.39 mg GAE/g). For flavonoids, the best response was observed at 120 min/70% ethanol (50.76 mg QE/g). Statistical modeling showed limited predictive power for yield ($R^2 = 47.01\%$) and phenolic content ($R^2 = 69.06\%$), but demonstrated a strong and significant fit for flavonoids ($R^2 = 91.10\%$; $p < 0.05$). The global desirability analysis indicated 120 min/70% ethanol as the overall optimal condition ($D = 0.83$), favoring the recovery of bioactive compounds, especially flavonoids. Overall, these findings reinforce the biotechnological potential of *H. speciosa* and emphasize the importance of optimized extraction protocols to promote the valorization of native Cerrado species.

Keywords: Mangaba; ultrasound assisted; phenolic compounds; flavonoids; Central Composite Design





Prospecting for Circular Miniproteins in the Leaves of *Pombalia atropurpurea*.

Alexsandro Davi Mantovani de Oliveira¹, Ana Letícia Pires dos Santos¹, Juliana de Paula Souza², Vanderlan da Silva Bolzani¹

alexsdavi.working@gmail.com

1-Institute of Chemistry, São Paulo State University-UNESP-IQ, Araraquara, SP, Brazil;. 2-Department of Biological Sciences, Federal University of Santa Catarina-UFSC, Santa Catarina, SC, Brazil.

Circular miniproteins, also known as cyclotides, are a class of cyclic peptides found in plant families such as Violaceae, Rubiaceae, and Fabaceae. Their distinctive structure, with a circular backbone of 28 to 37 amino acid residues and a head-to-tail cyclization, is stabilized by an arrangement of three disulfide bonds that form the Cyclic Cystine Knot (CCK). This unique configuration gives them remarkable stability and resistance to proteolytic degradation. With over 720 structures cataloged in the Cybase database, cyclotides have been the focus of research due to their role in plant defense and their varied biological activities, including antimicrobial, anti-HIV, and antitumor effects. Aiming to fill a gap in the national literature, our research group is currently investigating these compounds in native Brazilian plant species. Cyclotides from leaves of *Pombalia atropurpurea* (Violaceae), were extracted, defatted, and lyophilized, resulting in the crude extract, which was submitted to SPE-C18 cartridges and eluted with a mixture of 20%, 80%, and 100% buffer B (90% CH₃CN, 0.1% CF₃COOH) in an aqueous solution of 0.1% CF₃COOH. The 80% fraction showed rich concentration in cyclotides, which were isolated and identified. 3 cyclotides were isolated and 3 are new in the literature.

Keywords: *Circular miniproteins, cyclotides, cyclic peptides, Pombalia atropurpurea, Violaceae.*





**ECOLOGICAL INTERACTIONS AS DISCOVERY TOOLS: CO-CULTIVATION OF
ENDOPHYTIC AND PATHOGENIC PERSIMMON FUNGI IN SEARCH FOR
BIOCONTROL AGENTS**

Gabriela de Oliveira Almeida^{1*}, Paulo Cezar Vieira¹

gabi.almeida@usp.br

*1- Department of BioMolecular Sciences, Ribeirão Preto School of Pharmaceutical Sciences,
University of São Paulo, Ribeirão Preto, SP, Brazil.*

Plant diseases cause annual losses of up to 15% of major global crops, of which about 80% are attributed to pathogenic fungi. The chemical agents traditionally used for pest control have proven unsustainable, being one of the main causes of environmental degradation. Reduced agricultural productivity and excessive agrochemical use, combined with rapid population growth, have put food security at risk. In this context, sustainable strategies such as biocontrol agents emerge as promising alternatives. Endophytic fungi are valuable resources for discovering new natural products, and the co-cultivation strategy enables activation of silent biosynthetic genes, mimicking natural microbial interactions and yielding antifungal metabolites not observed under standard conditions. This study evaluated the antifungal activity of crude extracts from co-cultures of the endophytic fungus *Lasiodiplodia* sp. (EC1), isolated from persimmon (*Diospyros kaki*), and four phytopathogens of the same fruit (*Lasiodiplodia* sp. PC3, *Fusarium* sp. PC4, *Penicillium* sp. PC5, and *Neopestalotiopsis* sp. PC6), in rice medium. Cultures (axenic and co-cultures) were extracted with ethyl acetate and fractionated by vacuum liquid chromatography to remove rice triglycerides. The methanolic fraction (0.5 mg/mL) was tested in agar dilution assays in triplicate. Results showed that axenic RP4 extract inhibited EC1 (85.67 ± 7.86), while co-culture RE1,P4 inhibited EC1 (86.13 ± 3.37) and PC4 (88.20 ± 1.48). Co-culture RE1,P6 was active against EC1 (56.05 ± 4.45) and PC6 (62.10 ± 1.10). Extracts with inhibition above 50% (RE1,P4 and RE1,P6) were analyzed by UHPLC-MS/MS and ¹H NMR for chemical profiling. Mass data were pre-processed in MZmine (v4.7.3), and molecular networking in GNPS2 revealed exclusive and shared metabolites, including epiquisetine, polanrazine B, and lasiodiplodin. These extracts will undergo further purification and structural characterization by ¹H NMR and LC-MS/MS. Overall, the findings highlight endophytic-phytopathogen co-cultivation as a promising strategy for prospecting antifungal metabolites with potential biocontrol applications, contributing to sustainable agriculture. The authors thank the support from their institutions and the financial support of FAPESP scholarship #2024/01273-5.

Keywords: *fungi; persimmon; antifungal activity; co-cultivation; molecular networking.*





ETHANOL/NaOH BIPHASIC SYSTEMS: A SUSTAINABLE APPROACH FOR BIOCOSMETIC FORMULATION

Samuel Leite Cardoso^{*1}, Artur Borges Fiuza Arantes¹, Patrícia Marques Rodrigues¹, Joel Abreu¹, Ana Luisa Leoncio Rodrigues¹, Guilherme Martins Gelfuso², Yris Maria Fonseca-Bazzo¹, Damaris Silveira¹, Perola de Oliveira Magalhães¹

Samuca93@gmail.com

¹Natural Products Laboratory, University of Brasilia, Brasilia, zip code 70910-900, Brazil.

²Laboratory of Food, Drugs, and Cosmetics, University of Brasilia, Brasilia, zip code 70910-900, Brazil

Biphasic systems (TPS) represent a sustainable alternative for the separation and purification of biomolecules, reducing the need for toxic organic solvents. In this study, we investigated a TPS composed of ethanol and sodium hydroxide (NaOH), an inorganic salt, highlighting its viability as a green technology. Ethanol, a biodegradable and low-toxicity solvent, minimizes environmental impacts and makes the system economically viable. We evaluated the partition efficiency of secondary metabolites from the ethanolic extract of *Morus nigra* L. leaves, rich in antioxidants, aiming at the direct formulation of a topical gel with anti-inflammatory activity. The results demonstrated high selectivity and recovery of bioactive metabolites in the salt-rich phase, with a reduction in the chlorophyll present in the extract, indicating that the ethanol-NaOH combination may be a promising platform for sustainable pharmaceutical formulations, in line with the principles of green chemistry. The chemical marker neochlorogenic acid present in the ethanolic extract of *M. nigra* L. leaves confirmed the partition of polar metabolites preferentially to the salt phase (NaOH), with the quantification of this marker by HPLC. The antioxidant and depigmenting activities of the extract were determined using the DPPH free radical scavenging assay and tyrosinase enzyme inhibition. The extract exhibited high antioxidant capacity, and inhibited greater than 90% of tyrosinase activity at concentrations above 10.81 µg/mL. Cytotoxicity was evaluated using the MTT cell viability assay, yielding IC₅₀ values of 800 µg/mL for L929 cells and 224.3 µg/mL for B16F10 cells, indicating low cellular toxicity and reinforcing the potential of the methanol-water biphasic system for obtaining bioactive compounds for sustainable cosmetic formulations.

Keywords: Biphasic systems; biopharmaceutical; secondary metabolites





**METABOLOMICS OF *PSITTACANTHUS CORDATUS* (HOFFMANN.) G. DON PARASITIZING
DIFFERENT HOST SPECIES**

Bruna Doimi Ortolan^{1*}, Mariana T. Hufnagel¹, Carlos A. Carollo², Flávio M. Alves³, Daniel
P. Demarque¹

brunadoimi@usp.br

1- Pharmacognosy Laboratory, Department of Pharmacy, Faculty of Pharmaceutical Sciences, University of São Paulo, São Paulo, SP 05508-000, Brazil. 2- Laboratory of Natural Products and Mass Spectrometry (LaPNEM), Faculty of Pharmaceutical Sciences, Food and Nutrition (FACFAN), Federal University of Mato Grosso do Sul, Campo Grande, Mato Grosso do Sul 79070-900, Brazil. 3- Laboratory of Botany, Institute of Biosciences (INBIO), Federal University of Mato Grosso do Sul, Campo Grande, Mato Grosso do Sul 79070-900, Brazil.

Psittacanthus cordatus, also known as “erva-de-passarinho”, is a parasitic plant from the Loranthaceae family that uses a specific organ, the haustorium, to uptake water and nutrients from its hosts. Parasitic plants, as agricultural pests, can damage and decrease crop productivity, but also disturb ecosystems and biodiversity. Thus, understanding host–parasite interactions is crucial for developing effective control strategies. In this study, we investigated the phytochemistry based on a metabolomic profile of *P. cordatus* growing on four different host species. The plants (parasites, hosts and non-parasitized plants) were collected in Pantanal-Brazil, the leaves and stem methanolic extracts of those groups were analyzed by HPLC-ESI-qTOF-MS untarget metabolomics and networking (GNPS platform) to compound comparison between the plants. In those networks, we identified some nodes with a shared distribution between both the host plants and their parasite, suggesting a possible parasite-host metabolite transference. Another networking, with all parasites, were also built to investigate differences between them, showing nodes with different distributions in each group. Multivariate ANOVA one-way statistics were used on MetaboAnalyst 6.0 to compare parasites data, showing nine ions with significant differences in their distribution, depending on the host to which the parasite was associated. At last, in the annotation process of *P. cordatus*, the GNPS library matched with several flavonoids and flavonoid O-glycosides. Other compounds that were not able to identify and will be subjected to further investigation and isolation process. We concluded that, so far, it is possible to see differences in the chemical profile of the species, based on the host association. These findings contributed to a better understanding of the biochemical interactions between parasites and hosts plants. The authors acknowledge FCF-USP for providing the infrastructure and FAPESP (processes 2024/18203-0; 2022/08191-9) for financial support.

Keywords: Metabolomics, parasitic plant, phytochemistry, Loranthaceae, natural products





LC-HRMS BASED METABOLITE AND PHYTOCHEMICAL ANALYSIS OF *Maranta arundinacea* L. FOR THE FUNCTIONAL ASSESSMENT OF UNCONVENTIONAL FOOD PLANTS (UFP)

Yasmine Fernandes Oliveira^{1*}, Jorge Luiz Souza Simão¹, Rodolfo Dantas Lima Junior², Maurício Vicente Cruz³, Kátia Flávia Fernandes³, Patricia Santos Lopes⁴, Taícia Pacheco Fill² and Vanessa Gisele Pasqualotto Severino¹

yasminefernandes@discente.ufg.br

1 - Universidade Federal de Goiás, Chemistry Institute, 74690-900 Goiânia, Goiás, Brazil. 2 - Universidade Estadual de Campinas, Chemistry Institute, 13083-970, Campinas, São Paulo, Brazil. 3 - Universidade Federal de Goiás, Biological Science Institute, 74690-900 Goiânia, Goiás, Brazil. 4 - Universidade Federal de São Paulo, Institute of Environmental, Chemical and Pharmaceutical Sciences, 09972-270, Diadema, São Paulo, Brazil.

The growing demand for healthy and affordable food has increased interest in Unconventional Food Plants (UFP), which remain undervalued despite their high nutritional value⁽¹⁾. This trend aligns with the United Nations Sustainable Development Goal 2, which emphasizes food security and sustainable agriculture. Among UFP, *Maranta arundinacea* L. (“aratura”) is noteworthy for its starch-rich rhizomes and the largely unexplored nutritional and pharmacological potential of its aerial parts⁽²⁾. This study investigated the anti-nutritional profile, annotated compounds using public spectral libraries, and evaluated the cytotoxic activity of *M. arundinacea*. Aerial (AP) and rhizomatic (RP) parts (SISGEN A2DB3EC) were collected in Goiânia, Brazil, washed, lyophilized, and extracted with methanol via ultrasound-assisted extraction for 1 h at 15 °C. The extracts were then tested for trypsin and α -amylase inhibitory activities, analyzed by LC-HRMS, and dereplicated through Feature-Based Molecular Networking (FBMN) using the Global Natural Products Social Molecular Networking (GNPS) platform. Phenolic compounds, flavonoids, and proanthocyanidins were quantified spectrophotometrically, and antioxidant activity was assessed using ABTS⁺, DPPH, and FRAP assays. Cytotoxicity was evaluated using HaCaT (HE662121) cells using the neutral red assay⁽³⁾. LC-HRMS analysis of AP and RP extracts enabled Level 3 annotation of 48 compounds in [positive](#) and 9 in [negative](#) ionization mode, curated through GNPS spectral libraries. Rutin (m/z 611.1612), quercetin (m/z 303.0504), and kaempferol 3-hexoside-6-hexoside-hexoside (m/z 741.2236) were detected and they are known for several pharmacological activities. The antioxidant potential of both extracts was confirmed by the ABTS⁺ (0.11 ± 0.05^A and 0.05 ± 0.02^B mmol TE/g), DPPH (3.27 ± 0.03^A and 8.32 ± 0.15^A), and FRAP (0.07 ± 0.03^A and 0.03 ± 0.02^A mmol TE/g) assays. Toxicological assessment classified the RP extract as Dermal Toxicity Category 5 (IC_{50} 3.61 ± 0.53 mg/mL) according to OECD guidelines, indicating low acute toxicity with potential risk only for vulnerable groups. The AP extract was non-cytotoxic, maintaining cell viability above 93%. Overall, both extracts exhibit bioactive profiles combined with low toxicity, making them promising candidates for safe application in food products and dietary supplements.

Keywords: *Maranta arundinacea* L., Unconventional food plants, UHPLC-HRMS/MS, Molecular networking, Antioxidant activity.

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CHEMICAL COMPOSITION OF COUROUPITA GUIANENSIS FRUITS (LECYTHIDACEAE)

Bonifácio José Mause^{1,2}, Victória Pinheiro Guedes², Fernanda Das Neves Costa^{2*}

bmausse.gaza@gmail.com

1-Eduardo Mondlane University, Department of Chemistry, Maputo, Maputo, 3453, Mozambique. 2 - Federal University of Rio de Janeiro, Walter Mors Institute of Research on Natural Products, Rio de Janeiro, RJ, 21941-902, Brazil.

Couroupita guianensis exhibits high phytochemical complexity, producing a wide variety of secondary metabolites responsible for its diverse pharmacological activities. These bioactive constituents are distributed across different parts of the plant, including the fruit pulp. This chemical diversity not only reinforces the multifunctional medicinal value of the species but also raises relevant questions regarding its biosynthetic pathways, ecological roles, and potential technological applications. The fruits of *C. guianensis* represent a public safety issue, since, when ripe, they detach from the trunk and may cause accidents. Pruning is an alternative, but it leads to the accumulation of organic waste in landfills. Despite the limited chemical studies available, it is known that the pulp of this species is rich in indigo and other structurally related compounds. The valorization and utilization of this material have been directed toward the study of indigo and related alkaloids. The reuse of organic waste is directly related to several Sustainable Development Goals (SDGs) of the United Nations 2030 Agenda. In this context, the present work aims to explore the reuse of *C. guianensis* Aubl. (Lecythidaceae) fruits, popularly known as “abricó-de-macaco” (monkey apple). This Amazonian-origin tree is widely available in urban centers and throughout the UFRJ campus. The pulp of ripe fruits collected at the UFRJ Fundão campus was extracted with water. The material was lyophilized and subsequently partitioned by Soxhlet extraction using hexane, acetone, and methanol (in increasing order of polarity). The isolated substances were analyzed by thin-layer chromatography (TLC) and gas chromatography coupled to mass spectrometry (GC-MS), and subsequently sent for ¹H NMR analysis. The fermentation step of the fruit pulp of *C. guianensis* proved to be crucial for increasing the indigo content in the crude extract, in addition to contributing to the reduction of the overall process time. The isolation method adopted allowed the recovery of some alkaloids, including indigo.

Keywords: *Couroupita guianensis*; Indigo; Secondary metabolites; Soxhlet extraction; Sustainable reuse.

SHARMA, R. et al. Phytochemical complexity of *Couroupita guianensis*: secondary metabolites from flowers, bark, leaves, pulp, and seeds. *Journal of Pharmacognosy and Phytochemistry*, v. 12, n. 6b, p. 14774, 2023. DOI: 10.22271/phyto.2023.v12.i6b.14774.





ULTRASOUND-ASSISTED EXTRACTION OPTIMIZATION OF BIOACTIVE COMPOUNDS FROM *Dipteryx alata* LEAVES USING RESPONSE SURFACE METHODOLOGY

Feliciano Da Silva Neto¹, Juliana Panato Didonet¹, Nathália A. A. Nunes¹, Aline Biggi Maciel Del Conte², Elisandra Scapin^{1,2*}

scapin@uft.edu.br

1-Curso de Engenharia Ambiental, Universidade Federal do Tocantins, Palmas, Tocantins, CEP 77001-090, Brazil. 2 -Programa de Pós-graduação em Biodiversidade e Biotecnologia - BIONORTE, Universidade Federal do Tocantins, Palmas, Tocantins, CEP 77001-090, Brazil.

The Brazilian Cerrado is one of the most biodiverse savannas in the world and a valuable source of phytochemicals. *Dipteryx alata* Vogel (baru), a native species used in folk medicine, has been studied mainly for its fruits and seeds, while its leaves remain underexplored. These leaves contain bioactive metabolites, particularly phenolic compounds and flavonoids, relevant to pharmaceutical and cosmetic applications. This study aimed to optimize ultrasound-assisted extraction (UAE) of *D. alata* leaves, focusing on yield, phenolics, and flavonoids. A Central Composite Design (CCD) and Response Surface Methodology (RSM) were employed, considering extraction time (60, 90, 120 min) and ethanol concentration (30, 50, 70%) as independent variables. Leaves collected in Palmas-TO, Brazil, were identified at the UNITINS herbarium (voucher HUTO 8056), dried, powdered, and extracted in an ultrasonic bath (200 W, 40 kHz). Extracts were lyophilized and analyzed for yield, total phenolic content (Folin–Ciocalteu, mg GAE/g), and total flavonoid content (quercetin method, mg QE/g). The maximum yield (42.51%) was obtained with 30% ethanol at 120 minutes, while the highest phenolic (136.46 mg GAE/g) and flavonoid (23.45 mg QE/g) levels occurred with 70% ethanol at 60 minutes. Statistical models showed good predictive capacity ($R^2 > 78\%$ for phenolics and flavonoids; 90% for yield). RSM revealed ethanol concentration as the most influential factor, and global desirability indicated optimal conditions at 60 minutes and 70% ethanol. In conclusion, UAE proved efficient for recovering phenolic compounds and flavonoids from *D. alata* leaves. The application of RSM enabled the identification of optimal conditions, maximizing extraction efficiency and reducing experimental effort. These results support the valorization of *D. alata* leaves as a promising phytochemical source and highlight statistical optimization as a valuable tool in green extraction processes.

Keywords: Baru; Cerrado biome; phenolic compounds; flavonoids; Phytochemical valorization, Statistical optimization





DIVERSITY AND PHYTOTOXIC POTENTIAL OF EXTREMOPHILIC FUNGI PRESENT IN SOIL FROM THE LONGYEARBREEN GLACIER, SVALBARD ARCHIPELAGO, NORWAY

Sara Lemes de Souza^{1*}, Vívian Nicolau Gonçalves¹, Luiz Henrique Rosa¹.

sara.souza1905@gmail.com

1-Instituto de Ciências Biológicas, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Stressful conditions to which the fungal community in extreme ecosystems is subjected may be responsible for selecting fungi that produce secondary metabolites with phytotoxic activity. These compounds may be relevant for the development of natural herbicides, as weeds account for up to 90% of global crop losses. This study aimed to investigate the diversity and phytotoxic potential of the fungal community from the Longyearbreen Glacier soil, located in the Svalbard Archipelago, Norway. Soil samples were collected at five points along a glacial chronosequence, processed in quadruplicate, and the isolated fungi were subjected to an extract preparation protocol involving solid-state fermentation, lyophilization, metabolite extraction with dichloromethane, and drying. The extracts were screened at 1 mg/mL for herbicidal activity using *Lactuca sativa* (lettuce) and *Allium schoenoprasum* (chive) seeds as eudicot and monocot models, respectively. Seed germination assays were conducted in 24-well plates incubated at 26 °C under continuous light for 10 days (*L. sativa*) and 14 days (*A. schoenoprasum*). Extracts that inhibited germination were reproduced and retested to determine the Minimum Inhibitory Concentration (MIC). Extracts that maintained activity were further analyzed by Nuclear Magnetic Resonance (NMR) spectroscopy and scaled up for purification. A total of 233 filamentous fungi were isolated and grouped into 166 morphotypes, based on macromorphological features and confirmed by molecular biology. One representative of each morphotype was selected for extract production. To date, 143 extracts have been tested, of which 11 inhibited seed germination, and two retained phytotoxic potential in MIC assays. Sequencing of the ITS4 region identified these fungi as *Penicillium piltunense* UFMGCB 20823 and *P. samsonianum* UFMGCB 20935. Preliminary NMR analyses suggest that the metabolic profile from *P. samsonianum* UFMGCB 20935 has aromatic groups that may be interesting for future studies, indicating promise for large-scale purification and structural elucidation. These findings highlight the potential of extremophilic fungi as a source of novel metabolites with applications in sustainable weed management.

Keywords: Extremophilic fungi, secondary metabolites, phytotoxic activity, natural herbicides, sustainable weed management





EVALUATION OF THE ANTIOXIDANT POTENTIAL OF LEAVES OF *CURITIBA PRISMATICA* (MYRTACEAE)

Suelen dos Santos^{1*}, Fernanda Caroline Knob², Karin Carla dos Santos Schmidt², Tatiane Luiza Cadorin Oldoni², Vanderlei Aparecido de Lima²

Suhellen1105@gmail.com

1-Graduate Program in Applied Chemistry (PPGQA), State University of Central-West (UNICENTRO) – CEDETEG Campus, Alameda Élio Antonio Dalla Vecchia, 838, Vila Carli, Guarapuava, PR, 85040-167, Brazil. 2-Graduate Program in Technology of Chemical and Biochemical Processes (PPGTP), Federal University of Technology – Paraná (UTFPR) – Pato Branco Campus, Via do Conhecimento, s/n – KM 01, Fraron, Pato Branco, PR, 85503-390, Brazil.

Brazilian biodiversity represents a vast source of bioactive compounds. However, the antioxidant potential of many native plant species remains unexplored, including *Curitiba prismatica* (Myrtaceae), an endemic tree from Southern Brazil (found in the highlands of Paraná and Santa Catarina), popularly known as “guamirim” or “murta”. This study aimed to evaluate the antioxidant profile of the ethanolic leaf extract of *C. prismatica*. Leaves were collected in Irati, Paraná, dried in an oven (40°C/6 days), ground, and stored frozen. For extraction, 2 g of dried leaves were mixed with 25 mL of 45% ethanol and subjected to constant agitation (85 rpm/24 h), repeated every 24 h for 6 days. Extracts were filtered, combined, evaporated (40°C, 100 mbar, 100 rpm), frozen, and lyophilized. Antioxidant activity was evaluated using DPPH radical scavenging, ABTS radical cation decolorization, ferric reducing antioxidant power (FRAP), and Folin–Ciocalteu reagent (FCR) assays. The antioxidant potential of the ethanolic extracts of *C. prismatica*, as determined by the methods, was: FCR: 348.46 ± 7.80 mg gallic acid equivalents (GAE) g⁻¹ dry extract; ABTS: 3568.44 ± 80.28 µmol Trolox equivalents (TEAC) g⁻¹ dry extract; DPPH: 2770.27 ± 50.73 µmol TEAC g⁻¹ dry extract; FRAP: 7314.30 ± 166.40 µmol Fe²⁺ g⁻¹ dry extract. Comparable results have been reported for other Myrtaceae species, such as *Syzygium malaccense*. This first report provides new insights into the antioxidant profile of *C. prismatica* and contributes to the phytochemical knowledge of Brazilian endemic species.

Keywords: *Curitiba prismatica*, Myrtaceae, Antioxidant activity, Phenolic compounds, Brazilian biodiversity





PHYTOCHEMICAL EVALUATION OF PSITTACANTHUS ACINARIUS (Mart.) Mart.

IN DIFFERENT HOSTS

Mariana T. Hufnagel^{1*}, Bruna D. Ortolan¹, Carlos A. Carollo², Flávio M. Alves³, Daniel P. Demarque¹

mari.tedesco@usp.br

1-Department of Pharmacy, Faculty of Pharmaceutical Sciences, University of São Paulo, São Paulo 05508-900, Brazil. 2-Faculty of Pharmaceutical Sciences, Food and Nutrition, Laboratory of Natural Products and Mass Spectrometry, Federal University of Mato Grosso do Sul, Campo Grande, Mato Grosso do Sul 79070-900, Brazil. 3-Laboratory of Botany, Institute of Biosciences, Federal University of Mato Grosso do Sul, Campo Grande, Mato Grosso do Sul 79070-900, Brazil.

Parasitic plants obtain nutrients from their hosts through haustoria, specialized structures that connect to the vascular system and enable the exchange of water, nutrients, and metabolites. Although they can negatively affect crop productivity and health, they may also possess relevant medicinal properties. Descriptive phytochemical studies are crucial to elucidate their chemical diversity and ecological interactions; however, research in this field remains scarce, as only a small fraction of parasitic species has been thoroughly investigated, limiting our understanding of their biological and therapeutic potential. The present project aims to explore the chemical constituents of *Psittacanthus acinarius* (Mart.) Mart. in different hosts, focusing mainly on the species *Astronium fraxinifolium* Schott and *Andira inermis* (W.Wright) DC. The species were collected in the Pantanal, comprising parasitized and non-parasitized hosts, as well as the parasite. From the powdered plant material, a small-scale extraction was performed using methanol/water, followed by analysis with HPLC-ESI-qTOF-MS. The data were processed using DataAnalysis and MZMine, and clusters were generated via the online platform GNPS. From these clusters, a detailed data analysis was carried out, revealing that one of the parasite species, when compared with its parasitized and non-parasitized hosts, presented an unidentified compound (m/z 399.1259) absent in the others. Sequential maceration was then conducted with hexane, ethyl acetate, and ethanol, and the fractions related to the unidentified compound were evaluated by HPLC to initiate the isolation process. A chromatographic column was prepared in an attempt to reduce chemical variability; however, the isolation process will continue with preparative HPLC. In conclusion, our study revealed the presence of a chemical compound not identified in existing databases, which may have been generated through the parasite–host interaction. This finding promoted the ongoing process of isolation and structural elucidation. The authors acknowledge FCF-USP for providing the infrastructure and FAPESP (processes 2024/15443-0; 2022/08191-9) for financial support.

Keywords: *Metabolomics, natural products, parasite plants, phytochemical profile, chromatography.*





PHYTOCHEMICAL STUDY OF LEAVES AND BRANCHES FROM *Jacaranda obovata* (BIGNONIACEAE)

Davi Veiga Dutra,^{1*} Lucienir Pains Duarte,¹ Grasiely Faria de Sousa.^{1*}

[*grasielysousa@ufmg.br](mailto:grasielysousa@ufmg.br), davivtr@ufmg.br

I-Neplam, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Bignoniaceae Juss. is a dicotyledonous family comprising about 700-800 species grouped in 100-125 genera, being especially common in the tropics of South America, with lower representation in temperate regions. The genus *Jacaranda*, belonging to this family, includes 49 species around the world that are native to Central and South America and the Caribbean. Of these, 39 taxa are endemic to Brazil.¹ This genus has demonstrated pharmaceutical potential due to metabolites exhibiting several biological effects, including anti-inflammatory and antimicrobial activities.² Despite the genus diversity and its potential, there are still a few studies that clarify the secondary metabolites present in the species and their respective biological activities. *Jacaranda obovata* Cham., commonly known as “Carobinha”, is an example of an understudied species of *Jacaranda*. In this context, the present work aimed to advance the identification and isolation of metabolites synthesized by *Jacaranda obovata* searching for compounds with biological activity in their leaves and branches. A total of 698.3 g of dried and powdered leaves and branches were subjected to successive maceration with hexane, chloroform, and ethanol at room temperature. Following each extraction step, the extracts were filtered and subsequently concentrated under reduced pressure using a rotary evaporator, affording the corresponding crude extracts. The 12.38 g of chloroform extract were subjected to silica gel column chromatography to purify the compounds. The characterization was performed using ¹H, ¹³C and DEPT-135 NMR spectroscopy. To date, approximately 900 mg of 3 β -hydroxy-urs-12-en-28-oic acid (ursolic acid) have been identified. Ursolic acid is a natural product with recognized biological activity, such as anti-inflammatory, antioxidant, and anticancer activities.³ These findings indicate that, in addition to its intrinsic activity, ursolic acid also holds potential for the synthesis of derivatives in future studies aimed at pharmacological applications.

Acknowledgments: CAPES, CNPq, FAPEMIG

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Keywords: Phytochemistry Bignoniaceae, *Jacaranda obovata*





CHEMICAL STUDY OF *Litchi chinensis* SEEDS CRUDE EXTRACT.

Viviani Motta Ferreira^{1*}, Carolayne Cavalcante Brasil¹, Gabriele Sousa Trovo¹, Patrícia Mendonça Pauletti¹

viviani.motta.ferreira@hotmail.com

1-University of Franca, UNIFRAN, Franca, Brazil, 14404-600

Lychee (*Litchi chinensis* Sonn.) was introduced in Brazil in 1810 and is cultivated mainly in the Southeast region. Although the seeds play an important role, they are often discarded during consumption of the fruit, resulting in waste of a potentially valuable material. In traditional medicine, the seeds of *L. chinensis* have commonly been used to relieve neuralgic pain, abdominal pain, bloating, and testicular pain. The predominant chemical constituents in *L. chinensis* seeds include cyclopropanoic fatty acids, terpenes, flavonoids, phenolic compounds, glycosidic fatty acids, and lignans. This study aimed to isolate chemical compounds of *L. chinensis* seeds crude extract, since this extract showed antifungal and anti-insecticidal activity in preliminary assays. The dry seed material (2.7 kg) was extracted with ethanol, yielding 158.1 g of crude extract, which was subjected to a liquid-liquid partitioning with *n*-hexane, ethyl acetate, and *n*-butanol. The ethyl acetate fraction was further purified by Vacuum Liquid Chromatography (VLC) using silica and chloroform/methanol as mobile phase, furnishing six subfractions. Subfraction 4 (1.79 g) was purified by Sephadex LH-20 column, eluted with methanol, furnishing 4,5-dihydroxy benzoic acid, which had been previously isolated in earlier research. Further investigations are being conducted to isolate additional metabolites and to assess the biological properties of the obtained fractions and compounds.

Keywords: *Lychee*, *phenolic compounds*, *Sapindaceae*, *seeds*





CHEMICAL PROFILE ANALYSIS AND ANTIOXIDANT POTENTIAL OF MALBEC WINE FERMENTED WITH *HANSENIASPORA VINEAE*

Luis Felipe Lima Guimarães^{1*}, Paolla Xavier de Amorim¹, Izadora Viana Maia¹, Ana Carolina Souza Parreira¹, Isabella Marques do Nascimento¹, Jerônimo Raimundo de Oliveira Neto³, Luiz Carlos da Cunha³, Yuri Arrates Rocha¹, Andréa Rodrigues Chaves¹, Júlio César Gonzaga da Silva³, Eric de Souza Gil³, Esther Pedroso Theisen², Vanessa Gisele Pasqualotto Severino¹

luis.lima@discente.ufg.br

1-Universidade Federal de Goiás, Institute of Chemistry, 74690-900, Goiânia, GO, Brazil. 2-Universidade Federal do Pampa, Dom Pedrito Campus, 96450-000, Dom Pedrito, RS, Brazil. 3-Universidade Federal de Goiás, Faculty of Pharmacy, 74605-170, Goiânia, GO, Brazil.

During vinification, sugars are converted into ethanol and other metabolites through the metabolic activity of yeasts, traditionally *Saccharomyces cerevisiae* [1]. In recent years, non-*Saccharomyces* species have gained attention for their ability to metabolize diverse aromatic precursors [2]. Among these, *Hanseniaspora vineae* has emerged as a promising alternative for modulating wine composition [2]. This study aimed to characterize the chemical profile and evaluate the antioxidant potential of wines from the Malbec cultivar using two vinification strategies: inoculation with *S. cerevisiae* alone (T3) and co-inoculation with *H. vineae* and *S. cerevisiae* (9:1, T4). Physicochemical characterization was performed by FT-IR. Total phenolic compounds, flavonoids, proanthocyanidins, anthocyanins, and antioxidant activity (DPPH• and ABTS•⁺) were determined spectrophotometrically. Antioxidant capacity was also assessed by electroanalytical methods. Volatile profiles were analyzed by HS-SPME-GC-MS using CAR/PDMS fiber and the NIST11s library. Data were processed by PCA and Venn diagrams. The fixed profile was analyzed by HPLC-ESI-(+)-MS/MS and submitted to GNPS. Sensory analysis was conducted with 25 wine experts. Physicochemical analyses showed faster malolactic fermentation in T4, with increased pH (3.80), higher lactic acid (2.20 g/L), reduced total acidity (6.90 g/L), and lower malic acid (0.50 g/L). Spectrophotometric results indicated higher phenolic compounds (1048.41 mg GAE/L) and proanthocyanidins (252.90 mg CE/L), but lower flavonoids (355.79 mg QE/L) and anthocyanins (586.00 mg Mv-3G/L). Targeted analysis identified seven compounds, mainly flavonoids such as quercetin-hexoside (*m/z* 465.1028) and the tannin procyanidin B2 (*m/z* 579.1498). Twenty-three volatile compounds were detected, predominantly acetate esters (e.g., phenylethyl acetate) and alcohols (e.g., hexanol), associated with fruity and floral notes. PCA and Venn diagrams revealed that *H. vineae* enhanced the production of highly aromatic esters. Sensory evaluation indicated that T4 had greater intensity of ripe black fruit, stewed black fruit, and dried fruit notes, suggesting that co-inoculation favored acetate ester production. Overall, *H. vineae* co-inoculation modulated Malbec wine composition, increasing aromatic complexity and potential functional properties.

Keywords: Aromatic profile, *H. vineae*, Malbec wine, co-inoculation, HS-SPME-GC-MS

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FUNGAL CO-CULTIVATION DYNAMICS AND SECONDARY METABOLITE PRODUCTION: A MULTI-PHASE INVESTIGATION OF ANTAGONISTIC INTERACTIONS AMONG SEVEN PLANT PATHOGENIC SPECIES

Mustapha Ngaski Abubakar^{1*}, Paulo Cezar Vieira¹

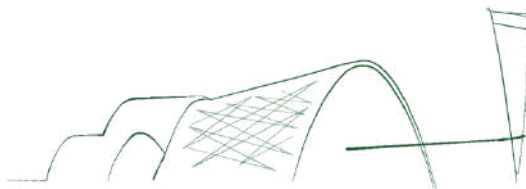
mngaskyii@usp.br

¹Faculdade de Ciências Farmacêuticas de Ribeirão Preto, USP - Avenida Professor Doutor Zeferino Vaz, s/n - 14040-903 - Ribeirão Preto, SP, Brazil

This study investigated the complex interactions and secondary metabolite production patterns among six economically important plant pathogenic fungi: *Fusarium guttiforme*, *Pestalotiopsis diospyri*, *Colletotrichum horii*, *C. gloeosporioides*, *F. sacchari*, and *F. verticillioides* as well as an endophyte *Neofusicoccum ribis*. A systematic three-phase experimental approach was employed to evaluate fungal interactions in axenic, dual, and triple co-cultivation systems across multiple growth media. Phase I examined axenic cultures and triple permutations of selected species on rice and potato dextrose broth (PDB) media, revealing enhanced chemodiversity and metabolite yields in rice-based systems. Phase II expanded the investigation to include dual co-cultivation systems using rice medium exclusively, based on Phase I optimization results. Phase III, currently in progress, focuses on three species (*P. diospyri*, *C. gloeosporioides*, and *N. ribis*) selected for their demonstrated overexpression and novel metabolite production capabilities. These organisms were cultivated on rice, rice flakes, and modified Czapek-Dox media with alternative carbon sources (glycerol and suspended flakes), employing varied inoculation ratios and strategic temporal introduction of challenger and inducer strains. Antagonistic interactions predominated across all cultivation systems, with α -pyrone polyketides from *P. diospyri* and *N. ribis* governing the competitive dynamics, consistent with phenotypic observations on potato dextrose agar. Notably, four novel metabolites were isolated from axenic *C. gloeosporioides* cultures grown on rice medium. Metabolite identification employed classical and advanced high-performance liquid chromatography methods, while structural elucidation utilized nuclear magnetic resonance spectroscopy, liquid chromatography-mass spectrometry, and high-resolution mass spectrometry. Principal component analysis is being applied for statistical evaluation of Phase III culture permutations. Promising extracts will undergo scale-up production followed by comprehensive antifungal and protease inhibitory activity assessments. These findings contribute to understanding fungal chemical ecology and may inform biotechnological applications for natural product discovery.

Keywords: Fungal pathogens, co-culture, secondary metabolites, culture-media, bioactivity





BIOPROSPECTING OF NATIVE SPECIES FROM THE BRAZILIAN CAATINGA AND CERRADO FOR THE DEVELOPMENT OF MICROEMULSIONS WITH ANTIOXIDANT POTENTIAL.

Micaela Sousa Coutinho Silva^{1*}, Catarina Silva Guimarães², Paulinne Moreira Lima², Maria Alice Sousa Marinho², Jayne Ferreira da Silva Oliveira², Yolanda Trindade de Oliveira², Isabela Dias dos Santos¹, Lara Beatriz de Andrade Silva¹, Gabriel Azevedo de Brito Damasceno^{1,2}, Juliano Geraldo Amaral^{1,2}.

micaela.coutinho@ufba.com

1-Instituto Multidisciplinar em Saúde, Campus Anísio Teixeira, Universidade Federal da Bahia, Vitória da Conquista, Bahia, Brazil. 2-Programa de Pós-Graduação em Biociências, Campus Anísio Teixeira, Universidade Federal da Bahia, Vitória da Conquista, Bahia, Brazil.

Brazil, with its vast biodiversity combined with the demand for sustainable alternatives, has driven the research and development market. Licuri (*Syagrus coronata*), a palm tree native to the Brazilian semiarid region, is a species with notable biotechnological potential. Similarly, pequi (*Caryocar brasiliense* Camb.), widely found in the Cerrado, is composed of bioactives that confer antioxidant and emollient properties. Although the peel and outer mesocarp constitute a large part of the fruit, they are still considered waste with potential for use. Plant-based active ingredients have been widely used in microemulsions due to their advantages: increased skin permeability, sensory properties, and formulation stability. Therefore, this study aimed to develop microemulsions using the spontaneous emulsification method, using *S. coronata* kernel oil as the oily phase, supplemented with the aqueous extract of *C. brasiliense* residue. The species were registered in the National System for the Management of Genetic Heritage and Associated Traditional Knowledge (SisGen) under registration AFD6D69. The *C. brasiliense* extract was obtained by ultrasound-assisted extraction and tested for total flavonoid content and 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging capacity, showing antioxidant activity of 84.62% and a total flavonoid content of 93.36 µg EQ/mg. A pseudoternary phase diagram delimited the regions with macroscopic aspects typical of microemulsions, defining the relationships between the oil phase (*S. Coronata*) and the emulsifier (*Hydrogenated Castor Oil PEG-40 and Sorbitan Oleate*). The formulations were subsequently subjected to the freeze-thaw cycle and accelerated stability. Among the analyzed formulations, the selected one presented parameters such as mean particle diameter (MAD) of 38.83 nm, polydispersity index (PDI) of 0.230, and zeta potential (ZT) of |24 mV|, values considered satisfactory for the incorporation of *C. brasiliense* extract at 0.1%. The formulation demonstrated stability even after subjection to thermal stress, demonstrating its potential. The incorporation of pequi residue conferred multifunctional properties, in agreement with the nanostructured system..

Keywords: *Caryocar brasiliense*, *Syagrus coronata*, Microemulsion, antioxidant, pequi residue





ISOLATION OF AMYRINIC TRITERPERNES FROM PROTIUM HEPTAPHYLLUM OLEORESIN

Stefany Marques da Silva (IC)^{1*}, Michelle Frazão Muzitano (PQ)¹, Danilo Ribeiro de Oliveira (PQ)², Shaft Côrrea PINTO (PQ)¹.

*stefolegario@gmail.com

1-Laboratório de Produtos Bioativos, UFRJ-Macaé, Av. Aloísio da Silva Gomes, 50, Macaé, RJ, 27930-560, Brazil. 2-Laboratório de Bioprospecção e Etnofarmacologia Aplicada, UFRJ-Fundão, Av. Carlos Chagas Filho, 373, Rio de Janeiro, RJ, 21941-170, Brazil.

The oleoresin of *Protium* has been traditionally employed in the treatment of several pathologies and has attracted pharmacological and cosmetic interest (Albino et al., 2021). In this context, the present study aims to fractionate this oleoresin in order to isolate and identify amyrinic triterpenes, providing material for quality control and future biological assay. For this purpose, the oleoresin (401.6 mg) was fractionated by HSCCC under the following conditions: biphasic solvent system Hex:AcN (1:1, v/v), mobile phase = lower phase, column volume (V_c) = 113 mL, flow rate 2.0 mL/min, rotation = 850 rpm (stopped at $K_D = 2$, $VR = 207.36 \sim$ tube 52), $S_f = 84\%$, 4.0 mL/tube, extrusion with the stationary phase (SP). Fractions were screened by TLC (silica gel F254, $CHCl_3$ 100% v/v, vanillin–sulfuric acid), compared with α -amyrin standard. Fractions containing amyrins were analyzed by HPLC-DAD: isocratic elution (95% AcN, 5% H_2O + 0.05% TFA); $\lambda = 202$ nm; flow = 1.0 mL/min; column: Luna C18 (250mm $\times$ 4.6mm $\times$ 5 μ m); $T=40^\circ C$. Isolation of amyrins was performed by semipreparative HPLC-DAD under the same conditions as for the qualitative analysis, except for the use of a Luna C18 column (250mm $\times$ 10mm $\times$ 5 μ m) and a flow rate of 3.0 mL/min. Fractions 67–77 showed indications of amyrin presence when compared to the commercial standard and were analyzed individually by HPLC-DAD, and those with similar patterns were combined in order to increase the mass available. So, fractions were grouped into three sets: 68–69, 70–72, and 73–77. Comparing the chromatographic profile of fraction 70–72 with the results of Haralampidis et al. (2001), the presence of γ -amyrin, α -amyrin, and β -amyrin was suggested. Continuing with the separation process by HPLC-DAD, fraction 70–72 resulted four isolated substances, which will be subjected to NMR. The remaining combined fractions will also undergo semipreparative separation. In conclusion, the biphasic solvent system employed for resin partitioning led to the obtainment of an amyrin mixture, as suggested by TLC and HPLC-DAD results. Finally, semipreparative HPLC-DAD enabled the isolation of four peaks, which will be characterized by NMR techniques, including ^1H , ^{13}C , HSQC, HMBC, COSY, and NOESY, and compared with existing literature data.

Keywords: *Protium*, oleoresin, isolation, amyrin, chromatography.





**EXPLORATORY STUDY OF VOLATILE NATURAL PRODUCTS FROM A
LAMIACEAE SPECIES**

Mariana Godoi Anunciação^{1*}, Maria Rita Scotti², Diogo Montes Vidal¹

*marigodoi@ufmg.br

1-Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

2- Instituto de Ciências Biológicas, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

The Lamiaceae family is the sixth largest group of angiosperms and includes many familiar aromatic herbs, such as rosemary, thyme, and oregano, which are commonly used as spices. In addition to their extensive use in the food industry, species from this family have been traditionally employed in medicine for centuries, largely due to their diverse biological activities.¹ In this context, the World Health Organization highlights the importance of investigating Lamiaceae plants with a well-documented history of use and validated therapeutic properties in order to uncover additional biological activities and potential pharmacological applications.² Another relevant application of this family lies in agricultural pest management, since the development of sustainable pesticides is increasingly necessary.³ Small bioactive molecules, such as monoterpenes and sesquiterpenes, hydrocarbons and oxygenated compounds, can be isolated from Lamiaceae species.⁴ In the present study, volatile compounds from a Cerrado species of the Lamiaceae family were investigated using two different approaches: dynamic headspace and essential oil extraction, the aim of conducting an exploratory analysis of their natural products and contributing to the growing body of research on Lamiaceae species. The resulting extracts were characterized by GC–MS to compare their chemical profiles. The dynamic headspace showed higher proportions of monoterpenes, including α -thujene, α -pinene, and sabinene, whereas essential oil extraction resulted in a larger proportion of sesquiterpenes, such as β -caryophyllene, germacrene D, and caryophyllene oxide. In conclusion, the method employed plays an important role in determining the volatile compounds extracted. Future investigations should focus on the biological properties of these compounds to determine their potential applications.

Keywords: Natural products, Lamiaceae, cerrado, volatile extraction, essential oil, terpenes

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ANTI-INFLAMMATORY EFFECTS OF AQUEOUS EXTRACTS OF ROSMARINUS OFFICINALIS AND ORIGANUM VULGARE, ALONE AND IN COMBINATION, IN IN VITRO AND IN VIVO MODELS

Joana Cristina Farias Cayres^{1*}, Ana Beatriz Loures², Laura Loures¹, Rebeca R. Rodrigues¹, Fernand Medaglia¹, Jull Chay¹, Rogério de Carvalho¹, Sandra B. R. Castro¹, Alessandra P. Carli²

joana.cayres@ufvjm.edu.br

1- Federal University of the Jequitinhonha and Mucuri Valleys, 39803-371 Teófilo Otoni - Minas Gerais, Brazil. 2- Federal University of the Juiz de Fora, Governador Valadares Campus Minas Gerais, Brazil.

Abstract

Natural products rich in phenolic compounds, such as *Rosmarinus officinalis* (rosemary, ALE) and *Origanum vulgare* (oregano, ORO), have been associated with the modulation of inflammatory pathways. This study evaluated the anti-inflammatory effect of the aqueous extracts (AE) of these species—tested individually (AE-Ale, AE-Oro) and in combination (AE-Ale + AE-Oro)—using a cellular model of inflammation. Murine macrophages (RAW 264.7) were exposed to the extracts at 333, 100, 33.3, and 10 µg/mL. Cytotoxicity was assessed by MTT, and the inflammatory response by nitric oxide (NO) production. The AEs exhibited low cytotoxicity under all conditions, with cell viability $\geq 70\%$ at 100, 33.3, and 10 µg/mL. A significant inhibition of NO was observed at nearly all concentrations: reductions of $\sim 60\%$ at 333, 33.3, and 10 µg/mL and $\sim 66\%$ at 100 µg/mL. The combined extract (AE-Ale + AE-Oro) achieved $\sim 60\%$ inhibition, with an effect comparable to or better than the isolated extracts. Taken together, the results indicate that the combined aqueous extracts of rosemary and oregano reduce NO production with no relevant cytotoxicity, supporting their anti-inflammatory potential and in vitro safety. These findings suggest that combining rosemary and oregano aqueous extracts is a promising and original strategy for controlling acute inflammation.

Keywords:

Rosmarinus officinalis; *Origanum vulgare*; RAW 264.7 macrophages; nitric oxide; inflammation

Reference

ISO 10993-5:2009 – Biological evaluation of medical devices — Part 5: Tests for in vitro cytotoxicity. Geneva: ISO, 2009.





**PLAKORTIDES AND COLESTANE STEROIDS FROM THE MARINE
SPONGE *Plakinastrella microspiculifera***

Ana Luíza Vidal Pimentel Santos^{1*}, Johanna de Carvalho Girão¹, Lidilhone Hamerski
Carbonezi¹, Roberto Carlos Campos Martins¹.

alvpsantosufrj@gmail.com

1-Instituto de Pesquisa de Produtos Naturais Walter Mors, Centro de Ciências da Saúde,
Universidade Federal do Rio de Janeiro-UFRJ, Av. Carlos Chagas Filho, 373, Bloco H, Rio de
Janeiro, RJ, Brazil

Sponges, belonging to the phylum Porifera, are sessile marine organisms with approximately 600 species widely distributed along the Brazilian coastline, from north to south. Among marine organisms, they stand out as prolific producers of bioactive metabolites of interest to humans. For the sponges themselves, these compounds act as chemical defense mechanisms against predators and are also very important in roles in defense, nutrition, and adaptation processes for these invertebrates. Sponge *Plakinastrella microspiculifera* (Plakinidae) occurs in the Fernando de Noronha Archipelago and on the northern coast of the state of Rio de Janeiro. Preliminary data indicate the presence of substances with potential antitumor and cytotoxic activities. A specimen of this sponge was collected in Fernando de Noronha, and an extract was prepared using a CHCl₃:MeOH (1:1) solvent mixture. This extract was lyophilized and subjected to liquid-liquid partitioning with *n*-hexane, dichloromethane, and ethyl acetate. Due to the chemically diverse profile observed by thin-layer chromatography (TLC), the insoluble fraction from the MeOH:H₂O (9:1) resuspension — used for solubilizing the extract prior to partitioning — was further fractionated by adsorption column chromatography using hexane, ethyl acetate, and methanol as eluents. The most apolar fractions, obtained in small amounts, were analyzed by gas chromatography-mass spectrometry (GC-MS), employing a DB-5 column and electron impact ionization (70 eV), for the identification of their chemical constituents. The results obtained so far indicate the presence of plakortides, aliphatic cyclic peroxides previously isolated from other sponge species, and steroids with a cholestane skeleton. Preliminary NMR data support the proposed structures and are currently undergoing advanced stages of structural elucidation. Some of these compounds, according to the literature, exhibit known biological activities such as antimicrobial and cytotoxic effects.

Keywords: Sponge, Porifera, Natural Products





IDENTIFICATION, QUANTIFICATION OF FLAVONOIDS, AND ANTIOXIDANT ACTIVITY ASSESSMENT OF *Passiflora setacea* D.C (Passifloraceae) LEAVES

André Santos Alkimim^{1, 2*}, Juliana Rodrigues Vasconcelos^{1, 2}, Cláudia Gontijo Silva¹, Wagner Campos Otoni³, Julio Cesar Dias Lopes⁴, Claudinei da Silva Souza³, Vera Lúcia de Almeida¹, Priscilla Rodrigues Valadares Campana²

vera.almeida@funed.mg.gov.br

1-Serviço de Fitoquímica e Prospecção Farmacêutica, Fundação Ezequiel Dias, Rua Conde Pereira Carneiro, 80, Belo Horizonte - MG, Brazil 30510-010 2-Faculdade de Farmácia, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil 31270-901 3- Departamento de Biologia Vegetal, UFV, Av. P. H. Rolfs, s/n - Campus Universitário, Viçosa - MG, Brazil 36570-900.4-Departamento de Química UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil 31270-901 3

Passifloraceae family stands out for its role in natural product utilization. The wild species *Passiflora setacea* D.C, known as "maracujá-do-sono" has chemical and pharmacological properties which are important to food and pharmaceutical industries. This species presents greater resistance to pathogens compared to commercial counterparts. Although the chemical composition and biological activity of *P. setacea* have been studied, further investigation is still needed. This study aimed to identify and quantify flavonoids in the hydroalcoholic extract of *P. setacea* leaves using thin-layer chromatography (TLC), high-performance liquid chromatography (HPLC), ultra-performance liquid chromatography with diode-array detector and mass spectrometer (UPLC-DAD-MS), and spectrophotometric methods. The antioxidant potential of the extract was evaluated through DPPH free radical scavenging, the β -carotene/linoleic acid lipid peroxidation method, and the liposome peroxidation assay (TBARS). Apigenin 6-C- β -D-glucopyranoside and luteolin 6-C- β -D-glucopyranoside were identified by TLC, HPLC, and UPLC-DAD-MS, while isovitexin-2"-O-xyloside and apigenin 6,8-di-C- β -D-glucopyranoside were detected by UPLC-DAD-MS. The total flavonoid content, expressed as apigenin, was 4.44 ± 0.13 (% w/w). Apigenin 6-C- β -D-glucopyranoside and luteolin 6-C- β -D-glucopyranoside contents were quantified by HPLC, with values of 0.44 ± 0.009 and 0.83 ± 0.087 (% w/w). Antioxidant activity was detected by the β -carotene/linoleic acid method (EC_{50} 61.93 ± 3.07). However, no activity was found in the DPPH and TBARS assays. This phytochemical investigation contributes to understanding the chemical characteristics and biological activity of this understudied species, which has pharmaceutical and agronomic relevance.

Keywords: *Passiflora setacea*, HPLC, UPLC-DAD-MS, DPPH, TBARS, β -carotene





EPIGENETIC MODULATORS AIMING AT IMPROVEMENTS IN THE METABOLIC PRODUCTION OF THE ENDOPHYTIC FUNGUS HYPOMONTAGNELLA MONTICULOSA ISOLATED FROM THE RED MARINE ALGA DICHOTOMARIA MARGINATA

Ariele Maria Morelli*, Lucas Henrique Silva Moura, Victor Hugo Lino Rufino, Yan Michel Lopes Fernandes, Natasha Grizzo Cesário, Dulce Helena Siqueira Silva.

am.morelli@unesp.br

Universidade Estadual Paulista – UNESP, Instituto de Química, Araraquara – SP

Recent studies have revealed a wide variety of fungi associated with marine algae, showing great biotechnological potential and pharmacological properties. Complementarily, the modification of gene expression through epigenetic modulators can activate the production of novel metabolites via silenced biosynthetic pathways, contributing to chemical diversity. In this context, this work aimed to evaluate the chemical profile of the fungus *Hypomontagnella monticulosa*, isolated from the red alga *Dichotomaria marginata*, focusing on metabolic changes induced by epigenetic modulators. The fungal strain was first cultivated on potato-dextrose-agar (PDA) plates for 35 days and subsequently inoculated into Erlenmeyer flasks containing liquid Malt Extract medium under control conditions and supplemented with sodium butyrate (NaBut, 1 mM) and 5-azacytidine (5-AZA, 100 µM). A growth curve of the fungus in liquid medium was performed with ethyl acetate (EtOAc) extractions at 5, 10, 15, 20, 25, 30, and 35 days to assess metabolic variation during growth. Results showed that both mycelial dry weight and extract yields increased with longer cultivation times. However, cultivation in the presence of modulators was performed specifically at 15, 20, and 25 days, as these time periods presented the most significant fungal growth results in terms of biomass and extract yield. After EtOAc extraction, the samples were analyzed by HPLC-DAD under different chromatographic conditions. Four analyses were performed using gradient elution (5% to 100%) with methanol (MeOH/H₂O), MeOH/H₂O with 1% formic acid, acetonitrile (MeCN/H₂O), and MeCN/H₂O with 1% formic acid. Acidified solvents provided sharper and more intense peaks than non-acidified ones, suggesting that compounds in the extract are more stable or detectable in acidic media, possibly due to facilitated protonation. Epigenetic modulators promoted more intense peaks compared to the control, indicating possible activation of silent biosynthetic pathways. This work reinforces the effectiveness of epigenetic modulators and distinct chromatographic conditions in the detection of fungal secondary metabolites, while also directly contemplating UN Sustainable Development Goals related to Good Health and Well being (SDG 3) and Life under water (SDG 14).

Keywords: Red algae, epigenetic modulators, marine fungi, chemodiversity.





FIRST REPORT OF THE ISOLATION AND CHARACTERIZATION OF ENT-16 α ,17-DIHYDROXY-KAURAN-3-ONE FROM *EUPHORBIA TIRUCALLI* LEAVES (EUPHORBIACEAE)

Anndreisa Christiny Monteiro^{1*}, Simone Grecco dos Santos¹, Patricia Sartorelli¹

anndreisa.monteiro@unifesp.br

1- Instituto de Ciências Ambientais, Químicas e Farmacêuticas, UNIFESP, 09972-270, Diadema-SP, Brasil.

Euphorbia tirucalli is a species belonging to the Euphorbiaceae family, popularly known as aveloz¹. It is a plant widely used in folk medicine to treat various diseases, due to its numerous reported medicinal properties². To contribute to the phytochemistry from the genus *Euphorbia*, the present study aims to isolate and identify the chemical constituents from *E. tirucalli* leaves. The leaves of *E. tirucalli* were collected from the medicinal garden of the Eldorado campus of UNIFESP, followed by drying, grinding, and extraction until exhaustion with *n*-hexane and, subsequently, with methanol. The methanolic extract was subjected to a liquid-liquid partition procedure with *n*-hexane, DCM and EtOAc, to afford its respective partition phase fractions. The dichloromethane phase was fractionated on a silica gel column, with DCM/EtOAc, with an increasing polarity gradient, obtaining 18 fractions. Fractions ET-C8 to ET-C11 were combined and subjected to a new chromatographic fractionation with the same previous conditions, and at subfraction 21 was possible to observe a pure compound. The compound was analyzed by UHPLC-DAD-ESI-QTOF-HRMS/MS, ATR-FTIR, and NMR (¹H, ¹³C, DEPT 135, HSQC and HMBC), to perform its complete chemical characterization. The MS spectra displayed ions with *m/z* 321.2418 [M+H]⁺, 303.2316 [M-H₂O+H]⁺ and 285.2218 [M-2(H₂O)+H]⁺, corresponding to C₂₀H₃₂O₃ molecular formula. The ¹H and ¹³C NMR spectra revealed signals corresponding to a kaurane diterpene derivative, evidenced by the characteristic signals at δ_H 2,46 (t, *J*= 14,8 Hz, H-2) and δ_H 3,51 (q, *J*= 10,7 Hz, H-16 e H-17), and at δ_C 79,80 (C-O; C-16), δ_C 70,00 (CH₂OH; C-16) and δ_C 218,3 (C=O). The presence of carbonyl was only confirmed in HMBC and at ATR-FTIR spectrum with an absorption band at 1700 cm⁻¹, characteristic of a ketone carbonyl group. After comparing the experimental data with the literature, it was possible to confirm the identification of the compound as *ent*-16 α ,17-dihydroxy-kauran-3-one, being the first time reported at *Euphorbia tirucalli*.

Keywords: *Euphorbia tirucalli*, Kaurane diterpene, chemical characterization, chromatographic isolation

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PREPARATION AND STABILITY EVALUATION OF A PHARMACEUTICAL FORMULATION CONTAINING SEED OIL AND FRUIT PEEL EXTRACT OF *CALOPHYLLUM BRASILIENSE* CAMBESS

Luciana Rabelo Quintela Iunes Araújo^{1*}, Maurília de Oliveira Souza¹, Cristiane dos Santos Giuberti¹, Rita de Cássia Ribeiro Gonçalves¹, Ricardo Machado Kuster¹, Rodrigo Rezende Kitagawa¹.

luquintela@gmail.com

1-Graduate Program of Pharmaceutical Sciences, Health Sciences Center, Federal University of Espírito Santo, Espírito Santo, 29047-105, Brazil.

Aligned with the global trend toward sustainability and upcycling — reusing waste and by product in new production cycles — the native species *Calophyllum brasiliense* Cambess, Calophyllaceae (guarandi) have demonstrated significant potential as a sustainable and medicinal raw material. However, one of the main challenges associated with natural products is their stability over time and under varying environmental conditions. This study aims to evaluate the behavior of a clean pharmaceutical formulation incorporating seed oil and crude extract fruit peel from *C. brasiliense*, from the point of manufacture through to the end of its shelf life. The selected formulations were emulsions composed exclusively of natural ingredients, including glycerin, Lexgard®, Natrosol, seed oil, and fruit peel extract from guarandi. To characterize the emulsions, assessments were conducted on physical and thermal stability, pH, general appearance, and emulsion type on the day of manufacture. After 90 days, the initial tests were repeated, and additional evaluations were performed, including spread ability and optical microscopy. Two emulsion samples were developed, sample A: containing 10% guarandi seed oil and sample B: containing 10% guarandi seed oil combined with 5% guarandi fruit peel extract. Both formulations were oil-in-water emulsions. Initial pH values were 6.0 for Sample A and 7.5 for Sample B, which decreased to 5.0 and 4.1, respectively, after 90 days. Initially, both samples exhibited a smooth, glossy, lump-free, homogeneous texture with a characteristic plant odor. After 90 days, only sample B showed alterations, including the presence of lumps and a heterogeneous appearance. Under physical and thermal stress conditions, both emulsions were stable on the first day. However, after 90 days, sample B failed both tests. Regarding spread ability, sample A demonstrated superior performance in terms of coverage area and responsiveness to applied pressure. Microscopic analysis revealed that both emulsions maintained rounded, uniform, and discrete droplets of the dispersed phase. Based on these findings, it is concluded that the developed emulsions were stable at the time of manufacture. However, by the end of the shelf life, particularly the formulation containing both oil and extract, the initial characteristics were not preserved. Further studies are required to obtain more comprehensive data.

Keywords: *Calophyllum brasiliense*, upcycling, pharmaceutical formulation

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**BIOACTIVITY AND CHEMICAL PROFILE OF THE OPTIMIZED EXTRACT OF
EUGENIA STIPITATA FRUITS**

Dayenne Alexsa A. de Souza^{1*}, Camila Fernanda B. Albuquerque¹, Eldrinei Gomes Peres²,
Hector Henrique F. Koolen², Pablo Luis B. Figueiredo³, Renan Campos Chisté⁴, Joyce
Kelly R. da Silva¹

dayenne@ufpa.br

1-LABITPNA, Laboratório de Bioprospecção e Inovação Tecnológica de Produtos Naturais da Amazônia, ICB, UFPA, R. Augusto Corrêa, 01, Belém, PA, Brazil. 2-CMABIO, Escola Superior de Ciências da Saúde, Universidade do Estado do Amazonas, Av. Carvalho Leal 1777, 69065-001 Manaus-AM, Brazil; 3-Laboratório de Química Dos Produtos Naturais, UEPA, Belém, PA, 66087-670, Brazil. 4- Faculdade de Farmácia, UFMG, Belo Horizonte, MG, 31270-901, Brazil.

The araçá-boi (*Eugenia stipitata* McVaugh - Myrtaceae) is a fruit species native to the Amazon and cultivated in some countries such as Brazil, Peru, Bolivia, Ecuador, and Colombia, which has great agro-industrial importance. Considering the growing search for bioactives from plant sources, this work proposed to optimize ultrasound-assisted extraction and evaluate the chemical profile and bioactivity of araçá-boi fruits. The experimental design was applied using a 2³-factorial design to construct a mathematical model and response surface. The input factors were ethanol (%) in water, solid/liquid ratio - SLR (m/v), and time (min), and the responses: total phenolics content (TPC) and antioxidant activity by DPPH radical inhibition (%DPPH). The SRL factor showed a significant effect for TPC and DPPH ($p < 0.05$), and a correction was observed between TPC and antioxidant activity (Person's $R = 0.843$, $p < 0.001$). The regression model was significant and predictive for both responses by the ANOVA F test ($p < 0.05$). The optimized parameters were EtOH 65%, solid/liquid ratio 1:5 and time of 25 min, resulting in 196.53 mg EAG/g of TPC and 86.03% DPPH inhibition. For the optimized extract, the total contents of flavonoids (131.20 mg EQ/g) and carotenoids (66.84 μ g/g) were determined. In addition, the extract displayed inhibition of lipid peroxidation in the system β -carotene/ linoleic acid (IC₅₀, 19.16 μ g/mL), Sun protection factor (7.0) and bacteriostatic effects against *Escherichia coli* (MIC, 62.5 μ g/mL) and *Staphylococcus aureus* (MIC, 125 μ g/mL). In annotation of the compounds present in the fruit of *E. stipitata* by HPLC-DAD-MS/MS, only the data obtained in negative mode were used, indicating that the majority was ellagic acid and the presence of its derivatives (ellagic acid glucoside, methylellagic acid, ellagic acid-rhamnoside, methylellagic acid rhamnoside) and other compounds (valoneic acid dilactone, trihydroxycinnamic acid-O-glucoside).

Keywords: bioactive, extract, process optimization, phenolic compounds, antioxidant activity, ellagic acid, antimicrobial activity





HALOGENATION OF PLANT NATURAL PRODUCT CRUDE EXTRACTS ENHANCES ACTIVITIES AGAINST TROPICAL PARASITES

Geraldo Célio Brandão¹, Isabela Penna Cerávolo², Mariza Gabriela Faleiro De Moura Lodi Cruz³, Daniela de Melo Resende⁴, Markus Kohlhoff^{5*}

markus.kohlhoff@fiocruz.br

¹ Escola de Farmácia, Universidade Federal de Ouro Preto (UFOP), Campus Morro Do Cruzeiro, 35402-163 Ouro Preto, Brazil; ² Immunopathologia, Instituto René Rachou (FIOCRUZ Minas), Av. Augusto de Lima, 1715, 30190-009 Belo Horizonte, Brazil; ³ Genômica Funcional de Parasitos (GFP), Instituto René Rachou (FIOCRUZ Minas), Av. Augusto de Lima, 1715, 30190-009 Belo Horizonte, Brazil; ⁴ Plataforma Bioensaios para triagem de drogas anti-Trypanosoma cruzi (PlaBio Tc), Instituto René Rachou (FIOCRUZ Minas), Av. Augusto de Lima, 1715, 30190-009 Belo Horizonte, Brazil; ⁵ Química de Produtos Naturais Bioativas (QPNB), Instituto René Rachou (FIOCRUZ Minas), Av. Augusto de Lima, 1715, 30190-009 Belo Horizonte, Brazil.

Plants are valuable sources of novel structures with biological activities. Organisms that produce halogenated natural products demonstrate that the presence of chlorine or bromine in the metabolite can be essential for their biological activity and the development and synthetic improvement of drug candidates from natural prototypes often involves the introduction of halogen atoms into lead structures.

In this project we collected plant material of ten *Bignoniaceae* species and halogenated chemically susceptible natural products of leaf and stem crude extracts using an environmentally friendly method to introduce chlorine, bromine or iodine [1]. We have developed an analytical microscale workflow to monitor halogenated compounds by their characteristic isotopic profiles using high resolution mass spectrometry (ESI-QTOF). Untreated as well as halogenated crude extracts were tested for activities against *Plasmodium falciparum*, *Leishmania infantum* and *Trypanosoma cruzi*, the protozoic parasites that cause Malaria, Leishmania and Chagas Disease, respectively. While all untreated extracts were inactive, some have shown remarkable activities after halogenation. Next, we intend to fractionate and screen active crude extracts at a microscale range (MTP96) to determine the formulas of active (halogenated) compounds by UHPLC-HRMS. Semi-preparative halogenation and mass monitored compound isolation should yield enough mass for structure elucidation by NMR and further biotests.

Keywords:

Bioactive Natural Products, Bignoniaceae, Halogenation, Mass Spectrometry, Tropical infection diseases

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**DEVELOPMENT OF AN EFFICIENT, HIGH-THROUGHPUT AND GREEN
PROCEDURE FOR METABOLIC PROFILING OF *Capsicum* spp.**

Leonardo de Oliveira Sartori^{1*}, Claudia Silva da Costa Ribeiro², Cristiano Soleo de Funari¹

l.sartori@unesp.br

1- Departamento de Bioprocessos e Biotecnologia, FCA/UNESP, Avenida Universitária, 3780, Botucatu, SP, Brazil. 2- Embrapa Hortaliças, Rodovia BR-060, Km 09 (Brasília/Anápolis), DF, Brazil

Fruits of *Capsicum* spp. are largely consumed worldwide. Chemical investigations have focused on few commercial species, neglecting local varieties and green chemistry principles. This work aimed to develop a sustainable, optimized analytical process for untargeted metabolomics of Brazilian *Capsicum* spp. Nineteen varieties were supplied by Embrapa Hortaliças and analysed by UHPLC-MS following the reference analytical procedure of Cervantes-Hernández et al., (2019). A principal component analysis (PCA) was performed separating the varieties in five clusters according to their metabolomic resemblance. A mixture with one sample of each of the five clusters was used to statistically develop a new, green and mathematically optimized analytical procedure (DoE), from sample preparation (dynamic maceration) to UHPLC-DAD/UV-MS metabolite profiling. The new analytical procedure demonstrated greater metabolite coverage, increasing the average number of chromatographic peaks from $151,0 \pm 5,0$ to $158,3 \pm 1,52$. Furthermore, the relative greenness of the new procedure was measured by the Analytical GREEnness Metric Approach and Software (AGREE), which assigned to the new procedure a score of 0.69, greener than that of the reference one (0.53). This was achieved mainly because the new sample preparation employed miniaturised, simultaneous extractions, allowing high sample throughput with recommended solvents (400 mg of plant/4 mL of EtOH:H₂O) followed by a syringe filtration before injection. The developed procedure proved to be advantageous for metabolite profiling *Capsicum* spp. from a comprehensive perspective, while being in line with the recommendations for a greener natural products chemistry (Funari et al., 2023) as well as with the goals 9, 12,13, 14 and 15 of United Nations Sustainable Development Goals. This study was financed, in part, by the São Paulo Research Foundation (FAPESP), Brasil. Process Number #2024/06494-0

Keywords: peppers, metabolomics, green chemistry, chemometrics, natural products, agrobiodiversity.

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CHEMICAL STUDY AND BIOACTIVE POTENTIAL OF THE SPECIES *Vitex orinocensis* Kunth. (Lamiaceae)

Juliene Aljahara Sousa Cardoso^{1*}, Aramys Silva dos Reis², Ivaneide Oliveira Nascimento⁴, Antônio José Cantanhede Filho¹, Juliana Aljahara Sousa do Nascimento³, Ana Karlla dos Santos Sousa², Maria de Fátima das Graças Fernandes da Silva⁵, Alan Bezerra Ribeiro²

jullienecardoso@gmail.com

1-Departamento de Química, Instituto Federal de Educação, Ciência e Tecnologia, Av. Getúlio Vargas, Campus Monte Castelo, São Luís, Maranhão, 65030-005, Brazil. 2-Centro de Ciência de Imperatriz, Universidade Federal do Maranhão, Campus Imperatriz, Imperatriz, Maranhão, 65900-410, Brazil. 3-Centro de Biociências, Universidade Federal de Pernambuco, Av. Professor Moraes, Recife, Pernambuco, 50670-420, Brazil. 4-Centro de Ciências Exatas, Naturais e Tecnológicas, Universidade Estadual da Região Tocantina do Maranhão, Brazil. 5-Universidade Federal de São Carlos, Rodovia Washington Luís, km 235, São Carlos, São Paulo, 13565-905

Vitex orinocensis Kunth is a native tree species from South America traditionally used in Brazilian folk medicine, especially in Maranhão state. Despite its ethnobotanical relevance, no phytochemical or biological data had been available in the scientific literature prior to this work. This study aimed to perform a comprehensive phytochemical investigation of the bark of *V. orinocensis* and to evaluate its potential against *Leishmania amazonensis*, the etiological agent of cutaneous leishmaniasis. Crude extracts were obtained by sequential solvent extraction (hexane, ethyl acetate, and methanol). The ethyl acetate was selected chromatographic fractionation using silica gel column chromatography. The isolation of secondary metabolites were performed by preparative high-performance liquid chromatography (HPLC), and compound structures were elucidated based on 1D and 2D Nuclear Magnetic Resonance (¹H and ¹³C NMR), supported by literature data. This approach allowed the isolation of four pentacyclic triterpenes, namely (3 β)-Olean-12-en-3-ol, (3 β)-3-Hydroxyurs-12-en-28-oic acid, (3 β)-3-Hydroxyolean-12-en-28-oic acid, and (3 β ,11 β)-dihydroxyurs-12-ene. The crude extracts were then tested against promastigote forms of *L. amazonensis*. The hexane and ethyl acetate extracts showed significant antiparasitic activity, with IC₅₀ values of 46.17 μ g/mL and 47.48 μ g/mL, respectively. In addition, cytotoxicity assays using RAW 264.7 macrophage cells revealed CC₅₀ values >240 μ g/mL for both extracts. Selectivity Index (SI) values of 5.23 (hexane) and 4.43 (ethyl acetate) suggest selective action against the parasite with low toxicity to host cells. Conversely, the methanolic extract exhibited low activity (IC₅₀ > 400 μ g/mL) but was non-toxic to mammalian cells (CC₅₀ > 400 μ g/mL), indicating potential utility in combination therapies. This is the first report on the chemical profile and antileishmanial effects of *V. orinocensis*, supporting its traditional use and highlighting its potential for phytopharmaceutical development.

Keywords: *Vitex orinocensis*, triterpenes, bioactivity, *L. amazonensis*





A PHYSICAL AND DIGITAL PLATFORM FOR THE VALORIZATION OF BOTANICAL ASSETS FROM AGRO-INDUSTRIAL BY PRODUCTS

Adriano Souza Fonseca^{1*}, Vitor Rossini¹, Isabel Duarte Coutinho², Ian Castro-Gamboa¹

adriano.s.fonseca@unesp.br

1-NuBBE, Instituto de Química, IQ-Araraquara, UNESP, Av. Prof. Francisco Degni, 55 - Jardim Quitandinha, Araraquara - SP, Brazil. 2-Natcrom Soluções Sustentáveis, Av. Jorge Fernandes de São Mattos, 311 - BOX 03 - 8º Distrito Industrial, Araraquara - SP, Brazil.

Food waste is a global challenge, with agro-industrial byproducts, such as fruit peels and seeds, often being discarded despite their high nutritional and bioactive value. In Brazil, where approximately 30% of food is wasted, the valorization of these residues is crucial for sustainability. This project's main objective was to develop a physical and digital platform for the prospecting and identification of botanical assets from fruit cultivation byproducts in the Araraquara region, SP. The methodological work was divided into three phases. Initially, a diagnosis of fruit farming residues in the Araraquara Region (comprising 16 municipalities) was carried out, based on information from technical document 128 of CATI-SP and Embrapa Cassava and Fruit Farming. Although data analysis identified oranges (83%) and bananas (7%) as the most economically significant crops, the initial chemical prospecting focused on pineapple (0.85%) and passion fruit (0.21%) byproducts. All data collected were systematized into standardized technical sheets. Subsequently, samples of these byproducts were processed and subjected to Soxhlet extraction. The obtained extracts were then analyzed by UPLC-MS and GC-MS. As the main result, a digital platform with a graphical user interface in Python (Tkinter) was developed, functioning as a library for chromatographic and spectral data. The system allows for data importation, searching for compounds by name, formula, or mass, and comparing experimental spectra with internal and external databases, such as MassBank. The platform proved to be a versatile tool, enabling not only the identification of compounds but also the management of a mapped chemical library for each fruit and the quantitative analysis of key substances. This facilitates the conversion of waste into standardized, high-value ingredients for the food, cosmetic, and pharmaceutical industries. The project contributes to the circular economy and is aligned with multiple Sustainable Development Goals (SDGs).

Keywords: *Agro-industrial Byproducts, Circular Economy, Bioactive Compounds, Mass Spectrometry.*





NANOEMULSIFIED L-CARVONE AND MENTHA SPICATA ESSENTIAL OIL AS POTENT DOSE-DEPENDENT ANTIFUNGAL AGENTS AGAINST THE WHITE ROT PATHOGEN SCLEROTIUM CEPIVORUM

Rodrigo Ribeiro Rocha^{1*}, Geraldo Humberto Siva¹, Lorena Alves de Melo Bessa¹

rodrigor.rocha@ufv.br

1-Laboratório Desenvolvimento de Agroquímicos, IEP, UFV-CRP, Rod. MG 230 KM 7, Cx.Postal 22, Rio Paranaíba, MG, 38810-000, Brazil.

The increasing demand for sustainable plant disease management has intensified interest in bioactive natural compounds, particularly essential oils (EOs), which are incorporated into nanostructured delivery systems to overcome the limitations of volatility and solubility. *Mentha spicata* EO and its major substance *L-carvone*, are known for *in vitro* antifungal properties; however, their efficacy against *Sclerotium cepivorum*, the etiological agent of white rot in *Allium* spp., remains unexplored. This study reports the dose-dependent antifungal activity of oil-in-water nanoemulsions containing *M. spicata* EO (NEOE) and *L-carvone* (NEOC) against *S. cepivorum*. Nanoemulsions were prepared via high-energy emulsification (Ultra-Turrax, 15,000 rpm, 5 min) with polyoxyethylene (20) sorbitan monooleate (Tween 80) at an oil:surfactant ratio of 1:2. Physicochemical characterization by dynamic light scattering revealed particle sizes of 33.53 nm (PdI = 0.432) for NEOE and 78.91 nm (PdI = 0.1591) for NEOC, indicative of stable, monodisperse systems. *In vitro* bioassays were performed on potato-dextrose agar (PDA) plates at concentrations from 100 to 4000 $\mu\text{g}\cdot\text{mL}^{-1}$. Controls included blank nanoemulsions (Tween 80 + water) and the synthetic fungicide iprodione. The mycelial growth area (cm^2) was quantified after incubation. NEOC achieved complete inhibition at 400 $\mu\text{g}\cdot\text{mL}^{-1}$ (MIC), whereas NEOE required 1600 $\mu\text{g}\cdot\text{mL}^{-1}$ for the same effect. Both formulations significantly reduced mycelial growth in a concentration-dependent manner ($p < 0.05$). These results align with previous findings, such as Kedia et al. (2014) on carvone's suppression of *Aspergillus flavus* and Maswanganye et al. (2025) on spearmint nanoemulsions inhibiting *Penicillium* spp. in postharvest fruit. The present study is the first report demonstrating the complete *in vitro* suppression of *S. cepivorum* by nanoemulsified *L-carvone* and *M. spicata* EO, highlighting their promise as biofungicidal agents for *S. cepivorum* management. The authors gratefully acknowledge CNPq and FAPEMIG for financial support, as well as Universidade Federal de Viçosa – Campus Rio Paranaíba (UFV-CRP) for technical assistance.

Keywords: *Mentha spicata*, *L-carvone*, nanoemulsions, essential oils, *Sclerotium cepivorum*.

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COMPARATIVE LC-UV-MS PROFILING OF COLOLOBUS SPECIES FROM THE ATLANTIC FOREST

Marilia Elias Gallon^{1*}, Marcelo Monge¹, Norberto Peporine Lopes¹

mariliagallon@usp.br

1 Núcleo de Pesquisa em Produtos Naturais e Sintéticos, Departament of BioMolecular Sciences, School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, São Paulo, Brazil.

The Atlantic Forest is globally recognized as a major Brazilian biodiversity hotspot, playing critical roles in the conservation of plant species and maintenance of ecological balance. The genus *Cololobus*, native to southeastern Brazil, comprises species that are predominantly endemic to this biome. Currently, five species have been formally described: *Cololobus argenteus*, *Cololobus hatschbachii*, *Cololobus longiangustatus*, *Cololobus rupestris*, and *Cololobus ruschianus*. Despite their ecological importance, the chemical composition and metabolic diversity of *Cololobus* species remain largely unexplored. Herein, we evaluate the chemical profiles of four *Cololobus* species. Plant extracts were analyzed by liquid chromatography with ultraviolet detection and coupled to mass spectrometry (LC-UV-MS). Comparative metabolic profiling revealed interspecific variations, showing high prevalence of phenolic compounds. Metabolites displaying ultraviolet absorption typical of flavonoids and hydroxycinnamic acid derivatives were especially prominent. Interestingly, we observed that *C. argenteus* exhibited a less diverse chemical profile (i.e, fewer detected signals), whereas *C. longiangustatus*, *C. ruschianus* and *C. rupestris* presented a more complex metabolic profile. The application of advanced spectrometric techniques enabled a comprehensive chemical characterization of the genus *Cololobus*, expanding the knowledge and providing new insights into the diversification of the Atlantic Forest. These results also strengthen methodological frameworks for investigating secondary plant metabolism and highlight the importance of developing strategies to promote and support the conservation and valorization of Brazilian biodiversity.

Keywords: *Asteraceae*, chemical characterization, secondary metabolites, flavonoids, hydroxycinnamic acid derivatives, natural products





BIOACTIVE POTENTIAL OF *Cariniana rubra* LEAVES: QUANTIFICATION OF SECONDARY METABOLITES AND OPTIMIZATION OF ULTRASOUND-ASSISTED EXTRACTION

Aline Biggi Maciel Del Conte^{1*}, Elis Ramos de Queiroz Jácome², Naísa Andrade da Silva², Rachel de Moura Nunes Fernandes³, Elisandra Scapin^{1,2,3}

aline.biggi@uft.edu.br

1-Programa de Pós-Graduação em Biodiversidade e Biotecnologia - BIONORTE, Universidade Federal do Tocantins, Campus de Palmas, 77001-090, Palmas, TO, Brasil. 2-Laboratório de Ensino e Pesquisa em Produtos Naturais e Biomassa, Universidade Federal do Tocantins, 77001-090, Palmas, TO, Brasil. 3-Laboratório de Química, Universidade Federal do Tocantins, 77001-090, Palmas, TO, Brasil

Cariniana rubra Gardener ex Miers, known as jequitibá-vermelho, is a native species of the Brazilian Cerrado, whose bark is traditionally used in folk medicine for the treatment of inflammations, infections, and disorders of the urinary and reproductive tracts. Although some biological activities have been described for bark extracts, phytochemical studies remain scarce, and to date, there are no records involving the leaves. This study aimed to quantify phenolic compounds and flavonoids present in the leaves of *C. rubra*. For this purpose, ultrasound-assisted extraction (UAE) was employed, optimized by a central composite rotatable design (CCRD), evaluating ethanol concentration and extraction time. Response surface methodology (RSM) was applied to determine the optimal conditions of the process. Extractive yield was evaluated, and the total phenolic and flavonoid contents were determined using the Folin–Ciocalteu and AlCl₃ methods, with gallic acid and rutin as reference standards, respectively. For yield, the model was statistically significant ($p = 0.02416$), with an R^2 of 92.65% and optimal conditions at 50% (v/v) ethanol and 132 min of extraction. In contrast, the models for phenolics and flavonoids were not statistically significant ($p > 0.05$), presenting R^2 values of 55.81% and 73.37%, respectively. However, the desirability analysis associated with experimental validation indicated ideal conditions at 90 min and 50% ethanol, resulting in 440.56 ± 3.10 mg GAE g⁻¹ for phenolics and 169.22 ± 4.20 mg RE g⁻¹ for flavonoids, both with a desirability index equal to 1. The levels obtained exceeded those previously reported for the bark, suggesting a high antioxidant potential and highlighting the leaves as a promising source of bioactive metabolites, while reinforcing the relevance of optimization in the phytochemical investigation of underexplored native species.

Keywords: Phenolic compounds, Flavonoids, Response surface methodology, Cerrado medicinal species





**INTERACTIONS BETWEEN ENDOPHYTIC MICROORGANISMS AND
CARAMBOXIN PRODUCTION IN *Averrhoa carambola***

Beatriz Alborgheti Soares^{1*}, Jamicelly Rayanna Gomes da Silva¹, Norberto Peporine Lopes¹

beatrizalborgheti@usp.br

*1-Núcleo de Pesquisa em Produtos Naturais e Sintéticos (NPPNS), Faculdade de Ciências
Farmacêuticas de Ribeirão Preto (FCFRP), USP, Av. Prof. Dr. Zeferino Vaz, s/n, Ribeirão Preto, SP,
Brazil.*

Caramboxin is a neurotoxin found in the fruits of starfruit (*Averrhoa carambola*), structurally analogous to the aminoacids phenylalanine and tyrosine, and associated with severe intoxication cases, particularly in patients with renal insufficiency. Literature evidence indicates that several fungi are capable of synthesizing toxins derived from amino acid backbones. Preliminary studies from our group, using MALDI imaging, demonstrated that the toxin is localized in the outer region of the seed, raising the hypothesis that endophytic fungi may be involved in its biosynthesis. In this context, the present research aimed to isolate, identify, and investigate the ecological and chemical diversity of starfruit endophytic fungi, with emphasis on caramboxin detection. Samples were collected at different ripening stages, followed by fungal isolation and morphological characterization. Subsequently, culture media were used for the prospection of specialized metabolites produced by the cultivated microorganisms, analyzed by Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry (MALDI-TOF MS). The results revealed significant chemical diversity in microbial extracts, with detection of ions corresponding to amino acids, amines, alkaloids, phenolic compounds, flavonoids, and structural lipids, with emphasis on nitrogen-containing compounds in the 120–480 m/z range. Moreover, the HCCA matrix showed greater sensitivity for low abundance molecules, enabling the detection of metabolites potentially related to caramboxin biosynthesis, whereas the DHB matrix favored the visualization of more labile molecules, albeit with lower spectral intensity. The simultaneous presence of phospholipids and secondary metabolites suggests that the extracts reflect both the metabolic diversity of endophytic fungi and the preservation of cellular constituents. Altogether, these findings highlight the biotechnological potential of starfruit-associated endophytes and contribute to the understanding of their possible role in caramboxin biosynthesis.

Keywords: *Endophytic microorganisms; Averrhoa carambola; Caramboxin.*





BIOASSAY-GUIDED FRACTIONATION OF POTENTIAL BLOCKERS OF SARS-COV-2 RBD :ACE2 INTERACTION FROM STINGLESS BEE (*Melipona mondury*) GEOPROPOLIS BY COUNTERCURRENT CHROMATOGRAPHY.

Cristiane C. dos Santos^{1*}, Rafael F. dos Santos¹, Suzana G. Leitão³, Mariana F. Campos⁴,
Diego Allonso³, Gilda G. Leitão², Rosane N. Castro¹

ggleitao@yahoo.com.br

1- Instituto de Química, UFRRJ, Seropédica, Brazil. 2- Instituto de Pesquisas de Produtos Naturais, UFRJ, Brazil. 3- Fac. Farmácia, UFRJ, Brazil. 4- Prog. Biotecnol. Veg.e Bioproc., UFRJ, RJ, Brazil.

Geopropolis, a resinous bee product enriched with soil and clay and produced by stingless bees such as *Melipona mondury*, was investigated for its potential antiviral activity. Extracts were obtained via ultrasound-assisted extraction using 96°GL cereal alcohol (EEGP-U1) from geopropolis collected at Barra da Tijuca Forest (Rio de Janeiro, Brazil). The dried extracts were reconstituted in a methanol:water mixture (7:3, v/v) and subsequently partitioned with hexane (FrH) and dichloromethane (FrDCM). The inhibitory effect of these extracts on the interaction between the SARS-CoV-2 receptor-binding domain (RBD) and the human ACE2 receptor was evaluated using an *in vitro* bioluminescence assay (Lumit®-Promega). The EEGP-U1 extract showed 60.90% inhibition, while FrH, FrDCM, and the MeOH:H₂O extract exhibited 38.20%, 79.23%, and 75.71% inhibition, respectively. Based on these results, FrDCM was selected for further fractionation using countercurrent chromatography (CCC), a liquid-liquid partition technique that enables purification without solid supports. Solvent system optimization for CCC was performed using shake-flask experiments, in which 2 mg of FrDCM was tested in various proportions of petroleum ether, ethyl acetate, methanol (or ethanol), and water. The system composed of petroleum ether-ethyl acetate-methanol-water (1:0.8:1.1:0.6, v/v) was selected for the fractionation of 123 mg of FrDCM in normal elution mode (2.0mL/min, 3mL fraction), dissolved in 5 mL of both phases and injected into a 112 mL column of an HT Prep, yielding 80 fractions. CCC fractionation successfully led to the isolation and purification of vanillin (2.1 mg, 70% purity by HPLC-DAD), demethoxymatteucinol (8.8 mg, 91% purity), and cryptostrobin (3 mg, 77% purity), along with a mixture of 40:60 C-methylated flavanones, strobopinin and cryptostrobin, respectively (14.3 mg). These results demonstrate the efficiency of CCC in separating bioactive constituents from *M. mondury* geopropolis and provide access to highly purified compounds for future evaluation of their antiviral activity.

Keywords: C-methylated flavanones, countercurrent chromatography, coronavirus

Acknowledgments: to CAPES, FAPERJ and CNPq





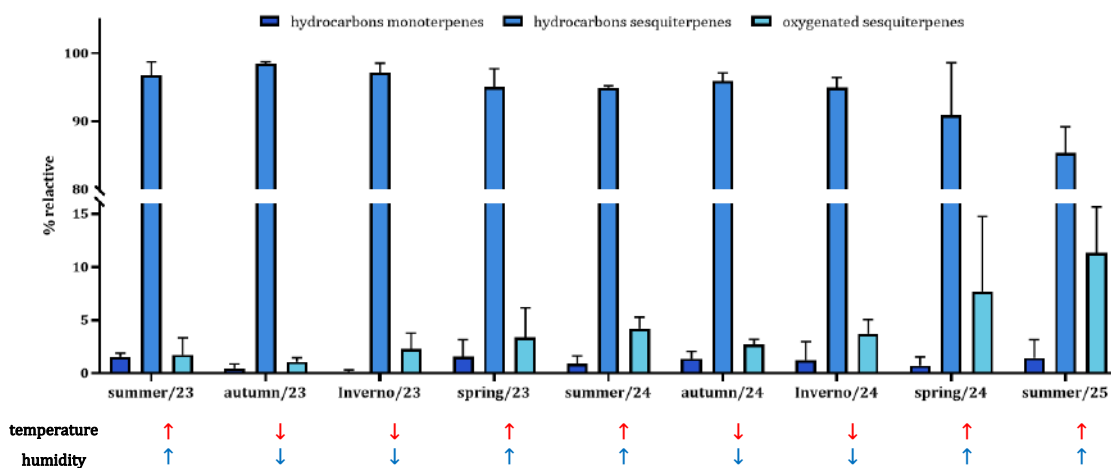
INFLUENCE OF MICROCLIMATIC PARAMETERS AND SEASONALITY ON THE COMPOSITION OF ESSENTIAL OILS FROM *Vernonanthura polyanthes* (ASTERACEAE)

Felipe S. Sales*, Carlos Henrique T. dos Santos, João Henrique G. Lago

felipe.sales@ufabc.edu.br

Center for Natural Sciences and Humanities, Federal University of ABC, Santo André, Brazil

Vernonanthura polyanthes, belonging to the Asteraceae, is chemically composed of triterpenes, sesquiterpene lactones, and flavonoids.¹ The essential oil composition revealed a predominance of sesquiterpenes, with zerumbone as the main compound.² However, the literature does not contain any information about the dynamics of the essential oil chemical composition. Therefore, in the present study, aerial parts of *V. polyanthes* were monthly collected from January/2023 to January/2025 (for a total of 25 samples) and the essential oils were extracted by hydrodistillation, in triplicate. After dereplication using GC-MS and determination of Kovats index, the data were regrouped by season: summer (January, February, March), autumn (April, May, June), winter (July, August, September), and spring (October, November, December). Chemically, a predominance of hydrocarbon sesquiterpenes – from 91 ± 7 % (spring/2024) to 99 ± 1 % (autumn/2023) was observed, with β -caryophyllene (16 ± 1 – 18 ± 1 %), α -humulene (15 ± 2 – 19 ± 1 %), germacrene D (22 ± 4 – 25 ± 1 %), and bicyclogermacrene (18.6 ± 0.7 – 22.4 ± 0.8 %) as the main compounds. Oxygenated sesquiterpenes, however, were identified as minor compounds but showing more intense variation (1.1 ± 0.4 – 11.0 ± 0.9 %), with humulene (0.13 ± 0.09 – 0.95 ± 0.09 %) and caryophyllene (1.0 ± 0.1 – 3.3 ± 0.6 %) oxides were predominant. Similarly, the amount of β -pinene, the only monoterpene identified in the analyzed oils, ranged from 0.11 ± 0.09 to 1.56 ± 0.08 %. These results suggest that variation in chemical composition (Figure 1) may be associated with microclimatic parameters (especially temperature and humidity) and seasonality. This finding is consistent with our previous studies on *Pittosporum undulatum*³ and *Guarea macrophylla*⁴.



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³Lago et al. *J. Braz. Chem. Soc.* **2006**, 17, 1334; ⁴Oliveira et al. *J. Braz. Chem. Soc.* **2019**, 30, 1395.

Keywords: essential oils, sesquiterpenes, seasonality, assa-peixe. **Acknowledgment:** CNPq, CAPES, FAPESP.





ANTIMICROBIAL ACTIVITY OF THE COMPOUND SELINA-1,3,7(11)- TRIEN-8-ONE

CHRISTIANO CATTANI BELINI^{1*}, JOCIANI ASCARI¹, ERIKA IZUMI¹, STEFANY
DE SOUZA QUINTINO¹, MARCOS FELIPE MACIEL PEREIRA¹

*cbelini@alunos.utfpr.edu.br

*1-UTFPR, Federal Technological University Of Paraná, Campus Santa Helena, Santa Helena,
Paraná, Brazil.*

Eugenia uniflora L. (Myrtaceae) popularly known as pitanga, it's a fruit native to Brazil, occurring in the Northeast, Central-West, Southeast, and South regions, as well as in other countries in South and Central America. The species is widely valued for its therapeutic properties, associated with bioactive components derived from secondary metabolism, which have antioxidants, antimicrobial, antiviral, and other activities. The essential oil from the leaves of *E. uniflora* is predominantly composed of sesquiterpene compounds, including selina-1,3,7(11)-trien-8-one and selina-1,3,7(11)-trien-8-one oxide. In this study, the compound selina-1,3,7(11)-trien-8-one was isolated from the essential oil of *E. uniflora* leaves obtained from local markets. The compound was isolated by fractionation in a silica gel 60 chromatographic column accompanied by thin-layer chromatography of silica gel 60 HG/254, and its structure was determined by nuclear magnetic resonance using a Bruker DRX-400 spectrometer. The antimicrobial activity of the compound was evaluated using the broth microdilution assay, standardized by the Institute for Clinical and Laboratory Standards. The microorganisms used in the study were *Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* ATCC 27587, *Staphylococcus aureus* ATCC 29213, *Enterococcus faecium* ATCC 6569, and *Candida albicans* ATCC 13231. The compound was solubilized in Tween 20 and then diluted in an appropriate culture medium, added to a microplate at a maximum concentration of 1000 µg/mL, followed by serial dilutions to approximately 7.8 µg/mL. The dilutions were performed so that the maximum concentration of Tween 20 did not exceed 0.3%. The compound selina-1,3,7(11)-trien-8-one had a more pronounced antifungal action, with a minimum inhibitory concentration against *C. albicans* of 62.5 µg/mL. Regarding antibacterial action, MIC values of 125 and 250 µg/mL were observed for *E. faecium* and *S. aureus*, respectively. Against *E. coli* and *P. aeruginosa*, inhibition was similar at 500 µg/mL for both species. The compound selina-1,3,7(11)-trien-8-one, present in pitanga essential oil, has antimicrobial potential that had not yet been reported, showing that even well-known plant species can harbor molecules of interest to human health.

Keywords: *Eugenia uniflora*, pitanga, essential oil, sesquiterpene.





EUGENIA UNIFLORA* ESSENTIAL OIL: ONTOGENETIC CHEMICAL VARIATIONS, RESPONSES TO ELICITORS, AND ACARICIDAL ACTIVITY AGAINST *TETRANYCHUS URTICAE

Mirian Luzinete da Silva^{1*}, Daiane Maria Barbosa dos Santos¹, Rodolfo Rodrigues da Silva¹, Marcilio Martins de Moraes¹, Claudio Augusto Gomes da Camara¹.

myrianmelo765@gmail.com

1-DQ, Departamento de Química, Universidade Federal Rural de Pernambuco, Rua Dom Manuel de Medeiros, s/n - Dois Irmãos, Recife, Pernambuco, (81) 3320-6001, 52171-900. Brazil.

The genus *Eugenia* L. comprises approximately 600 species, of which 240 occur in the Brazilian Atlantic Forest, with 202 being endemic. Among them, *Eugenia uniflora* L. (pitangueira) stands out for its high production of essential oils (EOs), recognized for their insecticidal and acaricidal activities. However, most studies focus on adult plants, although chemical variations have already been associated with developmental stages and responses to biotic and abiotic stresses. In this context, the aim of this study was to analyze variations in chemical composition and acaricidal activity of *E. uniflora* EOs at different ontogenetic stages and under stress induced by elicitors, with emphasis on their effects against the mite *Tetranychus urticae*, a major agricultural pest of economic relevance, targeting the mite *Tetranychus urticae*, an agricultural pest of economic importance. The seeds of *E. uniflora* were cultivated in 5 L pots under greenhouse conditions, and leaves were collected at 2, 17, and 24 months of age, as well as from adult plants. Additionally, different pots containing 17-month-old plants were treated with methyl jasmonate (MJ), methyl salicylate (MS), and nerolidol (NE). Essential oils were obtained by hydrodistillation and analyzed by GC-MS. Acaricidal activity was evaluated through toxicity bioassays against *T. urticae*, using the lethal concentration (LC₉₀) of the commercial acaricide Azamax[®] as reference. The highest oil yield was observed in adult plants (0.66%). Ontogenetic analysis revealed significant differences in chemical composition ($p < 0.05$), with curzerene being the major compound predominant in all phases, especially in adult plants (40.63%), while the compound atractylone presented the highest percentage in seedlings (16.03%). In elicitor-treated groups, an increase in eudesma-5,11(13)-dien-8,12-olide was observed in NE (18.48%) and MJ (22.33%) treatments, whereas MS treatment enhanced germacrone production (15.34%). Differences in the chemical composition of EOs were confirmed by multivariate analyses (Heatmap and PCA). Bioassays demonstrated that the oils exhibited high toxicity against *T. urticae*, with the strongest effect in 2-month-old plants (89.0%), followed by 17-month-old plants (86.5%) and adults (76.11%). In conclusion, the chemical composition and acaricidal potential of *E. uniflora* essential oils vary according to developmental stage and elicitor-induced stress, highlighting the potential of this species as a source of bioactive molecules for agricultural applications.

Keywords: Myrtaceae, Chemical variation, GC-MS analysis, Botanical acaricide, chemometrics, PCA.





BIOCONTROL OF *MAGNAPORTHE ORYZAE* BY *WAITEA CIRCINATA*: INTEGRATION OF BIOASSAYS AND METABOLOMIC CHARACTERIZATION

Matheus Santos de Souza Teodorico^{1*}, Geovanna Silva Reis¹, Leila Garcês Araujo², Lucilia Kato¹

matheusteodorico@ufg.br

1-Instituto de Química, IQ, UFG, Avenida Esperança s/n, Câmpus Samambaia, Goiania, GO, 74690-900, Brazil. 2- Instituto de Ciências Biológicas IV, ICB-IV, UFG, Avenida Esperança s/n, Câmpus Samambaia, Goiania, GO, 74690-900, Brazil

Rice blast, caused by *Magnaporthe oryzae*, is one of the most severe threats to global rice production.¹ While biological control offers a sustainable management alternative, the potential of *Waitea circinata* as a biocontrol agent remains largely unexplored². This study presents the first evaluation of the antagonistic activity of three individuals of *W. circinata* (W1, W2, and W3) against *M. oryzae*, combining biological, chemical, and microscopic analyses. In vitro dual-culture assays revealed a high and consistent inhibition rate of the phytopathogen: 95.63% (W1), 93.36% (W2), and 94.68% (W3), with no statistically significant differences among the individuals. For chemical characterization, extracts were obtained using ethyl acetate and chloroform and analyzed by LC-MS/MS. MS data were processed with MZmine 4.0 and submitted to GNPS and RStudio. Principal component analysis (PCA) did not reveal discrimination between extracts according to solvent, suggesting a consistent metabolic profile. Molecular annotation indicated the presence of coumarins, terpenes, terpenoids, and flavonoids, metabolite classes widely reported for antifungal activity. Microscopic observations suggested a direct physical antagonistic interaction between mycelia during in vitro assays, currently under detailed investigation using scanning electron microscopy (SEM). Inhibition zones observed in co-culture also indicated metabolite release, pointing to complementary chemical and physical mechanisms of action. Overall, the results demonstrate that *W. circinata* exhibits strong biocontrol potential against *M. oryzae*, likely mediated by a combination of antifungal secondary metabolites and direct mycelial interactions. The findings suggest that *W. circinata* can be considered a potent antagonist of the rice blast fungus and highlight its relevance as a promising and underexplored source of natural products for sustainable management strategies.

Keywords: biocontrol, *Waitea circinata*, *Magnaporthe oryzae*, metabolites, natural products;

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2 Sousa, K. C. I. Pesq. Agropec. Trop., Goiânia, v. 52, e72707, 2022





BIOSURFACTANT PRODUCTION BY *Pseudomonas aeruginosa* USING PALM OIL (*Elaeis guineensis* Jacq.) WASTE AS RAW MATERIAL

Jeovane Barros Silva^{1,3*}, Alan Moura Feio^{2,3}, Antonia Gabriela Brito de Oliveira^{1,3}, Emanuele Pereira Lima³, Giovana Eveli Martins Silva³, Paulo de Souza Jesus^{3,4}, Emilly Cruz da Silva⁵, Sidnei Cerqueira dos Santos^{1,2,3}

jeovanebarros0605@gmail.com; sidnei.cerqueira@unifesspa.edu.br

1-Programa de Pós-Graduação em Química, Universidade Federal do Sul e Sudeste do Pará (PPGQ/Unifesspa), Marabá - PA, Brasil. 2-Programa de Pós-Graduação em Biodiversidade e Biotecnologia (PPG-BIONORTE/Unifesspa), Marabá - PA, Brasil. 3-Laboratório de Bioensaios e Bioprocessos (L@bio/Unifesspa), Marabá - PA, Brasil. 4-Programa de Pós-Graduação em Reprodução Animal na Amazônia, Universidade Federal Rural da Amazônia (ReproAmazon/UFRA), Castanhal - PA, Brasil. 5-Laboratório de Estudos de Materiais para Adsorção e Sensoriamento, Universidade Federal de Roraima (LEMAS/UFRR), Boa Vista - RR, Brasil.

Biosurfactants (BS) are amphiphilic molecules that exhibit surface-active properties comparable to those of synthetic, petroleum-derived surfactants. This study aimed to evaluate the production of rhamnolipid BS by *Pseudomonas aeruginosa* P23G-02, isolated from a gas station tank in the city of Marabá, Pará, using oil palm (*Elaeis guineensis* Jacq.) residues as a raw material. BS production occurred in Erlenmeyer flasks containing Vegetable Saline Medium (VSM), with palm oil residues (sludge, fiber, and a combination thereof) as the sole nutrient source. The flasks were incubated on a shaker for 10 days at 36 °C and 200 rpm. BS were extracted with a chloroform-methanol solvent mixture (3:1, v/v). Rhamnolipid quantification was performed by determining rhamnose using the orcinol method. Surfactant activity was assessed by the emulsification index (%), using mineral oil. The rhamnose dosage of the BS was 0.75 µg/mL with the sludge, 0.63 µg/mL with the fiber and 0.38 µg/mL with the combination of residues, after the application of the correction factor (3.2), the rhamnolipid concentration was 2.40 µg/mL, 2.02 µg/mL and 1.21 µg/mL respectively. The emulsification index of the BS with the sludge was 45%, of the fiber 43% and 40% of the combination. The results demonstrate that palm oil residues are a low-cost alternative source for bacterial production of BS. Thus, the biotechnological applicability of this residue could strengthen the palm oil production chain, reducing the risk of improper disposal and promoting sustainable development and a circular economy in the Amazon region.

Keywords: Biotechnology, bacteria, palm oil, surfactant.





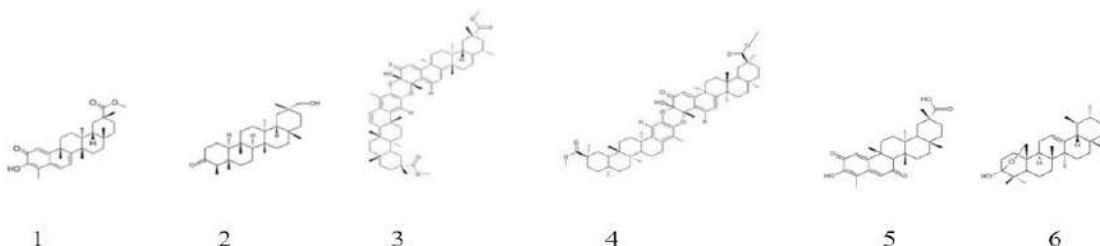
*Phytochemical study of the hexane–ethyl ether extract from the roots of **Salacia grandifolia***

Luiz Carlos de Carvalho Farias,^{1*} Leila Renan Oliveira,¹ Diogo Montes Vidal,¹ Lucienir Pains Duarte,¹ Grasiely Faria de Sousa¹

Luizccf@ufmg.br, grasielysousa@ufmg.br

¹Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brasil.

The Celastraceae family is considered an abundant source of quinonemethide triterpenes, natural compounds associated with various biological activities, such as antiangiogenic, antitumor, antiviral, and anti-inflammatory.¹ This class of compounds is regarded as a chemical marker of the Celastraceae family and is found in the roots. The species *Salacia grandifolia* belongs to the Celastraceae family and can be found in areas of the Atlantic Forest in Brazil. However, there are no records of phytochemical studies on the roots of this species. To isolate chemical constituents from the roots, 1 kg of dried plant material was used. The extract was prepared using a 1:1 mixture of hexane and ethyl ether in a Soxhlet apparatus. During partial solvent removal in a rotary evaporator, an orange solid precipitated and was filtered under vacuum. The supernatant, referred to as EHER (hexane-ether extract from the roots), was used for this study. Successive chromatographic purifications by silica gel column and preparative layer chromatography resulted in the isolation of the following compounds: pristimerin (**1**, 449.0 mg), 3-oxo-29-hydroxyfriedelane (**2**, 7.4 mg), escutinin α A (**3**, 15.9 mg), escutinin α B (**4**, 3.0 mg), dispermoquinone (**5**, 2.0 mg), and a new compound, lantanol (**6**, 4.1 mg). The structures of the compounds were determined by ¹H and ¹³C NMR analyses, in comparison with data available in the literature. The structure of the new compound was elucidated through 2D NMR, including HSQC, HMBC, COSY, and NOESY experiments.



Keywords: Dimeric triterpenoids, Celastraceae, Lantanol

References: ¹ Santos, J. P. dos; Coelho, W. X. O.; Vieira-Filho, S.A.; Pereira, R.C.G.; Sousa, G.F. de; Gouveira, V.A.; Sabino, A. de P.; Evangelista, F.C.G.; Takahashi, J.A.; Moura, M.A.F.; Almeida, F.B.; Duarte, L.P Química Nova, 2020, 43, 558-567.

Acknowledgments: CAPES, CNPq, FAPEMIG





**ENHANCED RECOVERY OF FLAVONOIDS FROM SUGARCANE BAGASSE
USING GREEN EXTRACTION WITH NADES: ANTIOXIDANT BIOACTIVITY IN
*DROSOPHILA MELANOGASTER***

Gabriela Cremasco^{1*}, Mirella Thaisa Ferreira Ranzeti², Luísa de Toledo Tury³, Marina Piacenti-Silva³, Daniel Rinaldo^{1,2}

gabriela.cremasco@unesp.br

1-Greenbiotech network, FC, Unesp, Av. Eng. Luiz Edmundo Carrijo Coube, 14-01, Bauru, SP, Brazil. 2-Chemistry Institute, Unesp, Av. Prof. Francisco Degni, 55, Araquara, Brazil. 3-School of Sciences, Unesp, Av. Eng. Luiz Edmundo Carrijo Coube, 14-01, Bauru, SP, Brazil

Sugarcane is the second-largest agricultural crop worldwide, with Brazil as its principal producer. Despite its significance to the sugar–energy industry, this production chain generates large volumes of solid residues, such as bagasse (250–280 kg per ton). The utilization of this byproduct remains limited, although it is a rich source of flavonoids with well-recognized antioxidant activity. Conventional extraction of these compounds employs toxic solvents, such as methanol, which restricts their application in biological systems and contravenes the principles of green chemistry and the Sustainable Development Goals. In this context, Natural Deep Eutectic Solvents (NADES) have emerged as sustainable, biodegradable, and safe alternatives for the valorization of agroindustrial residues. Ten NADES systems were evaluated for the extraction of flavonoids from sugarcane bagasse using Microwave-Assisted Extraction (MAE) at 50 °C and 60 min, a miniaturized and efficient technique. Extraction yields were evaluated and compared with those obtained using methanol by HPLC-DAD. The bioactivity of the extracts was assessed using *Drosophila melanogaster* *in vivo* model, through survival and locomotor performance assays, parameters associated with the antioxidant response. Among the ten NADES tested, nine demonstrated higher extraction efficiency than methanol, with the choline chloride: lactic acid (CL:LA) (1:1 mol/mol) system proving most promising. In biological assays, the extract obtained with this NADES led to an increased lifespan and enhanced locomotor performance in the flies, whereas the methanolic extract significantly diminished these parameters. The combination of NADES and MAE was effective for the recovery of flavonoids from sugarcane bagasse, yielding superior results compared to methanol both in terms of extraction efficiency and biological activity. . These findings underscore the viability of this approach as a sustainable strategy for valorizing agroindustrial residues, in alignment with global targets for responsible consumption and production. The authors acknowledge financial support from the CNPq, grant #303887/2024-9, and the FAPESP, grant #2025/03036-3 and #2025/14225-1, Brazil.

Keywords: green chemistry, MAE, *in vivo* alternative model, cost-effective bioassay





POTENTIAL OF *DIPTERYX ALATA* (BARU) UNDEREXPLORED PARTS AS RAW MATERIALS FOR COSMETIC INDUSTRY: CHEMICAL AND BIOACTIVE PROPERTIES

Matheus Silva de Barros^{1*}, Jaqueline Alves Barbosa¹, Isadora Gonzaga da Silva², Larissa Silva Costa³, Jessica Cristina Amaral⁴, Philipp Gabor⁵, Lorena Ramos Freitas de Sousa², Patricia S. Lopes³, Maria Fátima das Graças Fernandes da Silva⁴, Alexander Weng⁵, Vanessa Gisele Pasqualotto Severino¹.

barrosmatheus@discente.ufg.br

1- Instituto de Química, Universidade Federal de Goiás, Goiânia, GO, Brazil. 2- Instituto de Química, Universidade Federal de Catalão, Catalão, GO, Brazil. 3- Universidade Federal de São Paulo, Campus Diadema, Diadema, SP, Brazil. 4- Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP, Brazil. 5- Institute of Pharmacy, Freie Universität Berlin, Berlin, Germany.

Dipteryx alata Vogel (Baru), a native tree of the Brazilian Cerrado, is mainly valued for its edible nuts, while other fruit parts remain underexplored despite their promising biotechnological and commercial potential. This study investigated the chemical composition and cosmetic potential of ethanolic extracts from epicarp, mesocarp, endocarp, and nut. Extracts were obtained by maceration and subsequently fractionated by liquid-liquid extraction with solvents of increasing polarity, to afford fractions. The chemical profiles of extracts and fractions were characterized by UHPLC-QTOF-MS/MS. Data were processed with MS-DIAL for feature detection and alignment, and Feature-Based Molecular Networking (FBMN) was carried out on GNPS2 for spectral organization and dereplication. This workflow allowed the annotation of over 30 metabolites, including phenolic acids (gallic, caffeic, ellagic), flavonoids (liquiritigenin, isoliquiritigenin, luteolin, eriodictyol, formononetin), coumarins (umbelliferone, daphnetin, scopoletin, isofraxidin), and hydrolyzable tannins (galloylated compounds), several of which have reported bioactivities relevant to cosmetic applications. Biological assays were selected to evaluate skin-protective and anti-aging properties, including intracellular antioxidant activity (ROS reduction in HaCaT keratinocytes), elastase and tyrosinase inhibition, anti-inflammatory response (IL-6 and TNF- α modulation), cytotoxicity (MTT assay in HaCaT cells, following OECD/GHS criteria), and regenerative potential in 3D keratinocyte spheroids. Extracts exhibited potent intracellular antioxidant activity, particularly in the ethyl acetate fraction of the endocarp. Regarding anti-inflammatory activity, the endocarp extract demonstrated a significant selectivity index (SI = 4.8), indicating selective anti-inflammatory effects. Notably, nut extracts demonstrated remarkable regenerative activity, with up to 28.45% increase in 3D viability. The integration of chemical and biological data suggests that the metabolites annotated in bioactive fractions may underlie the observed antioxidant and anti-inflammatory effects. Overall, the underexplored fruit parts of *D. alata* represent a rich chemical space associated with relevant bioactivities, supporting their potential as sustainable cosmetic ingredients and contributing to the valorization of Cerrado biodiversity.

Keywords: *Dipteryx alata*; MS-DIAL; GNPS2; flavonoids; coumarins; antioxidant; elastase; cosmetics.

Reference: UNITED NATIONS. GHS. 9th rev. ed. New York; Geneva: United Nations, 2021.





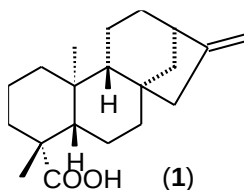
XYLOPIA POLYANTHA R. E. FRIES (ANNONACEAE): A NEW NATURAL SOURCE OF ENT-KAURANE DITERPENES

Karollen da Gama Serrão^{1,*} and Emmanoel Vilaça Costa¹

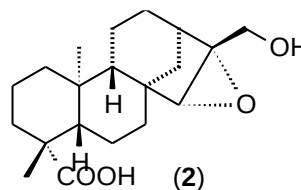
* karollen.serrao@ufam.edu.br / evc@ufam.edu.br

1. GEQBiom, Programa de Pós-Graduação em Química, ICE, Universidade Federal do Amazonas, Av. General Rodrigo Octavio Jordão, 6200, Manaus, AM, Brazil.

Xylopia polyantha R. E. Fries (Annonaceae), commonly known as “pindaíba” and “embira,” is a tree species endemic to Brazil, occurring in the Amazon phytogeographic domain, particularly in terra firme forests. Its distribution extends across the North and Central-West regions of the country. According to the literature, no phytochemical studies have been reported for *X. polyantha*, making this an unprecedented investigation. The hexane extract of the bark of *X. polyantha*, obtained by maceration (room-temperature extraction), was subjected to classical chromatographic techniques (CC, CCDA, and CCDP), resulting in the isolation and identification of two compounds belonging to the *ent*-kaurane diterpene class, identified as kaurenoic acid and 15 β ,16 β -epoxy-17-hydroxy-*ent*-kaurane-19-oic acid. The presence of kaurenoic acid is remarkable in this species, accounting for approximately 50% of the hexane extract. Structural elucidation was performed through 1D/2D ¹H and ¹³C NMR experiments, along with comparisons with data previously reported in the literature. Although both diterpenes are already known, this is the first report of their occurrence in *X. polyantha*. The high concentration of kaurenoic acid in the bark of this species highlights *X. polyantha* as a new and significant natural source of this diterpene, reinforcing the importance of the genus *Xylopia* within the Annonaceae family as a reservoir of bioactive metabolites. Moreover, this study contributes to chemosystematic knowledge, considering that kaurenoic acid has been recognized as a chemical marker present in nearly all investigated species of *Xylopia*. Research on this species is still ongoing; however, the preliminary results described herein not only expand the chemical and chemophenetic knowledge of the genus but also provide a basis for future studies, including the biological evaluation of these diterpenes and their potential pharmacological applications.



(1)



(2)

Keywords: *Xylopia polyantha*; Annonaceae; *ent*-kaurane diterpenes; kaurenoic acid.

Acknowledgments: CAPES, CNPq, FAPEAM, UFAM, Pró-Amazônia/CNPq Processo N° 445615/2024-9, and CA/CAM/UFAM.





PHYTOCHEMICAL CHARACTERIZATION OF ZIZIPHUS (RHAMNACEAE) SPECIES AND THE ISOLATION OF METABOLITES BY COUNTERCURRENT CHROMATOGRAPHY (CCC)

Felipe Costa Cardoso^{1*}, Wallace Rodrigo de Jesus Barbosa^{1,2}, Fernanda das Neves Costa¹, Roberto Carlos Campos Martins¹

felipecardoso@ufri.br

1-Walter Mors Institute of Research on Natural Products (IPPN), UFRJ, RJ, Brazil. 2- Federal Institute of Education, Science and Technology of Rio de Janeiro (IFRJ) campus Nilópolis, RJ, Brazil.

The genus *Ziziphus* (Rhamnaceae) is a promising source of bioactive secondary metabolites, particularly cyclopeptide alkaloids, which exhibit several pharmacological activities, including the potential to inhibit enzymes like α -glucosidase, a key therapeutic target in diabetes management (1). This work focused on the phytochemical study of the Brazilian native species *Ziziphus joazeiro* and *Ziziphus undulata*, employing chromatographic techniques to isolate their chemical constituents, and evaluate their biological activities. Ethanolic extracts were prepared from the leaves and twigs of *Z. joazeiro* and *Z. undulata*. The crude extracts were subjected to liquid-liquid partitioning and fractionation by Countercurrent Chromatography (CCC), a support-free liquid-liquid partition technique. Biphasic (BPSS) and triphasic solvent systems (TPSS) were used to optimize the separation. Additionally, an acid-base extraction was performed to obtain alkaloid-enriched fractions. The phytochemical profile of the samples was monitored by Thin-Layer Chromatography (TLC) using specific spray reagents. The TLC analysis confirmed the presence of several classes of metabolites, including flavonoids, terpenoids, and alkaloids, in the extracts and fractions. The fractionation of the crude ethanolic extract from *Z. joazeiro* leaves (ELZJ) by CCC using the BPSS HEMWat (6:1:6:1, v/v/v/v) proved to be particularly effective, allowing for the direct isolation of a major compound, which was identified as methyl pheophorbide A (MPhA) by spectroscopic analysis by ¹H NMR (2). This study validated CCC as a practical tool for the fractionation of *Ziziphus* extracts, enabling the isolation of MPA in a single chromatographic step. The identification of diverse metabolic classes reinforces the pharmacological potential of the genus and establishes a foundation for further investigation. Future steps will include the application of TPSS and the use of molecular networking for dereplication and characterization of new compounds. Biological assays will be conducted to assess the therapeutic potential of the isolated substances.

(1) EL MAIDEN, E. *et al.* J. Ethnopharmacol, 259, 112950, 2020.

(2) HA, J. Y. *et al.* Appl. Biol. Chem., 65, 1, 52, 2022.

Keywords: *Ziziphus*, Countercurrent chromatography, α -glucosidase





EFFECT OF *Desmodium heterophyllum* AQUEOUS EXTRACT COMBINED WITH PHOTOBIOMODULATION THERAPY IN A MODEL OF ACUTE INFLAMMATION

Tássio Malber de Oliveira^{1*}, Roberta Maria Abrão², Luiz Gustavo Vilela Filho², Brendha Sena Costa², Gracimério José Guarneire², Nerilson Marques Lima², Sandra Bertelli Ribeiro de Castro², Caio César de Souza Alves³, Murilo Xavier Oliveira³, Alessandra de Paula Carli³

tassio.malber@ufvjm.edu.br

1-LAP, Departamento de Medicina, Fammuc, UFVJM, Rua. Do Cruzeiro, 01, Teófilo Otoni, Minas Gerais, Brazil. Universidade dos Vales do Jequitinhonha e Mucuri, Campus Mucuri, 39803-371.

Species of the genus *Desmodium* have bioactive compounds with anti-inflammatory and immunomodulatory properties. Photobiomodulation therapy (PBMT) has been attracting attention as a non-invasive alternative for modulating inflammatory processes. However, there are no studies evaluating the combination of these approaches. Therefore, we investigated the immunomodulatory potential of *Desmodium heterophyllum* aqueous extract combined with PBMT in an experimental model of acute inflammation. The study aimed to evaluate the immunomodulatory effects of *D. heterophyllum* aqueous extract, alone and in combination with PBMT, in a model of carrageenan-induced paw edema in mice, analyzing cell viability, nitric oxide production, and inflammatory cytokine profile. To this end, the species was collected, identified, and processed to obtain the aqueous extract, which was subsequently characterized by high-performance liquid chromatography (HPLC) and mass spectrometry. *In vitro* assays were conducted with J774A.1 and RAW 264.7 macrophages, evaluating cytotoxicity (MTT) and NO production (Griess). For *in vivo* assays, BALB/c mice were divided into groups and treated with the extract at different concentrations (50, 125, and 250 mg/kg), TFBM (780 nm), or a combination. Edema was induced with carrageenan (2.5%) and monitored for 4 hours. Cytokines (IL-1 β , TNF- α , IL-6, IFN- γ) were quantified by ELISA from tissue macerates. The extract presented a phytochemical profile rich in flavonoids, isoflavonoids, simple phenols, and saponins. *In vitro* cell assays demonstrated low cytotoxicity (>90% viability) and significant inhibition of NO production. In an animal model, a dose of 50 mg/kg reduced edema comparably to dexamethasone. TFBM alone also significantly reduced inflammation. The combination of the extract (250 mg/kg) with TFBM promoted edema reduction from the first hour, similar to dexamethasone. There was a significant decrease in TNF- α and IL-6 in treated groups, indicating modulation of the inflammatory response. This is the first time a study has evaluated the aqueous extract of *D. heterophyllum* combined with TFBM, demonstrating a promising and safe immunomodulatory effect. The combination showed innovative therapeutic potential, reinforcing the integration of phytotherapy and photobiomodulation as a relevant alternative for the control of acute inflammatory processes.

Keywords: *Desmodium heterophyllum*; photobiomodulation therapy; acute inflammation; phytotherapy.





COMPARATIVE EXTRACTION OF COSTIC ACID FROM *Nectandra barbellata* - CONVENTIONAL vs. SUPERCRITICAL CO₂ METHODS

Emmanuele Di Fabio^{1*}, Dalete C. S. Souza¹, Marina G. Monroe¹, Roberto B. P. Almeida², Priscila C. Veggi³, Juliana M. Prado⁴, João Henrique G. Lago¹, Bruno G. da Silva¹.

e.fabio@ufabc.edu.br

1-Center for Natural and Human Sciences, Federal University of the ABC, Santo André 09210-170, SP, Brazil.

2- Institute of Biosciences, University of São Paulo, São Paulo 05508-090, SP, Brazil. 3- Department of Chemical Engineering, Institute of Environmental, Chemical and Pharmaceutical Sciences, Federal University of São Paulo, Diadema 09913-030, SP, Brazil. 4- Engineering Modeling and Applied Social Sciences Center, Federal University of ABC, Santo André 09210-580, SP, Brazil.

In alignment with the guidelines that regulate the limits of residual organic solvents in pharmaceutical products (ICH Q3C)¹, this study evaluated the environmentally friendly approach of supercritical CO₂ for the extraction of costic acid, a promising antiparasitic - against the protozoal *Trypanosoma cruzi* - sesquiterpene from *Nectandra barbellata* (Lauraceae)², comparing it to the conventional maceration technique. In the maceration process, 16 g of dried plant material were extracted with 50 mL of solvent (hexane or EtOH) in six successive steps. For supercritical extraction, the conditions of 47.5 °C and 35 MPa were selected based on prior experimental design. After solvents removal under vacuum, the total yield and the costic acid content, quantified by HPLC-DAD, were determined. The results are summarized in Table 1. Supercritical fluid extraction (SFE) exhibited better selectivity, achieving the highest concentration of costic acid in the extracts (450 mg/g). Its productivity was markedly superior to conventional extraction methods, reflecting enhanced process efficiency. This superior performance, combined with reduced use of organic solvents, aligns SFE with green chemistry principles and supports more efficient, sustainable, and environmentally friendly processes to obtain this bioactive compound.

Table 1: Comparison among the yield and costic acid content of *N. barbellata* aerials parts extracts obtained by SFE and maceration techniques.

Extraction method	Yield (% d.b.)	CAC (mg/g extract)	CAC (mg/g RM d.b.)	Time (h)	Productivity (g h ⁻¹)
SFE	4.0 ± 0.2	450	18.01	0.8	0.4655
HEX	5.2 ± 0.2	358	18.71	240	0.0034
EtOH	12.2 ± 0.4	318	38.84	240	0.0078

RM raw material, CAC costic acid content, SFE extract obtained using supercritical fluid extraction, HEX extract obtained using hexane (maceration), EtOH extract obtained using ethanol (maceration), d.b. dry basis.

Keywords: Supercritical fluid extraction, costic acid quantification, green chemistry, sustainable extraction methods.

References: ¹ICH Q3C(R9), 2024. ²Londero, V. S. et al., *Bioorganic Chemistry*, **2019**, 95, 103510.

Acknowledgments: CAPES, CNPq, FAPESP.





BIOACTIVE FRACTIONS FROM SYAGRUS CORONATA FIXED OIL SELECTIVELY INHIBIT THE GROWTH OF COLORECTAL CANCER CELLS

Joyce Bezerra Guedes^{1*}, Andreza Larissa do Nascimento¹, Danieli Cristina Gonçalves¹, Débora Munhoz Rodrigues¹, Marcos Guilherme da Cunha¹, Beatriz Pelegrine Bosque¹, Maria Tereza dos Santos Correia², Rafael de Felício¹, Márcia Vanusa da Silva², Daniela Barretto Barbosa Trivella¹

joyce.guedes@lnbio.cnpem.br

1-National Laboratory of Biosciences, National Center for Research in Energy and Materials, Rua Giuseppe Maximo Scolfaro, 10000, Campinas, SP, Brazil.

2-Department of Biochemistry, UFPE, Av. Prof. Moraes Rêgo, S/N, Recife, PE, Brazil.

Syagrus coronata is a palm tree native to the Caatinga biome, belonging to the Arecaceae family, with significant socioeconomic and ecological relevance in the Brazilian semiarid region. Fixed oils extracted from plant seeds, such as those of *S. coronata*, stand out as promising sources of bioactive compounds, rich in fatty acids often associated with pharmacological activities, including anti-inflammatory and anticancer effects. Therefore, the objective of this study was to characterize and potentially isolate bioactive compounds from the fixed oil of *S. coronata* with anticancer activity against HCT-116 cells (colorectal cancer). The oil was supplied by the Cooperativa da Região do Piemonte da Diamantina (COOPES), in Capim Grosso, Bahia, Brazil. The sample was subjected to hydroalcoholic partitioning (methanol/water 8:2) to extract polar compounds. Approximately 5.5 g of the hydroalcoholic fraction was fractionated by silica gel column chromatography (normal phase) using a gradient of increasing polarity of organic solvents. The obtained fractions were grouped according to similar chemical profiles (monitored by TLC) and analyzed by liquid chromatography using an Acquity HClass UPLC system (Waters), equipped with a C18 BEH column (1.7 μ m). After separation, the analytes were subjected to tandem mass spectrometry (uhr-ESI-QqTOF Impact II, Bruker), in positive and negative ionization modes. In total, 12 chemically diverse fractions were obtained. Cytotoxicity assays were performed on HaCaT (non-tumorigenic) and HCT-116 (colorectal cancer) cell lines, using nuclear staining and High-Content Screening (HCS). Cells were stained with Hoechst 33342 and analyzed using the Operetta® system. Three fractions showed selective antiproliferative activity ($IC_{50} < 10 \mu$ g/mL; selectivity index > 4). UPLC-MS/MS analyses revealed complex chromatographic profiles in the active fractions, which are currently undergoing dereplication and structural characterization. To date, the study has yielded promising results, indicating that Licuri oil may contain bioactive compounds that could contribute to improving its production chain and enhancing the value of its extraction process.

Keywords: Caatinga, *Syagrus coronata*, cancer, chemical profile, cytotoxicity





Phytochemical Study of the Chloroform Extract from the Roots of Salacia grandifolia

Alika R. S. Brito^{1*}, Leila R. Oliveira¹, Diogo M. Vidal¹, Lucienir P. Duarte¹, Grasiely F. de Sousa¹

*alikarafaelad@gmail.com, grasielysousa@ufmg.br

¹Departamento de Química, ICEx, UFMG - Av. Pres. Antônio Carlos 6627, Pampulha, Belo Horizonte, MG

Among the diverse botanical families studied, the Celastraceae family stands out due to its rich variety of phytoconstituents with potential biological activities, such as antitumor, antiviral, and anti-inflammatory.¹ Quinonemethide triterpenes are among the chemical markers found in the roots of these plants,² as exemplified by the species *Salacia grandifolia*, which is present in areas of the Atlantic Forest in Brazil. However, there is a notable absence of documented phytochemical research on the roots of *Salacia grandifolia*. Therefore, this study aimed to isolate the phytoconstituents present in 1 kg of dry *Salacia grandifolia* roots. The plant material was subjected to maceration in chloroform, remaining immersed in the solvent at room temperature for 5 days. After each maceration period, simple filtration was performed, followed by solvent removal using a rotary evaporator. This cycle was repeated five times with the same plant material. The extracts were then grouped and designated as ECI (chloroform extract of the roots). Numerous purification steps by column chromatography led to the isolation of Pristimerin (40.3 mg) and Ursan-12-en-3-ol (α -amyrin, 3 mg). Identification of the isolated compounds was performed using Nuclear Magnetic Resonance (NMR) spectroscopy (¹H, ¹³C, and DEPT-135) and comparison with literature data.

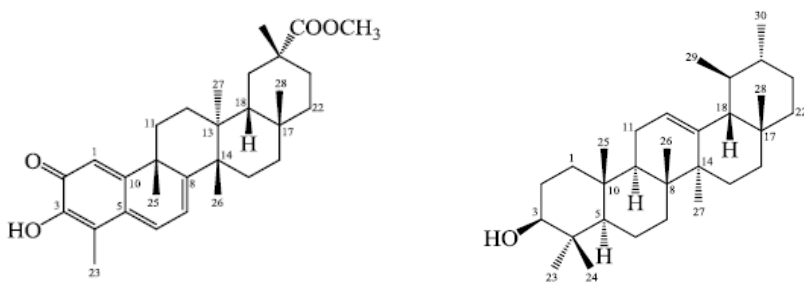


Figure 1: Pristimerin and ursan-12-en-3-ol

Keywords: Phytochemistry, Celastraceae, quinonemethide triterpene

References: ¹Camargo, K. C. et al. *Molecules* 2022, 27, 3. ²Jiang, H., et al. *Autophagy* 2024, 20, 7.

Acknowledgments: CAPES, CNPQ, FAPEMIG.





Isolation and Characterization of Flavonoids from *Maytenus quadrangulata*

Marcos L. D. de Souza^{1*}, Luiz C. de C. Farias¹, Mariana G. Aguilar¹, Grasiely F. de Sousa¹, Lucienir P. Duarte^{1*}

mldias1850@gmail.com; lucienir@gmail.com

1-NEPLAM, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Plant-derived natural products remain fundamental pillars in the discovery and development of new therapeutic agents, particularly in the current context of combating emerging viral diseases, which pose significant challenges to global public health. The genus *Maytenus* (Celastraceae) is recognized for its pharmacological relevance, with species exhibiting anti-inflammatory, antioxidant, and antiviral activities. *Maytenus quadrangulata*, in particular, has demonstrated potential against emerging arboviruses such as Zika and Mayaro. Previous studies isolated two bioactive flavonoids from the ethyl acetate leaf extract: 4'-O-methylepigallocatechin (**1**) and (-)-4'-O-methylepicatechin 5-O- β -D-glucopyranoside (**2**), the latter being reported for the first time in the literature, but only in insufficient quantities for adequate antiviral evaluation.¹ This work aimed to overcome this limitation by re-investigating the ethyl acetate extract and its constituents. Collected leaves were air-dried, ground, and subjected to exhaustive extraction with hexane, chloroform, ethyl acetate, and methanol. During concentration of the ethyl acetate extract, a precipitate (1.1 g) was formed, and the filtrate yielded the remaining crude extract (19.6 g). The precipitate was subjected to column chromatography on silica gel using a chloroform-methanol gradient. Fractions with similar profiles on thin-layer chromatography (TLC) were pooled and further purified using preparative chromatographic techniques. After purification, TLC analysis allowed the identification of compounds **1** and **2**, whose structures were confirmed by ¹H and ¹³C NMR in comparison with literature data. From the precipitate of the ethyl acetate extract, 3.3 mg of compound **1** and 9.2 mg of compound **2** were isolated. Despite these low yields, analysis of the remaining crude extract (19.6 g) indicated a substantial presence of both flavonoids, enabling their isolation in larger quantities. Future perspectives include: (i) fractionation of the crude extract to obtain additional quantities; (ii) evaluation of antiviral activity against Zika and Mayaro. These findings reinforce the potential of *M. quadrangulata* as a source of antiviral agents and highlight the importance of integrated approaches in natural products to address public health challenges.

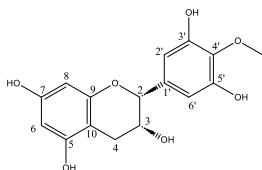


Figura 1: 4'-O-metilepigallocatequina

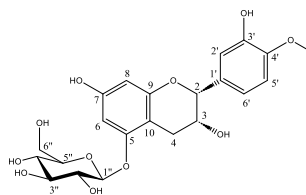


Figura 2: (-)-4'-O-metilepicatequina 5-O- β -D-glicopiranosídeo

Keywords: *Maytenus quadrangulata*, flavonoids, natural products, Celastraceae.

References: 1. Aguilar, M.G. et al. *Chemistry & Biodiversity*. 2024, 21, e202400636.

Acknowledgments: CAPES, CNPQ, FAPEMIG.





BIOTRANSFORMATION OF 6]-GINGEROL BY *Curvularia asianensis*

Beatriz Araujo L. Oliveira^{1*}, Fátima Miranda Nunes², Mariana da Cruz Passos¹, Rafael Ciro Marques Cavalcante¹, James Almada da Silva¹, Natália Nogueira Saraiva¹.

bia.oliveira010@gmail.com

1-, Departamento de Farmácia, Universidade Federal de Sergipe – Campus Lagarto, Av. Gov. Marcelo Déda, 13 - São José, Lagarto – SE, Brazil. 2- LABS, Departamento de química, Universidade Federal do Ceará, Av. Humberto Monte - Pici, Fortaleza - CE, Brazil.

[6]-Gingerol, the main phenolic compound of *Zingiber officinale*, exhibits several biological activities, such as antioxidant, anti-inflammatory, antimicrobial, cytotoxic, and gastroprotective effects. The chemical modification of this natural metabolite can enhance its pharmacological properties and open new possibilities for therapeutic applications. In this context, biotransformation using whole intact cells offers advantages over classical chemical synthesis: higher selectivity (chemo-, regio-, and enantioselectivity), reactions under mild temperature and pressure conditions, a wide diversity of reaction targets, and the generation of high value-added products. Endophytic fungi, such as the genus *Curvularia*, display great enzymatic potential with applications in bioenergy, bioremediation, and the synthesis of bioactive compounds. However, studies involving *Curvularia asianensis* and this substrate are still scarce. Therefore, the aim of this study was to evaluate the potential of *C. asianensis* as a biocatalyst agent on (5S)-5-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-decanone ([6]-gingerol) transformation. The substrate was isolated from *Zingiber officinale* rhizomes by classical liquid chromatography. Biotransformation experiments were carried out (in triplicate) for 7, 8, and 9 days, in Potato-Dextrose broth medium, under agitation (112 rpm), and the substrate at 0.5 mg/mL. Reaction products were extracted with EtOAc and analyzed by HPLC and ¹H NMR. Chromatographic analyses indicated that [6]-gingerol was consumed and that different products were formed. The ¹H NMR spectrum revealed the occurrence of at least three oxidative reactions. The disappearance of a singlet (δ 3.82 ppm), attributed to the methoxy group, indicates an O-demethylation reaction, while the disappearance of the quintuplet (δ 3.99 ppm), corresponding to the oxymethine hydrogen, suggests a reduction reaction and possible formation of paradol. The appearance of doublets at 1.14 and 0.99 ppm suggests an oxidation reaction in the aliphatic chain, specifically at the omega-1 carbon. Furthermore, new signals in the aromatic region suggest that the ring also underwent modifications. [6]-gingerol underwent different biotransformation reactions, mainly catalyzed by oxidoreductases.

Keywords: Biotransformation; Ginger; Gingerols, Endophytic fungi.





Diterpenoids from *Pinus cembra* isolated by HPLCC and HSCCC assisted by APCI-MS profiling

Matheus L. Silva^{1*}, Mohammad Al Ktifan, Pedro H. J. Batista¹, João H. G. Lago² and Gerold Jerz³

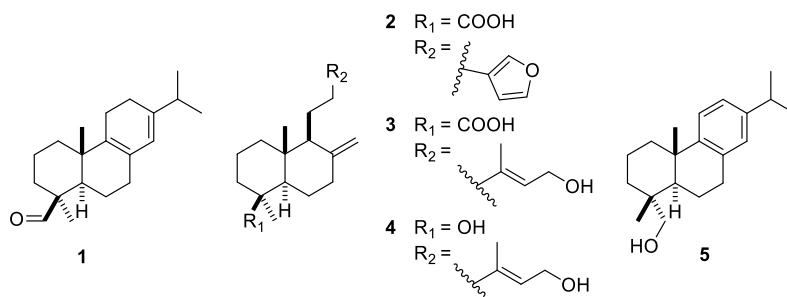
*matheus.silva@inpa.gov.br

¹Instituto Nacional de Pesquisas da Amazônia, 69060-001, Manaus, AM, Brazil.

²Universidade Federal do ABC, 09280-560, Santo André, SP, Brazil.

³Institute for Food Chemistry, Technische Universität Braunschweig, 38106 Braunschweig, Germany.

Pinus cembra, commonly known as Swiss stone pine, is an emblematic alpine conifer with ecological importance and a rich repertoire of secondary metabolites. While its seeds and essential oils are well documented, the chemical profile of cone scales has remained largely unexplored. In this work, air-dried cone scales (675 g) were extracted with *n*-hexane and yielded 8 g of crude extract. 650 mg of the hexane extract was fractionated using reversed-phase High-Performance Countercurrent Chromatography (HPCCC) with a *n*-hexane/ACN (1:1, v/v). 2 g of the same hexane extract was also fractionated with reversed-phase High-Speed Countercurrent Chromatography (HSCCC) with *n*-hexane/ACN/TBME (46:46:6, v/v/v). APCI-MS off-line injection profiling of HSCCC fractions enabled targeted tracking of diterpenoid-rich zones, improving fraction selection and structural assignment [1]. Subsequent purification by silica gel and RP-18 column chromatography afforded subfractions of high purity. Structure elucidation was carried out using NMR spectroscopy in combination with APCI-MS/MS fragmentation patterns. This workflow led to the isolation of five abietane diterpenoids: palustral (**1**), lambertianic acid (**2**), isocupressic acid (**3**), agathadiol (**4**), and 4-*epi*-dehydroabietol (**5**). This is the first time ¹³C NMR and MS data for palustral (**1**) shall be published. The findings not only contribute to chemophenetic understanding of *Pinus* genus but also open perspectives for potential bioactivity investigation from the isolated compounds.



Keywords: *Pinus cembra*, diterpenes, countercurrent chromatography, APCI-MS profiling, palustral

[1] Präßler *et al.*, *J. Chromatogr. A*, 2025





CHARACTERIZATION OF SECONDARY METABOLITES IN ETHANOLIC EXTRACTS AND HYDROSOLS OF *Piper tuberculatum* FROM THE ALTO SAN JUAN BIOLOGICAL CORRIDOR, RISARALDA, COLOMBIA

Oscar Marino Mosquera Martínez^{1*}, Gustavo Alfonso Cifuentes Colorado^{1*}, Jaime Alejandro Martínez Acosta¹, Juan David Yarce Botero¹

*omosquer@utp.edu.co, *gustavo.cifuentes@utp.edu.co

1-Grupo de Investigación Biotecnología-Productos Naturales, Escuela de Química, Facultad de Tecnología, Universidad Tecnológica de Pereira, Carrera 27 # 10-02, Barrio Álamos, Pereira-Risaralda, Colombia.

The biodiversity of the Alto San Juan biological corridor provides essential ecosystem services for the subsistence of Afro-descendant communities, whose plant resources are currently threatened by improper use and climate change. Bioprospecting emerges as a strategy for the conservation and valuation of these plant resources. This work aimed to phytochemically characterize and evaluate the antioxidant potential of the ethanolic extracts of leaves and stems and the hydrosol of *Piper tuberculatum* (Piperaceae). This species was selected participatively with community members for its use in traditional medicine. The main groups of secondary metabolites in ethanolic extract were identified by thin-layer chromatography (TLC). The antioxidant capacity was determined by three assays: DPPH radical scavenging, Total Antioxidant Capacity (TAC), and Oxygen Radical Absorbance Capacity (ORAC). The hydrosol was obtained by hydrodistillation, extracting the volatile compounds by headspace solid-phase microextraction (HS-SPME) followed by analysis by gas chromatography-mass spectrometry (GC-MS). The species *Piper tuberculatum* revealed the presence of **alkaloids, tannins, phenols, flavonoids, coumarins, anthraquinones, sterols, terpenes, saponins and triterpenes**. In the antioxidant evaluations, the ethanolic extract presented the following results: 35.8 ± 4.7 ($\mu\text{mol Trolox g extract}^{-1}$) for DPPH, a value of 105.9 ± 3.8 (mg GAE g extract⁻¹) for TAC, and 2131.9 ± 161.2 ($\mu\text{mol Trolox g extract}^{-1}$) for ORAC. The data obtained for the hydrosol were analyzed using molecular networking on the Global Natural Products Social Molecular Networking (GNPS) platform, where different molecular families such as **monoterpenes** and **sesquiterpenes** were grouped. The results highlight a wide variety of secondary metabolites and the bioactive potential of *Piper tuberculatum* as a promising source of natural antioxidants.

Keywords: antioxidant activity, phytochemical profile, bioprospecting, secondary metabolites, HS-SPME-GC-MS.





NIR SPECTROSCOPY FOR EFFICIENT SCREENING OF BIOACTIVE COMPOUNDS IN SORGHUM

Maria Lúcia Ferreira Simeone^{1*}, Valéria Aparecida Vieira Queiroz¹, Rafael de Araújo Miguel¹, Thaís Fernanda Silva², Emilly Rodrigues De Souza Santos², Cícero Beserra de Menezes¹, Maria Marta Pastina¹
marialucia.simeone@embrapa.br

1-Embrapa Milho e Sorgo, Rod MG 424, Sete Lagoas, MG, 35701-970, Brazil.

3- Universidade Federal de São João Del Rei, Campus Sete Lagoas, Minas Gerais, Brazil.

In recent years, there has been a growing interest in using sorghum for human consumption, mainly due to the demand for healthier, gluten-free foods with greater nutritional value. In addition, sorghum is a source of bioactive compounds with antioxidants, immunomodulatory, anti-inflammatory, and antimicrobial properties. The chemical characteristics of bioactive compounds become critical for human nutrition purposes, which influence their bioavailability and differ among sorghum genotypes. The reported high phenolic levels in sorghum have led to interest from sorghum breeding programs in developing and identifying germplasms with high phenolic levels, which requires screening many samples to find those with the highest levels. Since wet chemistry screening methods are slow, expensive, and destructive, the use of near-infrared (NIR) spectroscopy calibration models could be an alternative. The objective of this study was to develop NIR models for total phenols, condensed tannins, antioxidant activity, and total anthocyanin levels in a diverse set of ground grains of the 240 sorghum genotypes, and to assess the predictive value of NIR models to estimate these compounds in sorghum. A calibration model was developed using (NIRFlex 500, Buchi) (1,000 to 2,500 nm) and a chemometrics approach. Each compound estimated using NIR models was validated using an independent validation set. Calibration models correlations for total phenols, condensed tannins, antioxidant activity, and total anthocyanins were $R^2 = 0.91$, 0.84 , 0.84 , and 0.82 , respectively. Correlations between NIR-predicted values and reference values in the validation set were significant for total phenols ($R^2 = 0.90$), condensed tannins ($R^2 = 0.83$), antioxidant activity ($R^2 = 0.82$), and total anthocyanins ($R^2 = 0.80$). They indicated that sufficient variation for these compounds existed within sorghum and that NIR calibration models could be used to rapidly and non-destructively predict total phenols, condensed tannins, antioxidant activity, and total anthocyanins concentrations in ground grain sorghum.

Acknowledgments

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Keywords: *Sorghum bicolor*, functional foods, chemometrics, near-infrared, chemometrics





PHYTOCHEMICAL PROFILE AND EVALUATION OF THE ANTIOXIDANT POTENTIAL OF THE PLANT SPECIES *Lippia alba*, *Petiveria alliacea* Linn, AND *Eryngium foetidum* FROM THE ALTO SAN JUAN BIOLOGICAL CORRIDOR, RISARALDA, COLOMBIA

Gustavo Alfonso Cifuentes Colorado^{1*}, Oscar Marino Mosquera Martínez^{1*}, Jaime Alejandro Martínez Acosta¹, Juan David Yarce Botero¹

*Gustavo.cifuentes@utp.edu.co, *omosquer@utp.edu.co

1-Grupo de Investigación Biotecnología-Productos Naturales, Escuela de Química, Facultad de Tecnología, Universidad Tecnológica de Pereira, Carrera 27 # 10-02, Barrio Álamos, Pereira-Risaralda, Colombia.

Bioprospecting is presented as a key strategy to conserve and value the plant resources of the Alto San Juan biological corridor, which are vital for the subsistence of Afro-descendant communities and are threatened by misuse and climate change. This work aimed to characterize the phytochemical profile and evaluate the antioxidant potential of the ethanolic extracts of leaves and stems of *Lippia alba* (*Verbenaceae*), *Petiveria alliacea* Linn (*Petiveriaceae*), and *Eryngium foetidum* (*Apiaceae*), three species selected participatively with the communities for their use in traditional medicine. Se identificaron principales grupos de metabolitos secundarios por cromatografía de capa delgada (TLC). The main groups of secondary metabolites were identified by thin-layer chromatography (TLC). The antioxidant capacity was determined by three assays: DPPH radical scavenging, Total Antioxidant Capacity (TAC), and Oxygen Radical Absorbance Capacity (ORAC). In all three species, **tannins, phenols, anthraquinones, sterols, terpenes, saponins, and triterpenes** were detected. The presence of **flavonoids** in *Petiveria alliacea* Linn is highlighted. The ethanolic extract of *Lippia alba* showed a TAC value of 144.22 ± 2.8 (mg GAE g extract⁻¹), an activity 49% and 41% higher compared to the ethanolic extracts of *Petiveria alliacea* Linn and *Eryngium foetidum*, respectively. In the ORAC assay, the ethanolic extract of *Lippia alba* presented a value of 1772.2 ± 196.9 (μmol Trolox g extract⁻¹), this being 70% and 38% higher compared to the ethanolic extracts of *Petiveria alliacea* Linn and *Eryngium foetidum*, respectively. On the other hand, the three extracts show values close to 100 ± 10 (μmol Trolox g extract⁻¹) in the DPPH assay. The results highlight a high diversity of secondary metabolites and the bioactive potential of these plant species, positioning *Lippia alba* as a promising source of natural antioxidants.

Keywords: antioxidant activity, phytochemical screening, bioprospecting, secondary metabolites.





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FLAVONOID PROFILING OF CITRUS PEELS BY DART-HRMS

Yasmin Cunha da Silva^{1*}, Monica Costa Padilha², Valdir Florêncio Veiga-Junior¹

*ycunhasilva@gmail.com

¹Chemical Engineering Section, Military Institute of Engineering, Rio de Janeiro, RJ 22290-270, Brazil;

²Brazilian Doping Control Laboratory, Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, RJ 21941-909, Brazil.

Citrus fruits rank among the most widely cultivated and consumed fruits worldwide. Brazil stands out as one of the leading producers, not only in cultivation but also in the processing industry. As a result, millions of tons of waste are generated annually, contributing to potential environmental impacts. However, this by-product represents a valuable source of bioactive metabolites, particularly flavonoids and limonoids. Direct analysis of these raw materials, without the need for sample preparation, is crucial for obtaining a comprehensive and reliable characterization of the chemical profile of natural products. The aim of this study was to analyze the flavonoid composition of fresh peels from different citrus fruits using the DART-HRMS technique. The outer peels of various citrus fruits (lemons, oranges, and tangerines) were cut into pieces measuring 0.5 cm in width × 2.0 cm in height, placed on a QuickStrip® support, and subsequently analyzed by DART-HRMS. Samples were examined in both ionization modes (positive and negative) within the 70–1050 Da range. Mass spectra were processed using Xcalibur software, version 4.2 (Thermo Fisher Scientific), and interpreted based on comparison with literature data. Through the targeted analysis, both methoxylated and glycosylated flavonoids were identified across the different samples, compounds that are well-documented as characteristic of citrus fruits. Among the detected metabolites, ions corresponding to nobiletin (m/z 403.1400), tangeretin (m/z 373.1278), heptamethoxyflavone (m/z 433.1487), naringin/narirutin (m/z 581.1853), eriocitrin (m/z 597.1778), and hesperidin (m/z 611.1856) were observed. These findings demonstrate that DART-HRMS is an effective tool for the direct detection of metabolites in raw plant material, including those previously described in citrus extracts. The method is rapid, solvent-free, requires only a small amount of sample, and can be extended to the analysis of other natural products.

Keywords: Citrus, DART-HRMS, glycosylated flavonoids, and methoxylated flavonoid.



Sociedade Brasileira de Química
Divisão de Produtos Naturais





***EVALUATION OF THE PROBIOTIC POTENTIAL OF MICROORGANISMS
ISOLATED FROM COASTAL ECOSYSTEMS OF RIO GRANDE DO SUL, BRAZIL***

Rafaela Conceição de Souza^{1*}, Leidy Johana García Maza^{1,2}, Alexandre José Macedo^{1,2}

rafaela.csouzaedu@gmail.com

1- Centro de Biotecnologia, Universidade Federal do Rio Grande do Sul (UFRGS), Porto Alegre, RS, Brasil. 2- Faculdade de Farmácia, Universidade Federal do Rio Grande do Sul (UFRGS), Porto Alegre, RS, Brasil.

Scientific interest in probiotics has increased due to their role in maintaining human health and preventing various diseases. Initially associated only with intestinal balance, their effects are now recognized in metabolic, immunological, and allergic disorders (Yadav et al., 2019). Although *Lactobacillus* and *Bifidobacterium* species are widely used, they exhibit limitations such as low resistance to gastrointestinal conditions, reduced colonization capacity, and variable efficacy. These drawbacks highlight the need for novel and diverse natural probiotic sources, driving the development of next-generation probiotics. Marine ecosystems represent promising alternatives, harboring unique, underexplored microbial diversity and serving as reservoirs of bioactive molecules with biotechnological potential. This study aimed to prospect and characterize environmental microorganisms from marine ecosystems on the coast of Rio Grande do Sul, Brazil, as potential next-generation pre/probiotics. A total of 116 strains were isolated, and 10 candidates (3a, 6a, 12a, 13a, 15a, 24a, 30a, 48a, 51a, 90a) were selected for 16S rRNA sequencing to identify promising marine-derived bacteria. Selection criteria included preliminary tests: growth at 37 °C, anaerobic growth (identifying facultative anaerobes and microaerophiles), absence of virulence factors (gelatinase activity and γ -hemolysis), and antibiotic susceptibility. *Lactobacillus rhamnosus* ATCC 7469 served as a positive control. Six strains (3a, 6a, 12a, 13a, 15a, 30a) outperformed the control in antibiotic resistance profiles. These strains will be further assessed for tolerance to inhibitory substances and subjected to simulated gastrointestinal tract assays. This work was supported by Edital Universal/CNPq under the project “Brazilian biodiversity as a source of biotherapeutic products: a translational approach in the search for next-generation probiotics,” coordinated by REDE MaRe (Rede de Pesquisa dos Ecossistemas Mangue e Restinga) and funded by CNPq/PPBio.

Keywords: Probiotics; Marine bacteria; Restinga ecosystems; Microbial diversity.





***DEREPLICATION AND ISOLATION OF POLYKETIDES FROM WESTERDYKELLA
DISPERSA (Sporormiaceae)***

Letícia Pereira Pinto de Castro^{1*}, Isabela Macedo Silva¹, Angela Michelato Ghizelini²,
Andrew MacRae², Fernando Cotinguiba¹

*leticiappcastro@gmail.com

*1- Instituto de Pesquisa de Produtos Naturais Walter Mors, Av. Carlos Chagas Filho, 373 - Bloco H -
Cidade Universitária da Universidade Federal do Rio de Janeiro, Rio de Janeiro - RJ, 21941-599. 2-
Instituto de Microbiologia Paulo de Góes. Centro de Ciências da Saúde (CCS) – Bloco I – Cidade
Universitária – Fundão*

Fungi represent promising sources for the discovery of new bioactive compounds due to their ability to produce secondary metabolites with diverse biological activities. In this study, the fungus *W. dispersa* was selected for its largely unexplored chemical potential. Cultivation was carried out in a wheat-based medium, which demonstrated high efficiency in fungal biomass production in preliminary analyses. The extraction of metabolites was conducted with ethyl acetate, followed by analyses using ¹H NMR (500 MHz) and HPLC (C18 column) with a water/methanol gradient. The results revealed significant differences between the fungal extract and the control: new signals in the NMR spectra and additional peaks in the chromatograms indicated the production of secondary metabolites. Due to the complexity of the extract, fractionation by molecular exclusion was performed using Sephadex LH-20 with PA-grade methanol as the eluent, yielding eight distinct fractions. HPLC analysis of these fractions showed chromatographic profiles with well-resolved peaks, suggesting the presence of isolable compounds. Concurrently, high-resolution LC-MS/MS analysis was performed, and the data were processed on platforms such as MZmine and GNPS2. Two major compounds were identified: sulochrin and asteric acid. The suggestion of these compounds was made by the GNPS2 library and was validated by correlating the data with the signals observed in the NMR spectra of the corresponding fractions. This is the first time these substances have been identified in the genus *Westerdykella*. The next steps of this research include: (1) continuing the isolation of the major compounds, (2) complete structural elucidation through spectrometric and spectroscopic techniques, and (3) evaluation of the potential biological activities of the identified metabolites. The combination of chromatographic and spectroscopic techniques proved effective in the preliminary characterization of the secondary metabolites produced by this microorganism. This study highlights the potential of the fungus *W. dispersa* as a source of bioactive compounds, contributing to the knowledge of fungal chemical diversity and opening perspectives for future pharmacological investigations.

Keywords: Polyketides, secondary metabolites, fungi, *Westerdykella*, chromatography, mass spectrometry





CHEMICAL PROFILE OF TROPANE ALKALOIDS IN BRUGMANSIA SPP. (SOLANACEAE) FROM ZONA DA MATA (MINAS GERAIS, BRAZIL) USING HPLC-MS/MS AND GNPS MOLECULAR NETWORKING

Pedro Henrique Barbosa^{1*}, Raquel de Medeiros Silva¹, Fernando Cotinguiba¹

phenrique.barbosa.etm2020.2@gmail.com

¹Instituto de Pesquisas de Produtos Naturais Walter Mors (IPPN) – UFRJ. Av. Carlos Chagas Filho, 373, Centro de Ciências da Saúde, Bloco H. Cidade Universitária, Ilha do Fundão, Rio de Janeiro, RJ. CEP: 21941-902, Brazil

Brugmansia spp. (Solanaceae), popularly known as angel's trumpet, comprises species traditionally used in folk medicine for their analgesic, anti-inflammatory, and hallucinogenic properties. Their phytochemistry is dominated by tropane alkaloids, including hyoscyamine and scopolamine, which are associated with both therapeutic and toxic effects. Despite the rich history of chemical and pharmacological investigations on *Brugmansia*, modern approaches to metabolite annotation remain scarce. In this study, a dereplication workflow was applied using high-performance liquid chromatography coupled with tandem mass spectrometry (HPLC-MS/MS), combined with chemoinformatic tools such as MZmine 4 for feature detection and the Global Natural Products Social Molecular Networking (GNPS) platform for spectral-based annotation. Two extracts, one ethanolic and another obtained with ethyl acetate, were analyzed under this workflow, and molecular networking allowed the visualization of chemical space and the clustering of structurally related metabolites, facilitating the identification of tropane alkaloids. Several alkaloids were annotated, including hyoscyamine, scopolamine and anisodamine, with spectral matches confirmed using the GNPS public libraries. The plant material was collected in the Zona da Mata region of Minas Gerais, Brazil, a floristic domain where this genus remains poorly investigated from a phytochemical perspective. The novelty of this work lies in the integration of GNPS molecular networking into the dereplication of *Brugmansia* metabolites, representing one of the first systematic applications of this approach to the genus. Unlike previous studies, which relied only on classical dereplication or targeted analyses, molecular networking enabled the recognition of analog series and provided a more comprehensive chemical landscape. This methodological advance contributes to Natural Products Chemistry by reducing redundancy in compound isolation, enhancing confidence in metabolite annotation, and opening avenues for comparative metabolomics of *Brugmansia* and related Solanaceae species.

Keywords: Chemoinformatics; secondary metabolites; MZMine; annotation; dereplication





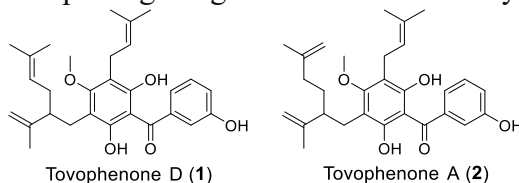
TOVOPHENONE A AND D: PRENYLATED BENZOPHENONES FROM *Tovomitopsis paniculata* (Spreng.) Planch. & Triana (Clusiaceae)

Mateus de Freitas Brito^{1*}, Adriana Quintella Lobão², Leandro Machado Rocha³, Lucas Silva Abreu¹

mateusfb@id.uff.br

1-LQPN, Departamento de Química Orgânica, Instituto de Química, UFF, Outeiro de São João Batista, S/N, Niterói, RJ, Brazil. 2- Herbário de Niterói, Instituto de Biologia, UFF, Outeiro São João Batista, S/N, Niterói, RJ, Brazil. 3-LTPN, Departamento de Tecnologia Farmacêutica, Faculdade de Farmácia, Niterói, RJ, Brazil.

Brazil is one of the most biodiverse countries in the world, making Brazilian flora a rich source for the search for new pharmaceutical products. Among Brazilian biomes, the Atlantic Forest is known for its numerous medicinal plants and for using ethnopharmacology as a reference for popular knowledge in this region, but its biodiversity is still poorly studied.¹ One example is *Tovomitopsis paniculata* (Spreng.) Planch. & Triana (Clusiaceae), a species endemic to the Brazilian Atlantic Forest, which has not yet been studied phytochemically. With the aim of exploring the chemical diversity of native plants belonging to the Atlantic Forest, this study describes the identification of tovo phenone D (**1**), a new benzophenone that is an isomer of tovo phenone A (**2**). The methodology involved maceration of *T. paniculata* roots in hexane, ethyl acetate, and methanol. The hexane extract was analyzed by HPLC-DAD and indicated that the chemical composition was mainly formed by a compound that was subsequently analyzed by NMR. The NMR spectra showed that the major component was a mixture of benzophenone tovo phenone A and an isomer not yet reported in the literature, allowing the structural proposal of tovo phenone D. The compound tovo phenone A has already been tested for oral carcinoma cell line KB and has an IC₅₀=10 ug.mL⁻¹, but the authors consider it inactive.² Therefore, in this study, it was possible to report the identification of tovo phenone A and propose the structure of a new benzophenone. This is the first report of the identification of these compounds in *T. paniculata*, a species endemic to the Atlantic Forest, reinforcing the need to continue exploring the great chemical diversity of Brazilian plants.



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Keywords: atlantic forest, Clusiaceae, *Tovomitopsis paniculata*, prenylated benzophenone





ANALYSIS OF THE CHEMICAL, ANTIOXIDANT AND ANTI-INFLAMMATORY PROPERTIES OF *Swinglea glutinosa* (Bl.) Merr.

Christian Fernando Lizalda-Aponte¹, Valentina Castaño Mosquera¹, Luz Angela Veloza¹, Juan Carlos Sepúlveda Arias², Monica Cala³, Francisco Javier Jiménez-González^{1*}

jjimenez@utp.edu.co

1-Grupo Polifenoles, Facultad de Tecnología, Universidad Tecnológica de Pereira, Pereira, Colombia. 2-Grupo Infección e Inmunidad, Facultad de Ciencias de la Salud, Universidad Tecnológica de Pereira, Pereira, Colombia. 3-MetCore, Vicerrectoría de Investigación e Innovación, Universidad de los Andes, Bogotá, Colombia.

Swinglea glutinosa (Bl.) Merr. (Rutaceae) is a shrub native to the Philippines. In traditional medicine, it has been used to treat skin conditions and hemorrhages, while in Colombia it is used for joint inflammation. Despite its ethnobotanical use, the information on its chemical composition and biological properties is limited, which motivated the present study. The research focused on the characterization of polar metabolites from the pulp, peel, and leaves of *S. glutinosa*, as well as the evaluation of its antioxidant and anti-inflammatory potential *in vitro*. Extracts were obtained from the fruits and leaves using butanol and water. These extracts were characterized by RP-LC-ESI/MS-QTOF, and their metabolites were annotated using bioinformatics tools such as MS-DIAL, SIRIUS, and GNPS molecular network. The antioxidant activity was determined through Folin-Ciocalteu, DPPH, and ORAC assays. The anti-inflammatory activity was evaluated in LPS-stimulated RAW264.7 murine macrophages. The levels of inflammatory mediators such as PGE₂, NO, IL-1 β , IL-6, IL-10, and TNF- α were measured using specific kits and reagents. The results of the molecular characterization of the *S. glutinosa* extracts showed the presence of glycosylated flavonoids, alkaloids, and hydroxycarboxylic acids, with a particular abundance of apigenin and its isomers. The total phenol content in the pulp and peel extracts was 31,3 and 9,3 mg EAG/g Extract, respectively. Regarding antioxidant activity, the pulp and peel extracts inhibited the DPPH radical by 22,9% and 19,5% (at 150 μ g/mL). The ORAC method highlighted the pulp and leaf extracts, with values of 2410,16 and 2802,9 μ molTE/g. In the evaluation of anti-inflammatory activity, the butanolic fruit extracts inhibited the biosynthesis of PGE₂, IL-1 β , and IL-6 by more than 50% after 24 h. Additionally, it was observed that the extracts modulated the mRNA expression of target genes such as iNOS, IL-1 β , and IL-6. Preliminary cytotoxicity assay results, in normal cells Hek-293 using the MTT method, indicate that the extracts do not contain lethal compounds.

Keywords: *Swinglea glutinosa*, LC-MS, anti-inflammatory mediators, ROS, phytochemistry, *In silico*.





LITERATURE REVIEW OF THE PHYTOCHEMISTRY OF THE GENUS *OXANDRA* (ANNONACEAE) AND ANNOTATION OF ALKALOIDS PRESENT IN THE LEAVES OF *OXANDRA MARTIANA*

Rayssa Cota Lopes^{1*}, Adriana Q. Lobão², Lucas Silva abreu¹
rayssacota@id.uff.br

1-Laboratório de Química de Produtos Naturais, Universidade Federal Fluminense, Niterói, RJ, Brazil. 2-Instituto de Biologia, Departamento de Biologia Geral, Universidade Federal Fluminense, Niterói, RJ, Brasil.

Natural products play a central role in modern science, serving as key sources of bioactive molecules. The Annonaceae family, with approximately 2,500 mostly tropical species, stands out for its phytochemical diversity. Within it, the genus *Oxandra*, comprising 29 recognized species, is promising for the search for bioactive compounds, although still poorly studied chemically and pharmacologically. *Oxandra martiana*, endemic to Brazil and found mainly in the Atlantic Forest, has no previous records regarding its chemical profile or biological activity. This study aimed to characterize the phytochemical profile of its leaf extract. A phytochemical database for the genus was first compiled through a literature review, which showed that only 6 of the 29 species had been chemically and/or pharmacologically studied, totaling 64 compounds from various classes. The crude ethanolic extract of *O. martiana* leaves was partitioned with hexane, dichloromethane, and butanol. Using the compiled database as reference, fractions were analyzed by HPLC-ESI-MS and dereplicated, allowing the annotation of several alkaloids. Precursor ions and fragmentation patterns matched known alkaloids: 5-hydroxy-6-methoxyonychine (m/z 242), anonaine (m/z 266), 7-hydroxy-5,6-dimethoxyonychine (m/z 272), liriodenine (m/z 276), aristolactam BII (m/z 280), norushinsunine (m/z 282), *N,N*-dimethylxylopine (m/z 324), parvinine (m/z 328), reticuline (m/z 330), corytenchine (m/z 342), and tetrahydropapaverine (m/z 344). Identification was based on MS/MS fragmentation patterns and confirmed by literature data. The alkaloid profile included various isoquinoline types, consistent with those reported in other species of the genus. This preliminary investigation provides essential insight into the chemistry of *O. martiana* and supports future studies on the isolation and characterization of bioactive compounds with pharmacological potential.

Keywords: *Oxandra martiana*, chromatography, phytochemistry, mass spectrometry (MS), literature review.

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IDENTIFICATION OF VOLATILE COMPOUNDS IN CURED VANILLA SAMPLES FROM ESPÍRITO SANTO USING HEADSPACE SOLID-PHASE MICROEXTRACTION COUPLED WITH GAS CHROMATOGRAPHY–MASS SPECTROMETRY

Amanda Almudin Garcia^{*1}, **Ana Caroline Campos Brunéle¹**, José Arcanjo Nunes², Juliana Aparecida Severi¹

ana.brunele@edu.ufes.br

1- Laboratório de Farmacognosia, Centro de Ciências Exatas, Naturais e da Saúde, Universidade Federal do Espírito Santo, Alto Universitário, s/n, Guararema, Alegre, ES, Brazil. 2- Prefeitura de Cachoeiro de Itapemirim, Centro Administrativo Hélio Carlos Manhães, Rua Brahim Antônio Seder, 96, Centro, Cachoeiro, ES, Brazil.

Vanilla is among the most valuable spices worldwide and finds extensive use in the food, perfumery, and cosmetics industries. Because its cultivation and curing processes are labor-intensive and delicate, vanilla is also one of the most expensive spices on the market. Despite synthetic substitutes, natural vanilla maintains high demand due to its complex aroma, primarily attributed to vanillin (4-hydroxy-3-methoxybenzaldehyde). Brazil has significant potential for the cultivation of both native and exotic species. In the state of Espírito Santo, some farmers have invested in vanilla cultivation and bean curing. However, the lack of studies on its chemical composition hampers the full valorization of this product. Therefore, this study aimed to characterize vanilla beans produced locally using gas chromatography coupled with mass spectrometry (GC–MS). Five locally produced samples were analyzed and compared with two established commercial products. Volatile compounds were extracted through solid-phase microextraction (DVB/CAR/PDMS) and analyzed according to Silva (2023). Peaks in the chromatogram were identified by comparing mass spectra with reference data. A total of 24 volatile compounds were detected and distributed among different chemical classes (aldehydes, alcohols, phenols, acids, esters, and others), highlighting the aromatic complexity of this spice. Vanillin was detected in all samples, confirming its role as the main quality marker. Based on peak areas, the analysis also indicated differences in vanillin content among the local samples, some even exceeding that of the commercial samples. We also observed that when vanillin content was lower, other sensory compounds, such as guaiacol and 4-methylguaiacol, were more prominent. These variations might be associated with cultivation conditions, stages of maturation, and curing processes. Therefore, the chemical characterization of vanilla beans from Espírito Santo not only enhances the value of the local product but also provides a scientific basis for future improvements in the production process, supporting small farmers and facilitating integration into the specialized market.

The authors gratefully acknowledge the support of FAPES, UFES, and Cáritas Diocesana-Cachoeiro de Itapemirim (ES).

Keywords: *Vanilla, vanillin, CG-MS, volatile compounds, Espírito Santo, small-scale farmers.*





PHYTOCHEMICAL INVESTIGATION OF PIPER HISPIDUM LEAVES: IDENTIFICATION AND CHARACTERIZATION OF FIXED CONSTITUENTS.

Helena Garcia Helena^{1*}, João Vyctor Calixto O. Santos², Alicia de Carvalho Souza¹, Magno Perêa Muniz³, Midiã Rodrigues de Oliveira¹, Sergio M. Nunomura³, Rita de Cássia Saraiva Nunomura¹

garciahelena252gmail.com

1- Universidade Federal do Amazonas-UFAM, Av. General Rodrigo Octávio, 6200, Coroado I, 69080-900, Manaus – AM, Brazil; 2- Escola Superior do Amazonas; 3- Instituto Nacional de Pesquisas da Amazonia-INPA, av. Andre Araujo, Petropolis, 69011-970, Manaus-AM.

Piper hispidum Sw., belonging to the family Piperaceae and popularly known in Brazil as jaborandi, is widely employed in traditional medicine, mainly for the treatment of inflammations, pain, and gastrointestinal disorders [1]. In parallel, the species has attracted scientific interest due to the presence of bioactive compounds with recognized therapeutic potential, which exhibit, among others, antioxidant, antimicrobial, antiplasmodial, and cytotoxic activities [2]. However, although the essential oils of *P. hispidum* have been extensively studied, the fixed constituents remain relatively unexplored, thus limiting a comprehensive understanding of the species' pharmacological potential. In this context, the present study aimed to expand knowledge regarding the fixed secondary metabolites of *P. hispidum* leaves, highlighting the occurrence of a flavonoid reported for the first time in this species. The leaves were collected in a secondary forest area, dried in an oven at 35 °C, pulverized, and subjected to exhaustive cold extraction with methanol, yielding the crude extracts. These were successively fractionated by liquid–liquid partition with solvents of increasing polarity and subjected to silica gel column chromatography (70–230 and 230–400 mesh), which enabled the isolation of the fixed constituents. Subsequent phytochemical analysis revealed the presence of the steroids β -sitosterol and stigmasterol, in addition to the flavonoid 5,7,4'-trihydroxyflavanone, identified for the first time in *P. hispidum*. Structural elucidation was based on 1D and 2D NMR data, corroborated by comparison with the literature. In summary, the isolated fixed constituents represent promising substances for future biological investigations, thereby reinforcing the importance of phytochemical exploration of this species in the context of the prospection of secondary metabolites with pharmacological relevance.

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Keywords: Flavonoid, Phytochemical, Piperaceae, NMR





“OSMAC Approach Applied to Modulate the Biosynthesis of Antimicrobial Natural Products in *Pseudonocardia* ICBG1860”

Guilherme José Brustello Vizin^{1*}, Rafael Gonçalves Padilha¹, Carlismari Oliveira Grundmann², Claudia Castania de Macedo¹, Mônica Tallarico Pupo¹

gjbvizin@usp.br

¹ School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, Brazil.

² Chemistry and Biochemistry Department, University of California, Santa Cruz, United States of America

The rise of microbial resistance poses a critical challenge to public health, underscoring the urgent need for new strategies in antibiotic discovery and development. Actinobacteria of the genus *Pseudonocardia*, symbionts of attine ants, are well known for producing bioactive metabolites with ecological and pharmaceutical relevance. In this study, we applied the One Strain Many Compounds (OSMAC) approach to *Pseudonocardia* sp. ICBG1860, which was isolated from *Paratrachymyrmex* ants. The study was conducted under the hypothesis that modifying culture conditions could activate silent biosynthetic pathways and promote the production of minor or novel antimicrobial metabolites. Among these metabolites is a putative tetracycline analogue, detected in previous work (GRUNDMANN, 2023), which is the main target of this study. The strain was cultivated in 11 media providing diverse nutrients, sugars, cofactors, and pH conditions. Solid cultures were extracted with ethyl acetate, while liquid cultures were processed using HP20 resin and acetone. The resulting extracts underwent solid-phase extraction (SPE, C18 cartridge) and were analyzed by HPLC-DAD-ELSD, enabling comparison of chromatographic profiles and identification of promising culture conditions. Among the tested media, D-Mannitol–Peptone Agar stood out by inducing a unique set of secondary metabolites that were absent under the other evaluated conditions. UV-Vis spectra suggested the presence of tetracycline analogues, while ELSD data revealed a marked increase in the production of a putative novel tetracycline analogue, previously detected only at low concentrations in ISP2 medium (GRUNDMANN, 2023). Accordingly, this medium was selected for large-scale cultivation (450 Petri dishes, 90 mm), followed by SPE fractionation into six fractions. The MeOH:H₂O (50% and 75%) and MeOH 100% fractions concentrated the elicited compounds and exhibited antimicrobial activity in overlay assays against *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Escovopsis* sp., a fungal pathogen of attine gardens. These results highlight the effectiveness of the OSMAC approach in modulating the metabolism of *Pseudonocardia* ICBG1860 and reinforce its potential as a source of novel bioactive compounds. Next steps include HPLC-MS/MS analysis, dereplication through molecular networking using the Atlas of Natural Products and GNPS platforms, followed by isolation and structural elucidation of the metabolites by NMR. The authors thank their institutions and acknowledge financial support from CAPES (Finance code 001) and FAPESP (grants 2013/07600-3; 2025/10223-4; 2024/21508-7).

Keywords: *Pseudonocardia*, antimicrobial, tetracycline, natural products, symbiosis, OSMAC





ISOLATION AND MORPHOLOGICAL CHARACTERIZATION OF ENDOPHYTIC FUNGI FROM *GUADUA ANGUSTIFOLIA* KUNTH IN THE COLOMBIAN COFFEE REGION

Aura María Blandón Osorio^{1*}, Gloria María Restrepo Franco², Oscar Marino Mosquera Martínez¹

aumablandon@utp.edu.co

1-GB-PN, Facultad de Tecnología, UTP, Carrera 27 No. 10-02, Pereira, Risaralda, Colombia. 2-IMBA, Facultad de Ciencias de la Salud, UCM, Carrera 23 No. 60-63 Manizales, Caldas, Colombia.

The Colombian Coffee Region represents a biodiversity hotspot harboring *Guadua angustifolia* Kunth, one of the most economically important bamboo species in Colombia with approximately 45,000 hectares. This species hosts diverse endophytic fungi that constitute an unexplored reservoir of microbial biodiversity with significant ecological importance. This research aimed to explore endophytic fungal diversity associated with *G. angustifolia* through systematic isolation and morphological characterization from different plant tissues. Plant material was collected from three representative sites: Botanical Garden of Universidad Tecnológica de Pereira (Risaralda), El Bambusal farm (Montenegro, Quindío), and El Paraíso farm (Belén de Umbría, Risaralda). Four tissue types were sampled: basal culms, middle culms, apical culms, and leaves. Surface sterilization involved sequential treatments with 75% ethanol (3 min) and 3% sodium hypochlorite (30, 90, and 180 s), followed by sterile water rinses. Sterilized segments were plated on potato dextrose agar supplemented with amoxicillin (300 ppm) and incubated at 25°C. Isolated fungi were purified through successive subculturing until axenic cultures were obtained. Morphological characterization included macroscopic analysis of colony texture, pigmentation, growth patterns, and microscopic examination of hyphal morphology and reproductive structures using lactophenol cotton blue staining and slide culture techniques. Results demonstrate successful isolation of endophytic fungi from all tissue types across three geographic locations, with 22 isolates obtained from site 1, 22 from site 2, and 28 from site 3, totaling 72 fungal isolates and revealing significant microbial diversity within *G. angustifolia*. Morphological characterization identified multiple distinct fungal morphotypes exhibiting diverse colony characteristics, growth rates, and microscopic features, indicating taxonomic diversity within the endophytic community. Colonization frequency varied among tissue types, with differential patterns between culm segments and leaves. This biodiversity survey contributes fundamental knowledge about fungal endophyte diversity in Colombian bamboo ecosystems and establishes a foundation for understanding ecological roles of these microorganisms in tropical biodiversity conservation. The authors thank the support from their institutions as well as the Ministry of Science, Technology, and Innovation of Colombia.

Keywords: *Guadua angustifolia*, endophytic fungi, biodiversity, Colombian Coffee Region, microbial diversity





**TURNING BY-PRODUCTS INTO BIOACTIVE ASSETS: DRYING
EFFECTS ON *Campomanesia adamantium* ESSENTIAL OIL FOR
COSMETIC APPLICATIONS**

Francisco Bitencourt Ottoni^{1*}, Andrielly Cristina Santana², Juliana Franco Mendes de
Siqueira³, Érica Luiz dos Santos², Nídia Cristiane Yoshida²

francisco.ottoni@ufms.br

1- Instituto de Biologia, Universidade Federal do Mato Grosso do Sul (UFMS), Brasil. 2- Laboratory
of Research on Bioactive Natural Products (PRONABio/UFMS), Instituto de Química, UFMS, Brasil
3- Faculdade de Farmácia e Nutrição, UFMS, Brasil

Known as guavira, *Campomanesia adamantium* (Cambess.) O. Berg (Myrtaceae) is the symbolic fruit of Mato Grosso do Sul state, where it represents both cultural identity and economic potential. The pulps are widely exploited for food purposes, whereas peels and seeds are often discarded due to large volumes generated and storage limitations requiring low temperatures. Considering the high potential of these residues, our Research Group PRONABio/UFMS has developed dermocosmetic formulations derived from *C. adamantium* residues (INPI, 2024). Within this context, the present study aimed to evaluate the influence of two distinct drying methods on the chemical composition and yield of the essential oils (EO) obtained from *C. adamantium* residues, as a strategy to overcome the challenges associated with its storage and refrigeration requirements. The residues (peels and seeds) were subjected to two drying treatments: in an oven at 40 °C and at room temperature (RT, ~22 °C). Extractions of OEs were performed at five different points (1, 2, 4, 6, and 8 days), with day 0 serving as the control. EOs were obtained by hydrodistillation, and the chemical composition was analyzed by gas chromatography coupled with mass spectrometry. The results showed a significant increase in EO yield from oven-dried samples, with fresh residues yielding 1.405 mg/g of plant material compared to 2.431 mg/g after drying, representing a 72.57% increase. The highest yields were observed after 6 and 8 days (81.79% and 81.43%, respectively). In both treatments, the main compounds identified were the monoterpenes *D*-limonene (31.40% RT; 23.55% oven) and β -pinene (12.01% RT; 11.22% oven), compared to control values of 29.14% and 7.46%, respectively. Notably, eucalyptol was absent in control but appeared in high concentrations in both treatments (18.99% RT; 18.38% oven). Other compounds also exhibited considerable variation compared to the control, including linalool (2.71% control; 6.39% RT; 8.02% oven), α -terpineol (2.66% control; 5.06% RT; 5.26% oven), and *D*-germacrene (1.21% control; 0.77% RT; 0.40% oven). In conclusion, both drying methods proved effective: oven drying significantly increased EO yield, while room temperature drying better preserved volatile compounds. Overall, thermal drying of the residues eliminates the need for refrigeration while maintaining EO quality, providing a sustainable approach for processing and value addition of this valuable raw material.

Keywords: Guavira, residue, GC-MS, chemical profile, monoterpenes





STUDY OF THE PHYTOTOXIC POTENTIAL OF SPHAGNETICOLA TRILOBATA ON IPOMOEA SPP AND LACTUCA SATIVA.

Olatoundji Abdou Rachidi Tidjani^{1*}, Anne Caroline Candido Gomes²

Carlos Rodrigues Pereira³, Naomi Kato Simas⁴

rachidit24@gmail.com

1-Departamento de Engenharia de Biosistemas, UFF, Rua Passo da Pátria, 156 bloco D sala 236 - São Domingos - Niterói - RJ - 24210-240, Brazil. 2- Instituto Federal do Rio de Janeiro, IFRJ, R. Sen. Furtado, 121/125 - Maracanã, Rio de Janeiro - RJ, 20270-021, Brazil, 3- Faculdade de Farmacia, LaProNEB/UFRJ, Avenida Carlos Chagas Filho, 373 Centro de Ciências da Saúde, Rio de Janeiro - RJ, 21941-902, Brazil

INTRODUCTION: The excessive use of chemical herbicides contributes to environmental degradation and biodiversity loss. Allelopathy emerges as a sustainable alternative, and *Sphagneticola trilobata*, a plant in the Asteraceae family, stands out for its allelopathic potential, containing phenolic and flavonoid compounds with inhibitory effects on other plants.

OBJECTIVE: To evaluate the phytotoxic effects of aqueous extracts of *S. trilobata* on model species *Ipomoea spp.* and *Lactuca sativa*, aiming to verify effects of growth stimulation or inhibition in addition to effects of impacts on non-target organisms.

METHODOLOGY: Dried leaves of *S. trilobata* were extracted in distilled water (12.5, 25, and 50 g/500 mL). Bioassays were conducted with *Ipomoea* and *Lactuca sativa* seeds exposed to different concentrations (25%, 50%, 75%, 100%) for 7 days in B.O.D.. Germination and root and hypocotyl growth/inhibition were evaluated by calculating the growth/inhibition index. Analysis of variance (ANOVA) was performed for the biological assays presented. The significance level was set at * $p < 0.05$. Results were expressed as mean $\pm$ standard deviation. Statistical analyses were performed using GraphPadPrism 5.0 software.

RESULTS: *S. trilobata* extracts exhibited dose-dependent effects. Lower concentrations (between 15.625 and 62.5 mg/L) significantly stimulated root and hypocotyl growth, particularly in *Ipomoea* and *Lactuca sativa*. Higher concentrations (≥ 125 mg/L), on the other hand, inhibited this growth, demonstrating a potential hormetic effect. Roots were more sensitive than hypocotyls.

CONCLUSION: *Sphagneticola trilobata* demonstrated phytotoxic potential with biphasic effects—stimulation at low doses and inhibition at high doses. This highlights its potential use as a natural bioherbicide, contributing to more sustainable agricultural practices.

Keywords: *Sphagneticola trilobata*, phytotoxic, *Ipomoea Spp*, *Lactuca sativa*





Detection of Diterpenes in the Oleoresin of *Eperua oleifera* Ducke (Fabaceae) and Isolation of a Naturally Occurring Methyl Ester of a Diterpenic Acid

Rayssa Ribeiro^{1*}, **Anna Cristina da Costa e Souza**¹, Henrique Marcelo G. Pereira², Monica Costa Padilha², Valdir Florencio da Veiga Junior¹

annasouz@gmail.com

1-Military Institute of Engineering, Rio de Janeiro, Praça General Tibúrcio, 80, Praia Vermelha, Urca, 22290-270, Brazil, 2-Federal University of Rio de Janeiro, Chemistry Institute, Brazilian Doping Control Laboratory (LBCD/IQ – UFRJ), Rio de Janeiro, RJ 21941-909, Brazil;

Oleoresins are plant exudates composed solely of terpenes, typically consisting of volatile monoterpenes and sesquiterpenes that solubilize heavier diterpenes and triterpenes. Studies on *Eperua* species, such as *E. purpurea* and *E. leucantha*, revealed compositions mainly of diterpenic acids and minor alcohols, particularly labdane-type diterpenes (copalic, cativic, and eperuic acids). Other plant parts of *Eperua* species have been reported to contain phenolic acids, flavonoids, sesquiterpenes, triterpenes, and abundant diterpenes. The oleoresin of *Eperua oleifera* Ducke, commonly known as “copaíba-jacaré,” is traditionally used in folk medicine for wound healing and as an antifungal and antibacterial agent, similar to species of the genus *Copaifera* (Fabaceae). Nevertheless, despite its pharmacological potential, few studies have investigated *E. oleifera* to confirm its bioactivity in relation to its chemical composition. In this context, the present study examined the oleoresin of *E. oleifera* collected in the Brazilian Amazon region. After derivatization, the sample was analyzed by GC-MS to identify its chemical constituents and characterize the volatile fraction, with the data compared against the literature, mass spectral libraries, and previously isolated standards. Furthermore, neutral and acidic fractions were separated using open-column chromatography and ion-exchange chromatography (KOH-impregnated silica as the stationary phase). This approach resulted in the identification of twelve diterpenes, including nine carboxylic acids and three alcohols, with hardwickiic and copalic acids as the primary components, which NMR fully characterized. Ion-exchange chromatography proved to be more selective, enabling the direct isolation—without subsequent steps—of a methyl ester identified by HRMS and NMR as the methyl ester of hardwickiic acid. This represents the first report of such a compound in oleoresins. We conclude that GC-MS analysis enabled the identification of diterpenes based on known fragmentation patterns. Furthermore, ion-exchange chromatography combined with infusion experiments allowed the isolation and detection of a naturally occurring methyl ester that, to our knowledge, had not been previously reported in oleoresins. This novel finding highlights the potential for discovering additional esters in oleoresins through infusion-based analyses.

Keywords: *Eperua oleifera* Ducke, GC-MS, diterpene acids, HRMS, Hardwickiic acid methyl ester





IN VITRO SCHISTOSOMICIDAL ACTIVITY AND MOLECULAR MODELING OF QUERCITRIN AND AFZELIN ISOLATED FROM COPAIFERA OBLONGIFOLIA LEAVES

João Victor Andrade^{1*}, Lizandra G. Magalhães², Rodrigo C. S. Veneziani², Renato Pereira Orenha², Márcio L. Andrade² e Silva, Mario F. C. Santos¹, Wilson R. Cunha²

joaovictorandrade927@gmail.com

1-Center for Exact, Natural and Health Sciences, Federal University of Espírito Santo, Alto Universitário, Alegre 29500-000, ES, Brazil 2-Center for Exact and Technological Sciences, University of Franca, Avenida Dr. Armando Salles de Oliveira, 201, Franca 14404-600, SP, Brazil

Schistosomiasis, a neglected tropical disease, has affected millions of people globally. Treatment depends mostly on praziquantel (PZQ), but the emergence of resistance justifies the search for new therapeutic alternatives. The enzyme Thioredoxin Glutathione Reductase (TGR) from *Schistosoma mansoni* is a validated target for the development of new drugs. Species of the genus *Copaifera* are recognized in traditional medicine for their pharmacological properties, making them promising sources for the discovery of bioactive compounds. This study investigated the *in vitro* and *in silico* schistosomicidal potential of compounds isolated from the leaves of *Copaifera oblongifolia*. The hydroalcoholic extract of *C. oblongifolia* leaves was partitioned and fractionated by chromatographic techniques, resulting in the isolation of the compounds quercitrin (1) and afzelin (2), identified by spectroscopic techniques (NMR ¹H, NMR ¹³C and ESI-MS). *In vitro* schistosomicidal activity was evaluated against adult worms of *S. mansoni* (LE strain) recovered from infected BALB/c mice. The parasites were incubated with the compounds (12.5–200 µM) and the crude extract (50 and 100 µg/mL) for 72 h. Mortality and reduction in motor activity were monitored every 24 h. Praziquantel (12.5 µg/mL) and culture medium were used as positive and negative controls, respectively. Molecular docking studies were performed with the GOLD software to evaluate the binding mode of the compounds to the active site of the TGR enzyme (PDB: 2V6O), using PZQ as a reference. The crude extract at the concentrations tested did not show significant activity. However, compounds 1 and 2 alone demonstrated potent schistosomicidal activity *in vitro*. Quercitrin (1) induced 100% mortality at the 50 µM concentration after 72 hours. Afzelin (2) was slightly less potent but still caused 100% mortality at the 200 µM concentration after 72 hours. The molecular docking results revealed that both compounds interact strongly with amino acid residues from the FAD binding site on the TGR enzyme, with binding energies (dG = -23.44 and -28.90 kcal mol⁻¹, respectively) comparable or even more favorable than that of PZQ (dG = -22.03 kcal mol⁻¹). This interaction, mediated by multiple hydrogen bonds and hydrophobic interactions, suggests a potential mechanism of action via inhibition of TGR, an enzyme crucial for parasite survival. The flavonoids quercitrin and afzelin, isolated from *Copaifera oblongifolia*, exhibited significant schistosomicidal activity *in vitro* and showed, by molecular modeling, a strong potential to inhibit the TGR enzyme of *S. mansoni*. These results highlight these compounds as promising candidates for future studies of drug development against schistosomiasis.

Keywords: Schistosomiasis; *Copaifera oblongifolia*; Quercitrin; Afzelina; Molecular Docking; TGR.





“FROM THE DEPTHS TO DISCOVERY: CHEMICAL DIVERSITY OF MARINE BACTERIA FROM THE BRAZILIAN CONTINENTAL SHELF”

Daniela Cristina Russo^{1,5,*}, Eduarda Antunes Moreira², Norberto Peporine Lopes², Paula Rezende-Teixeira³, Letícia Veras Costa-Lotufo³, Gabrielli Monzani de Lima⁴, Uesley Vieira Alves⁴, Massuo Jorge Kato⁴, Anelize Bauermeister⁵, Paula Christine Jimenez¹

[*daniela.russo@unifesp.br](mailto:daniela.russo@unifesp.br)

1-BioProsp, Departamento de Bioprodutos e Bioprocessos, UNIFESP, Rua Carvalho de Mendonça, 144, Santos, SP, Brazil. 2-CMMO, Departamento de Ciências Biomoleculares, Av. do Café, S/N, Ribeirão Preto, SP, Brazil. 3- LAFARMAR, Departamento de Farmacologia, ICB, USP, Av. Lineu Prestes, 2415, São Paulo, SP, Brazil. 4-LQPN, Departamento de Química Fundamental, IQ, USP, Av. Lineu Prestes, 748, São Paulo, SP, Brazil. 5-LEQUIM, Departamento de Química Fundamental, IQ, USP, Av. Lineu Prestes, 748, São Paulo, SP – Brazil

Herein, we reveal that deep-sea sediments from the Brazilian continental shelf along the Espírito Santo State coastline, collected in 2015 at approximately 1,500 m depth, harbor a unique diversity of chemically gifted Gram-positive bacteria with biotechnological potential. In this investigation, 41 strains were isolated from wood scraping biofilms and submerged animal bone biofilms preserved in the MicroMarin collection. Recovered strains were subjected to taxonomical identification based on 16S rDNA and their EtOAc extracts were subjected to spectral library annotation by classical molecular networking (CMN) on the GNPS platform, complemented by Dereplicator and Dereplicator+. Among the annotated metabolites, lipopeptides (surfactins, lipopeptide_NO), siderophores (acyl-DFO-D C7–C13), and indole derivatives (tryptamine, N-[2-(1H-indol-3-yl)ethyl]acetamide), are highlighted for their biological associated functions: membrane modulation, iron chelation, and cell signaling. The crude extracts were evaluated in two enzymatic assays (trypsin and chymotrypsin), one antioxidant assay (DPPH), and cytotoxicity assays against HCT-116 and MCF-7 cell lines. Strains identified within the genera *Bacillus*, *Mammaliicoccus*, *Micromonospora*, *Nocardiopsis*, *Streptomyces*, *Verrucosipora*, and *Williamsia* displayed positive activity in both enzymatic and DPPH assays (52.7%), whereas *Bacillus* sp., *Microbacterium* sp., and *Streptomyces* sp. exhibited cytotoxicity (8.1%). *Niallia* sp. BRB-316 strain was selected for further chemical assessments through a fractionation protocol, yielding the S7_3 subfraction obtained by column chromatography guided by TLC, preparative TLC, and purification by microsyringe. ¹H NMR analysis (500 MHz, CDCl₃) revealed key signals consistent with hydroxyl, amine, and methoxy groups. In summary, the integration of CMN, dereplication, and NMR data highlights deep-sea bacteria from the Brazilian continental shelf as a promising chemical reservoir, and the S7_3 subfraction illustrates the potential of rare taxa for biotechnological exploration.

Keywords: Marine Actinomycetota, Protease Inhibition, Cytotoxic Activity, *Niallia* sp., Marine Natural Products





STEROIDAL CHAIN FUNCTIONALIZATION MEDIATED BY ENDOPHYTIC FUNGI *Penicillium Citrinum* H7 AND *Talaromyces* sp. H4

Valmore Henrique Pereira dos Santos Sousa^{1,2*}, Eliane de Oliveira Silva².

hp20.2014@gmail.com

1- Campus Campo Formoso, Instituto Federal da Bahia, IFBA, Rua José Rufino, BA 220, KM 2,5, Campo Formoso, BA, 44790-000, Brazil. 2- Laboratório de Química de Microrganismos, LQM, Departamento de Química Orgânica, Instituto de Química, Universidade Federal da Bahia, UFBA, Rua Barão de Jeremoabo, 147, Salvador, B, 40170-115, Brazil.

Biotransformation has been successfully employed to conduct uncommon reactions, which would hardly be carried out by chemical synthesis¹. A wide diversity of compounds may be metabolized by fungi, leading to chemical derivatives through selective reactions that work under ecofriendly conditions². Endophytic fungi live inside vegetal tissues without causing damage to the host plant, making available unique enzymes for interesting chemical derivatization. Biotransformation of steroids by endophytic fungi may provide new derivatives as these microorganisms came from uncommon and underexplored habitats. In this study, endophytic strains isolated from *Handroanthus impetiginosus* leaves were assayed for biotransformation of progesterone, and its derivatives were identified through GC-EI-MS analysis. The endophyte *Talaromyces* sp. H4 was capable of transforming the steroidal nucleus selectively into four products through selective ene-reduction of the C4-C5 double bond and C-17 oxidation. The best conversion rate of progesterone (>90 %) was reached with *Penicillium citrinum* H7 endophytic strain that transformed the substrate into one derivative. The results highlight endophytic fungi's potential to obtain new and interesting steroidal derivatizations.

Keywords: Endophytic fungi, Steroids, Biotransformation, GC-MS.

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**CHARACTERIZATION OF POLYPHENOLS IN COFFEE HUSKS EXTRACTS
OBTAINED WITH DEEP EUTECTIC SOLVENTS BY HPLC-UV**

Soraia Cristina Gonzaga Neves Braga^{1,2*}, Keyller Bastos Borges³, Warley de Souza
Borges¹

soraia.braga@ifes.edu.br

1-Dep. de Química, CCE, Ufes, Av. Fernando Ferrari, s/n, Goiabeiras, Vitória-ES, Brazil.

2-Ifes, campus Viana, Rodovia BR 262, s/n, Universal, Viana-ES, Brazil

2- Dep. De Ciências Naturais, UFSJ, São João Del Rei-MG, Brazil

Coffee is the second-largest commodity in the world. In 2024, Brazil produced 54.2 million bags and exported approximately 50.5 million in the same period. During coffee processing, various residues are generated, and these residues differ depending on the processing method, which can be wet, semi-wet, or dry—the most common method used in Brazil. One of these residues are the coffee husks and in the study of chemical composition various extraction methods have been employed. An alternative to the use of harmful solvents are the deep eutectic solvents (DES). These solvents are produced by mixing two solids that, when combined, form a eutectic mixture with a drastically reduced melting point. In this work, the objective was quantify the polyphenols by HPLC in extracts of coffee husks produced with two different DES. The synthesized solvents used: Urea and Glycerol (URGLO) and Proline and Urea (PRUR) both optimized in a central composite design, with five replicates at the center point. For the DES synthesis, the reagents were weighed and placed in contact in a beaker at a constant temperature of 80°C, with times ranging from 10 to 120 minutes. The extraction of coffee husks was conducted using 0.400 ± 0.005 g and 2.000 mL of the corresponding solvent. The samples were extracted in an ultrasonic bath for 1 hour at 25°C, followed by centrifugation and collection of the supernatant. This supernatant was diluted in methanol, filtered and analyzed by HPLC-UV (1260 Infinity - Agilent technologies) equipped with a C18 Luna column (250mm, 4.5mm, 5microm-Allcrom) in a gradient elution using 5% of acetic acid solution and acetonitrile. Six compounds are analyzed: Trigonelline, gallic acid, caffeine, caffeic acid, p-coumaric acid and 3-CQA. These analyses were carried out after method validation with the ICH Q2(R2) guideline. The table showed the experiments with greater quantity of polyphenols in the extracts for each DES in µg/g.

	Trigonelline	Gallic acid	3-CQA	caffeine	Caffeic acid	p-coumaric acid
	µg/g					
URGLO (3)	561.0	ND	72.92	448.84	2.23	2.08
PRUR (4)	627.31	ND	79.40	485.92	2.89	2.78

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Keywords: coffee husks, deep eutectic solvent, HPLC, Polyphenols





BANK OF MOLECULES: AN INITIATIVE TO LEVERAGE COLLABORATIVE NATURAL PRODUCT-BASED DRUG DISCOVERY IN BRAZIL

***Rafael de Felicio^{1*}, Joyce B. Guedes¹, Andreza L. do Nascimento¹, Beatriz P. Bosque¹,
Marcos G. Cunha¹, Danieli C. Gonçalves¹, Daniela B. B. Trivella¹***

rafael.felicio@lnbio.cnpem.br

*¹Drug Discovery Division, Brazilian Bioscience National Laboratory (LNBio), Brazilian Center for
Research in Energy and Materials (CNPEM), Campinas/SP, Brazil*

Molecules from Nature (NPs) remain a main source of new drugs. Brazil, a biodiversity hotspot, harbors many molecules yet to be discovered and developed. The Brazilian scientific community is solid and needs to be connected to foster pharmaceutical innovation in Brazil. With this goal, we have established the Bank of Molecules, a multicollaborative initiative that aligns state of the art scientific infrastructure and expertise aimed to avoid early-stage drug discovery bottlenecks and to promote collaborative pharmaceutical innovation in Brazil. How it works: researchers interested in depositing their samples (extracts, fractions, pure compounds) to the Bank of Molecules (depositor) send their samples (2-10 mg) to LNBio/CNPEM, along with basic information that guarantees sample traceability. The samples are received by LNBio/CNPEM, where they are registered at a trackable certified database, processed and stored at low temperature under inert atmosphere, following automated processes under GLP practices. At this first stage, it will be performed two main analyses at LNBio/CNPEM: i) untargeted metabolomic analysis - quality control (t_0) and chemical space covered by the samples; and ii) biological evaluation in cellular assays (HCT-116, colon cancer, and HaCat, reference keratinocyte) – aiming to point natural samples with anticancer potential. The first results are expected within 90 days, which are delivered through standard reports on biological and chemical analyses, highlighting the main findings. From there, parties involved can discuss the next steps of the collaboration, including the publication in scientific literature or further developments from the obtained data, according to the interest of the depositor. Remaining samples are stored at LNBio/CNPEM for further analysis, remain property of the depositor, and require consent for use. At the same time, researchers interested in accessing the Bank of Molecules (users) can express their intents and will be connected to the depositor through our system. Once approved, the samples will be sent to the users in “assay ready plates”, containing typically 2.5 nL of the approved chemical samples (384-well format preferred). The “assay ready plates” can be promptly tested by the users, by dispensing their biological samples (bacteria, cells, target proteins, and so on) upon plate arrival at their laboratories. This enables the execution of medium to high throughput screenings at different institutions in Brazil, by avoiding bottlenecks of chemical sample pipetting and trackability, thus speeding up bioprospection in the country. The Bank of Molecules was just launched, attending researchers spanning all regions of Brazil. We invite all researchers to contribute to the Bank of Molecules by depositing their chemical samples, or by accessing them in their drug discovery projects in a collaborative fashion. For more information please consult: <https://lnbio.cnpem.br/>, Banco.Moleculas@lnbio.cnpem.br

Keywords: Drug discovery, Brazilian Biodiversity, Compound Management, Metabolomics, Bioassays





CHEMICAL PROFILE OF THE ESSENTIAL OIL FROM *CROTON COMPRESSUS* (EUPHORBIACEAE) BY GC/MS AND GC/FID

Gabriela Dinis Leonardo^{1*}, Luiz José Soares Pinto³, Lucas Silva Abreu¹, Rafael Ferreira da Silva²

gabriela_dinis@id.uff.br

1-Laboratório de Química de Produtos Naturais, Universidade Federal Fluminense (UFF), Niterói, RJ, Brazil 2-Laboratório de Fragrâncias e Aromas da Biodiversidade, Universidade Federal Fluminense (UFF), Niterói, RJ, Brazil 3- Faculdade de Formação de Professores /Universidade do Estado do Rio de Janeiro – FFP/UERJ

The Euphorbiaceae family includes about 300 genera, with *Croton* standing out for its ~1,300 species in tropical and subtropical regions, especially in Brazil. *Croton* species produce essential oils rich in monoterpenes, sesquiterpenes, and phenylpropanoids, with notable economic and pharmacological potential [1]. *Croton compressus*, native to Southeast Brazil, has no reported essential oil composition. This study aims to analyze its leaf oil to expand knowledge of the species and its potential bioactivity. The leaves of *Croton compressus* were collected in 2025 at Tijuca National Park, Rio de Janeiro. The essential oil were extracted from fresh and oven-dried leaves (72 h at 37 °C) and, in both cases, the plant materials were subjected in triplicate to hydrodistillation in a Clevenger apparatus for three hours. The oils were analyzed by GC/MS Agilent 6890N and GC/FID (Agilent 7820A GC with 5975C MSD) [2]. The components were identified by comparing their linear retention indices (IRL), obtained from n-alkane injections under the same conditions, and mass spectra with literature data [3]. Analyzing one of the triplicates in each case, 374.8 mg of essential oil (0.12% yield) were obtained from fresh leaves, with the main constituents being Bicyclogermacrene (8.6%), (Z) - α -trans-Bergamotol (6.9%), Germacrene D (5.9%), γ -Terpinene (5.5%), and Limonene (4.3%). From dried leaves, 677.7 mg were obtained (0.22% yield), with Bicyclogermacrene (7.1%), Germacrene D (5.1%), γ -Terpinene (5.4%), and 1,8-Cineole (5.3%) as the major constituents. Notably, in the oil from dried leaves, a compound accounting for 9.9% was detected as the major constituent, yet it has not been identified by the author. This same compound was also observed in the other triplicate analyses (from fresh and dried leaves) that have not yet been studied, remaining unidentified when compared with the available literature. As a future perspective, the complete characterization of the essential oil of *Croton compressus* is proposed, based on the comparison of the triplicates, aiming to broaden the understanding of this species and uncover the potential of its bioactive constituents.

Keywords: Essential oil, Chemical composition, Gas chromatography (GC), Mass spectrometry (MS)

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FLAVONOIDS ISOLATED FROM A NATIVE SPECIMEN OF *Ceiba pentandra* (L.) Gaertn.

Priscila Brasil Augusto de Souza^{1*}, Davi Santos Oliveira¹, Jennifer Araújo de Oliveira Lima¹, Estefane de Oliveira Picanço², Claudete Catanhede do Nascimento², Maria da Paz Lima²

priscilabrasil.souza@gmail.com

1-Instituto de Ciências Exatas, Programa de Pós-Graduação em Química, UFAM, Av. Gen. Rodrigo Octávio, 6200, Manaus, AM, Brazil. 2-Coordenação de Tecnologia e Inovação, Instituto Nacional de Pesquisas da Amazônia – INPA, Av. André Araújo, 2936, Manaus, 69067-375, Brazil.

Ceiba pentandra (L.) Gaertn., known as sumaúma or sapopema, is a tree species native to the Pantropical region and presents a rich diversity of secondary metabolites, such as fatty acids, steroids, triterpenes, sesquiterpenes, xanthenes, flavanolignans, flavonoids, and other phenolic compounds.^{1,2} Among these, flavonoids stand out as the class with the highest number of reports, whose biosynthesis is often associated with plant resistance.³ In this context, the present study aimed to isolate and identify flavonoids from a native specimen of *C. pentandra*. The wood residues originated from a tree that fell on the campus of the National Institute of Amazonian Research (INPA) due to termite attack on its tap roots. The residues were cut, dried, processed, and identified by comparison with samples available in the Xylotheque (INPA). The residues were then ground and subjected to extraction with hexane followed by methanol at room temperature. To fractionate the methanolic extract and obtain secondary metabolites, column chromatography was used with different stationary phases (silica gel 70-230, 230-400 mesh, and Sephadex LH-20), resulting in the isolation and identification of flavonoids (garbanzol [1], liquiritigenin [2], 7,4'-dihydroxyflavone [3], and 7,4'-dihydroxyflavan-3,4-diol [4]). The structures of these compounds were elucidated by one-dimensional (¹H and ¹³C) and two-dimensional NMR techniques (HSQC and HMBC), through comparison with literature data. This work represents the first phytochemical report of sumaúma wood and the identification of these flavonoids in the genus *Ceiba*.

Keywords: Flavanones, Flavone, Flavan-3,4-diol, Malvaceae, NMR.

¹Das, G., Shin, H. S., Ningthoujam, S. S., Talukdar, A. D., Upadhyaya, H., Tundis, R. Patra, J. K. (2021). Systematics, phytochemistry, biological activities and health promoting effects of the plants from the subfamily bombacoideae (family Malvaceae). *Plants*, 10(4), 651.

²Rai, M., Bhattarai, S., Feitosa, C. M. (Eds.). (2020). *Wild plants: the treasure of natural healers*. CRC Press.

³Treutter, D. (2005). Significance of flavonoids in plant resistance and enhancement of their biosynthesis. *Plant biology*, 7(06), 581-591.





INTEGRATED GENOME MINING AND MALDI-TOF-MS FOR THE PROSPECTION OF BIOACTIVE METABOLITES OF *BACILLUS SP.*

Maria José de Oliveira Pessoa^{1*}, *Clara Detúlio Martins Cavalcante*¹, *Júlia Firme Freitas*²,
*Lucymara Fassarella Agnez-Lima*², *Renata Mendonça Araujo*¹

maria.pessoa.117@ufrn.rdu.br

1-Lisco, Instituto de Química, CCET, UFRN, Campus Universitário, 59078-970, NATAL, RN, Brazil.

2-LBMG, Centro de Biociências, Campus Universitário, 59078-970, NATAL, RN, Brazil.

Bacillus species are promising sources of bioactive secondary metabolites, particularly non-ribosomal lipopeptides and polyketides. In this study, genome mining performed using the AntiSMASH platform was integrated with MALDI-TOF-MS analyses to explore the metabolic potential of a *Bacillus sp.* strain isolated from petroleum-contaminated sand sediments. Genome mining of *Bacillus amyloliquefaciens* BG1 revealed biosynthetic gene clusters (BGCs), including those related to the production of non-ribosomal lipopeptides, ribosomal peptides, and polyketides, previously associated with antimicrobial and antifungal activities. The presence of multiple NRPS and PKS systems highlights the high biosynthetic potential of the strain investigated. Comparative analysis between AntiSMASH predictions and MALDI-TOF-MS spectra of the ethyl acetate extract revealed mass peaks consistent with genomically predicted metabolites. [M+H]⁺ ions were putatively annotated as compatible with aurantini B (m/z 780.4732), surfactin (m/z 1035.5732), surfactin C (m/z 1021.5512), iturin A-7 (m/z 1070.5092), iturin C/bacillomycin D (m/z 1043.5292), and paenilarvin A (m/z 1111.4652), corroborating the correlation between genomic predictions and metabolic expression. These findings demonstrate that the integration of genome mining with mass spectrometry represents a rapid and targeted strategy for the prospecting of secondary metabolites with potential biotechnological applications. The results highlight the *Bacillus* strain studied as a promising candidate for future purification, structural elucidation, and biological activity evaluation studies.

Keywords: *Bacillus*, Genome mining, Mass spectrometry, Bioactive metabolites, Peptide

Acknowledgments: Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Programa de Pós-graduação em Química (PPGQ-UFRN) Laboratório de Isolamento e Síntese de Compostos Orgânicos (LISCO-UFRN), Laboratório de Biologia Molecular e Genômica (LBGM-UFRN), and Central de Espectrometria de Massas de Micromoléculas Orgânicas (CEMMO-USP/Ribeirão Preto).

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METABOLOMIC PROFILING AND CYTOTOXIC POTENTIAL OF UNCHARACTERIZED MARINE BACTERIA FROM THE BRAZILIAN COASTLINE AS A SOURCE OF NOVEL BIOACTIVE COMPOUNDS

Debora M. Rodrigues¹, Elthon G. Ferreira², Joyce B. Guedes¹, Nicolas A. Ledres², Gabriel O. dos Santos², Luciana C. Furtado², Andreza L. do Nascimento¹, Marcos G. da Cunha¹, Beatriz P. Bosque¹, Danieli C. Gonçalves¹, Daniela B. B. Trivella¹, Leticia V. Costa Lotufo², Rafael de Felício¹

debora.rodrigues@lnbio.cnpem.br

¹ Brazilian Biociences National Laboratory (LNBio), Brazilian Center of Research in Energy and Materials (CNPem), Campinas, SP, Brazil ² Marine Pharmacology Laboratory, Department of Pharmacology, Institute of Biomedical Sciences, University of São Paulo, São Paulo, SP, Brazil

Marine environments, particularly along Brazil's extensive coastline, represent a promising source of novel bioactive compounds. These regions host a high diversity of marine microorganisms, especially bacteria containing yet-undiscovered compounds with pharmaceutical potential. Advances in metabolomics are opening new avenues for drug discovery by improving the ability to predict, detect, and characterize novel compounds. In this context, the present study analyzed 98 previously uncharacterized marine bacterial strains isolated from ascidian *Herdmania pallida*, aiming to investigate their metabolomic profiles and biological potential through cytotoxicity assays. The isolated strains were cultured in A1 medium (starch 10 g/L, yeast extract 4 g/L, peptone 2 g/L) prepared with 75% seawater and incubated under agitation at 28°C and 200 rpm. After 7 days, liquid cultures were extracted with ethyl acetate (1:1). Extracts were sent to LNBio/CNPem through the collaborative project Bank of Molecules, where they were registered, stored under low temperatures and inert atmosphere, and further processed. Subsequently, UPLC-MS/MS analyses and cytotoxicity assays were performed on all samples. The LC-MS/MS data obtained (mzXML) were processed using the NP³ MS Workflow, and chemical annotations were performed with GNPS and UNPD databases. In total, 3,109 protonated compounds [M+H]⁺ were detected, of which 161 (5.17%) were annotated and classified into ten grouped chemical superclasses. The most representative annotated compounds belonged to "Alkaloids & Lactams" and "Terpenes & Carotenoids". The remarkably high proportion of unannotated compounds (94.83%), most of which occur in clusters exclusively associated with specific marine bacterial strains, highlights the potential novelty and uniqueness of this collection. Among all extracts evaluated in the cytotoxicity assay, 15 were selected for dose-response curve construction, of which 3 exhibited a selectivity index greater than 2 against the HCT-116 cell line. These findings suggest that these strains may be promising sources for the discovery of new antitumor compounds derived from Brazilian marine bacteria. Acknowledgement: Fapesp (proc. 2023/08735-1).

Keywords: Metabolomics, microorganism, marine bacteria, cytotoxic assays, NP³ MS Workflow





Chemical comparative study of *Byrsonima verbascifolia* (L.) DC and *Byrsonima sericea* DC and it's flavonoids by molecular networking

Gabriel Sardinho Greggio^{1*}, Daniel Rinaldo², Eduardo Ribeiro dos Santos³, Miriam Sannomiya¹

gabrielgreggio@gmail.com

1- Universidade de São Paulo, São Paulo, SP, USP Leste, 03828-000, Brasil 2- Universidade Estadual Paulista Julio de Mesquita Filho, Bauru, SP, Faculdade de Ciências, 17033-360, Brasil 3- Universidade Estadual do Tocantins, Palmas, TO, Fundação UNITINS, 77001-090

The genus *Byrsonima*, popularly known as murici, is widely used in folk medicine due to its anti-inflammatory and anti-ulcer activities, which justify its traditional use in the treatment of gastrointestinal disorders. Species of this genus frequently contain flavonoids derived from quercetin, proanthocyanidin derivatives, galloylquinic acid derivatives, and amentoflavone. However, some species of *Byrsonima* are considered neglected, meaning their industrial, nutritional, and chemical potential has been little explored. This is the case of *Byrsonima verbascifolia* and *Byrsonima sericea*, two species whose chemical arsenal remains poorly studied. One approach for evaluating the chemical profile of plants is the use of liquid chromatography coupled with mass spectrometry. Chromatographic peak areas and fragmentation profiles obtained by HPLC-ESI-IT-MS/MS can be processed in GNPS (Global Natural Products Social Network) to construct molecular networks, a resource that allows the visualization of structural relationships among detected compounds. In this way, it was possible to generate and compare the networks of hydroethanolic leaf extracts of *B. verbascifolia* and *B. sericea*, highlighting the diversity and relative abundance of their secondary metabolites. The molecular network comprised 57 nodes, with 32 indicating molecules exclusive to *B. verbascifolia*, 12 to *B. sericea*, and 13 shared between both species. Two clusters were formed, corresponding to the classes of terpenes and flavonoids. The terpenes identified included myrcene (m/z 159) and ebelactone and its derivatives. The main class of metabolites identified was flavonoids, particularly glycosylated quercetin derivatives, characterized by the aglycones at m/z 301 (quercetin), m/z 299 (diosmetin), and m/z 300 (peonidin), followed by the loss of sugars: -132 Da for pentoses (-Xyl, -Ara), -146 Da for deoxyhexoses (-Rha), -162 Da for hexoses (-Glu), or the loss of galloyl groups (-152 Da). The results are consistent with what is expected for the genus, as other *Byrsonima* species, such as *B. crassa*, *B. intermedia*, and *B. fagifolia*, have been reported to contain diverse glycosylated and galloylated quercetin derivatives. However, no reports of diosmetin or peonidin derivatives have been made in the genus. The data indicate a greater chemical diversity and molecular abundance in the hydroethanolic leaf extracts of *Byrsonima verbascifolia*, especially flavonoids, which may account for the biological activity of the extract, since both quercetin and diosmetin derivatives exhibit strong anti-inflammatory potential.

Keywords: *Byrsonima verbascifolia*, murici, GNPS, molecular networking, flavonoids.





Encapsulation of *Syzygium aromaticum* and *Cymbopogon citratus* Essential Oils using new technology with the Chitosan-Cholesteryl polymer and new methodology in homogenization by Ultrasound in a probe.

Danielle Fernandes da Silva¹, Jéssica Amaral¹, Regiane Bueno², João Pedro Bomfim², Toby Bruce³, David Buss³, Clare Hoskins⁴, Luis Guillermo Cuadrado¹, Moacir Rossi Forim¹, Maria Fátima das Graças Fernandes da Silva¹, João Batista Fernandes¹

1 – Universidade Federal de São Carlos, Dpto. de Química, Rod. Washington Luís, Km 235, São Carlos-SP, Brasil. 2- São Paulo State University “Júlio de Mesquita Filho” – UNESP School of Agricultural Sciences – FCA, Botucatu Campus Department of Plant Protection. 3- School of Life Sciences, Huxley Building, Keele University, Keele, Staffordshire, ST5 5BG, UK. 4- Dept. of Pure and Applied Chemistry Technology Innovation Centre University of Strathclyde 99 George Street Glasgow UK

Botanical pesticides are of great importance in Integrated Pest and Disease Management; they control insect pests and plant pathogens, pose no risk to natural enemies, and are environmentally friendly. However, they have some disadvantages that hinder their use in agriculture, making them poorly accepted by the agricultural community. These include a short period of activity due to their faster degradation due to their volatile nature. They are also insoluble in water. This study sought to optimize the activity of these pesticides by encapsulating the active ingredient, thereby increasing the availability of these compounds to protect plants and improving their water solubility. Previous studies with the oils *Syzygium aromaticum* and *Cymbopogon citratus*, popularly known as Clove and Lemongrass, showed promising activity against the corn pest *Spodoptera frugiperda*, so encapsulation methods for these oils were used in this study. These encapsulated formulations were produced as an emulsion using only water, the polymer, and the oil, and homogenization was performed using probe ultrasound. The polymer used was chitosan-cholesteryl, a novel molecule being tested for encapsulation of chemotherapy drugs for pancreatic cancer. After emulsion formation, they were quantified by GC-MS. The result was emulsions with excellent homogenization without precipitates or supernatants, and GC quantification demonstrated 80% encapsulation of the active ingredient.

Keywords: Insecticide, Essential oil, Encapsulation, Polymer





COMPARISON OF ESSENTIAL OIL AND AROMA FROM GUARANA FRUIT

Isaias Wallace Maciel da Silva¹, Alana Evelynne Tavares Batista², Sergio Massayoshi Nunomura³

wallaceisaias3@gmail.com

1-Post-Graduate Program in Chemistry, Federal University of Amazonas (UFAM), Manaus –AM, Brazil. 2- Chemistry Department, Federal University of Amazonas (UFAM), Manaus –AM, Brazil. 3- Coordination of Technology and Innovation, National Institute for Amazonian Research, 69067-375, Manaus-AM, Brazil.

The volatile compounds found in fruits and flowers play a crucial role in ecological interactions, particularly in pollination processes. The aroma of a fruit or flower results from a complex mix of volatile compounds that attract specific pollinators. Amazonian guarana, scientifically known as *Paullinia cupana* (Sapindaceae), is one of the primary forest products in the Western Amazon. The harvesting of non-timber forest products has gained increasing interest as an economic alternative for the region, with guarana being a significant export commodity. Products derived from Amazonian guarana have a distinctive chemical profile that is unique to the Amazon region¹. One factor influencing this uniqueness may be its pollination, which in the area is mainly carried out by stingless bees of the genus *Melipona*. To understand pollinator specificity, studies have been conducted on the chemical composition of propolis produced by guarana, which is exclusively pollinated by *Melipona seminigra*. Previous studies have shown that the non-volatile compounds present in guarana extracts share very similar compositions². We have now investigated the aromas and essential oils of guarana fruits to further explore pollinator specificity. Because essential oils and aromas are typically composed by different constituents, the studies employed two methods: Clevenger hydrodistillation extraction for essential oils and headspace by solid-phase microextraction (HS-SPME) to analyze the aromas. The essential oil and aroma were extracted from both the outer rind (epicarp) and the aril (white pulp) of the guarana fruit (*Paullinia cupana*). The essential oil extraction lasted for two hours, while aroma extractions used the HS-SPME technique with Polydimethylsiloxane (PDMS) and Carboxen-PDMS fibers. Compositional analyses of the essential oils and aromas were conducted using gas chromatography-mass spectrometry (GC-MS) and gas chromatography-flame ionization detection (GC-FID) techniques. Identification was based on retention indices and an analysis of the mass spectra, which were compared with existing libraries. The comparative analysis revealed that the essential oil and aroma of the guarana fruit possess distinct chemical profiles, allowing for the identification of terpenes, esters, alcohols, ketones, and aldehydes.

Keywords: *Paullinia cupana*, essential oil, volatile profile, HS-SPME; Amazonian biodiversity

¹Salles et al, *Food Chemistry*, V 371, p13068, 2022.

²Oliveira et al, *Biochemical Systematics and Ecology*, v. 112, p. 104769, 2024.





PHYTOCHEMICAL PROFILE AND BIOACTIVE POTENTIAL OF ROSMARINUS OFFICINALIS EXTRACT

Lívia Rodrigues Gamarano^{1*}, Lara Melo Campos¹, Priscila de Lima Paula¹, Ari Sérgio de Oliveira Lemos¹, Rodrigo Luiz Fabri¹.

liviagamarano2@gmail.com

1- Laboratório de Produtos Naturais Bioativos, Departamento de Bioquímica, Instituto de Ciências Biológicas, Universidade Federal de Juiz de Fora, Juiz de Fora, Minas Gerais CEP 36036-900, Brasil.

Since ancient times, plants have been valued as food and medicine due to their richness in bioactive compounds. Among them, Lamiaceae species stand out for their culinary and therapeutic uses, mainly attributed to phenolic compounds with antioxidant and anti-inflammatory properties. In view of the increasing global demand for natural bioactive ingredients, this study aimed to characterize the phytochemical composition and biological potential of *Rosmarinus officinalis* extract. Aerial parts of the plant were collected in Juiz de Fora (Minas Gerais) and extracted by static maceration with hydroalcoholic solvent (1:1). Phytochemical profiling by UFLC-QTOF-MS (Lemos *et al.*, 2020) and HPLC-DAD revealed a diverse composition, including phenolic acids, flavonoids, and diterpenes. Key compounds identified were rosmarinic acid, chlorogenic acid, hispidulin-7-glucoside, luteolin, pectolinarigenin, genkwanin, carnosol, and rosmadial. Chromatographic analysis also confirmed additional flavonoids, such as rutin, epicatechin, quercetin, isoquercitrin, and myricetin, contributing to the extract's chemical complexity. The coexistence of hydrophilic and lipophilic metabolites suggests potential synergistic interactions, in which phenolic compounds and diterpenes may act complementarily in modulating oxidative and inflammatory pathways (Francolino *et al.*, 2023). Rosmarinic acid, the predominant phenolic, is widely recognized for its strong antioxidant capacity through radical scavenging and metal chelation. Meanwhile, carnosol, an abietane diterpene, has been described as an anti-inflammatory agent and a regulator of cell signaling processes (Pais *et al.*, 2024). The presence of these multifunctional metabolites highlights the ability of the extract to act on multiple biological targets, reinforcing its potential as a source of functional ingredients. The phytochemical profile observed confirms *R. officinalis* as a promising candidate for nutraceutical and functional food applications, particularly in the management of metabolic disorders linked to chronic oxidative stress. These results support the relevance of exploiting this species not only in food formulations but also as a basis for developing dietary supplements and future active pharmaceutical ingredients. Further studies addressing safety, bioaccessibility, and in vitro bioactivities are essential to validate its translational potential and ensure its applicability in the health and wellness market.

Keywords: *Rosmarinus officinalis*; phenolic compounds; phytochemical profile; antioxidant activity; nutraceuticals





SCENTS FROM BRAZILIAN ATLANTIC FOREST: CHEMICAL PROFILE AND BIOACTIVITY OF ESSENTIAL OILS FROM THREE MYRCIA SPECIES (MYRTACEAE)

Pedro Peixoto dos Reis¹, Camila de Faria Nascimento², Thiago Fernandes³, Francisco P. Machado⁴, Lucas Silva Abreu⁵, Aislan, C. R. F. Pascoal⁶, Claudia Moraes de Rezende², Rafael Ferreira da Silva^{1,2}

pereis@id.uff.br; raferreirasilva@id.uff.br

¹Laboratório de Fragrâncias e Aromas da Biodiversidade, IQ – Universidade Federal Fluminense

²Laboratório de Análise de Aromas, IQ – Universidade Federal do Rio de Janeiro

³Instituto de Pesquisas, Jardim do Botânico do Rio de Janeiro

⁴Laboratório de Tecnologia de Produtos Naturais, FF – Universidade Federal Fluminense

⁵Laboratório de Química de Produtos Naturais, IQ – Universidade Federal Fluminense

⁶Laboratório de Pesquisa de Produtos Naturais e Moléculas Bioativas, ISN - UFF

Niterói city, in Rio de Janeiro's metropolitan region, preserves 56% of its territory as Atlantic Forest, a major biodiversity hotspot that still harbors endemic species with phytochemical potential. Among its representative groups, the Myrtaceae family stands out for its wide distribution and industrial relevance. A survey on Re flora Herbario Virtual recorded 96 Myrtaceae species in Niterói, 73% of which remain unstudied for their essential oils. This study is part of a broader project on the prospection of aromatic Myrtaceae in local reserves. Leaves of *Myrcia laranthifolia*, *M. rubiginosa*, and *M. ovata* were selected for their pleasant aromas. Samples were collected along a trail and subjected to hydrodistillation for 3 h in a Clevenger-type apparatus. Essential oils (1% in hexane) were analyzed by GC-FID and GC-MS with an HP-5MS column [1]. Percentage composition was determined by FID peak-area normalization, and components identified by NIST library, literature, and linear retention indices [2]. Antiproliferative activity was evaluated by the MTT method in the MG-63 cell line (osteosarcoma). Results showed sesquiterpenes predominating in *M. rubiginosa* (92%) and *M. ovata* (95%), while *M. laranthifolia* was rich in monoterpenes (>50%). The major compounds were (*E*)- β -Farnesene (26.8%) and (*E*)-Caryophyllene (25.9%) in *M. ovata*; α -pinene (33.7%) and β -pinene (6.7%) in *M. laranthifolia*; and (*E*)-Caryophyllene (15.3%), Bicyclogermacrene (12.3%), and Spirolepechinene (10.2%) in *M. rubiginosa*. In the analysis of antiproliferative activity, the essential oils were able to reduce cell viability at a dose of 125 μ g/mL. *M. laranthifolia* reduced cell viability by 23.25%, *M. rubiginosa* reduced cell viability by 72.89% and *M. ovata* by 37.11%. This is the first report on the chemical composition of the essential oil from *M. rubiginosa* and the oils showed slight cytotoxic activity in osteosarcoma.

Keywords: essential oils, volatile compounds, Myrtaceae, phytochemistry, biodiversity

[1] Silva et al. Journal of Essential Oil Research, 27:5, 417-420, 2015; [2] ADAMS, Robert P. 4.1 ed., 2017.





IDENTIFICATION OF MODIFIED FLAVONOIDS AND SUPPOSED BIOSYNTHETIC PRECURSORS IN WOOD RESIDUES OF *Peltogyne catingae* Ducke

Davi Santos Oliveira^{1*}, Priscila Brasil Augusto de Souza¹, Jennifer Araújo de Oliveira Lima¹, Gabriel Faria de Souza², Claudete Catanhede do Nascimento², Maria da Paz Lima²

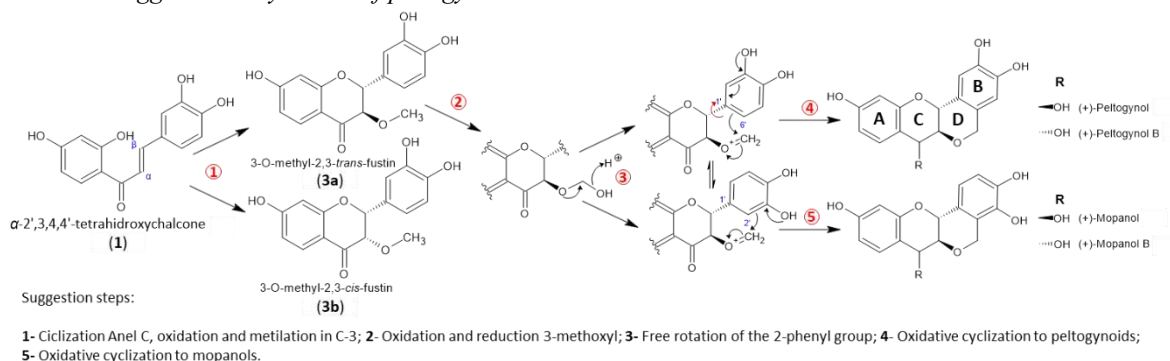
david.quimicas2@gmail.com

1-Instituto de Ciências Exatas, Programa de Pós-Graduação em Química, UFAM, Av. Gen. Rodrigo Octávio, 6200, Manaus, AM, Brazil. 2-Coordenação de Tecnologia e Inovação, Instituto Nacional de Pesquisas da Amazônia – INPA, Av. André Araújo, 2936, Manaus, 69067-375, Brazil.

Peltogyne catingae Ducke (Detarioideae, Fabaceae), known as “roxinho” or “pau-roxo,”¹ is an Amazonian species whose heartwood has a characteristic purple color due to the presence of peltoginoids, flavonoids modified by the addition of a D ring.² In addition to peltoginoids, other phenolics, such as flavones, flavonones, chalcones, and phenolic acids, have been reported in the wood of *Peltogyne* spp. In this context, the present study describes the isolation and identification of constituents present in wood residues of *P. catingae*. The wood waste was supplied by the Wood Technology Laboratory (LTM - INPA), dried, identified, and processed, and subsequently subjected to extraction with methanol at room temperature. In a previous study of the methanolic extract, we identified the peltoginoids (+)-peltoginol, (+)-mopanol, and their epimers,³ and continued fractionation by column chromatography using silica gel (70-230, 230-400 mesh) and Sephadex LH-20 resulted in the isolation and identification of chalcone α -2',3,4,4'-tetrahydroxychalcone (**1**), the peltoginoid 2,3-*trans*-pubschin (**2**) and the flavonoids 3-methoxy-2,3-*trans*-fustin (**3a**) and its epimer 2,3-*cis* (**3b**). We suggest that chalcone **1** and flavonoids **3a**, **b** are biosynthetic precursors of *P. catingae* peltoginoids, as shown in Scheme 1. The substances were identified by 1D and 2D NMR and Mass Spectrometry, with data confirmed by comparison with the literature. This study represents the first report of these substances in *P. catingae* and expands the phytochemical profile, highlighting the scientific value added to its wood residues.

Keywords: flavonoids, chalcone, isomers, Fabaceae, NMR

Scheme 1. Suggested biosynthesis of peltoginoids



[1] Kochanovski, F.J., Nogueira, L.H., Rosa, M.P., Mansano, V.F. & Sartori, Ângela L. (2025) *Phytotaxa* 688: 1–68.;

[2] Taga, Y.; Yamauchi, K.; Mitsunaga, T. (2025) *Wood Sci. Technol.*, 59: 11-33; Malan, E. & Roux, D. (1974). *Ptytochemistry*, 13: 1575-1579.

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PENTACYCLIC TRITERPENES FROM THE BRANCHES OF *Monteverdia acanthophylla* (CELASTRACEAE)

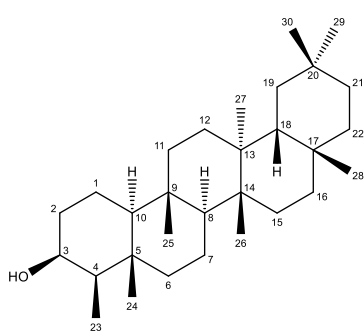
Rafael do Prado Gomes,^{1*} Lucienir Pains Duarte,¹ Grasiely Faria de Sousa.^{1*}

[*rafaelpgomes1@gmail.com](mailto:rafaelpgomes1@gmail.com), grasielysousa@ufmg.br

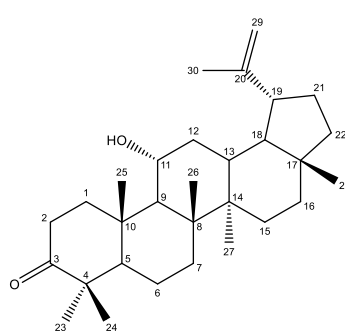
1- Neplam, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Monteverdia acanthophylla (basionym *Maytenus acanthophylla*) is a Brazilian species in the family Celastraceae, commonly known as “pau-de-jararaca” or “espinheira-santa”, occurring mainly in the states of Bahia and Minas Gerais and.¹ This study reports the phytochemical investigation of hexane and chloroform extracts obtained from the branches of the species. Chromatographic methods, including thin-layer chromatography (TLC) and column chromatography (CC), were employed to isolate the compounds. Structural elucidation was carried out by ¹H and ¹³C nuclear magnetic resonance (NMR) spectroscopy, supported by 2D NMR experiments (HSQC, HMBC, COSY, and NOESY). The pentacyclic triterpene friedelan-3 β -ol (**1**, friedelane-type skeleton) and the lupane-type triterpenes 11 α -hydroxylup-20(29)-en-3-one (**2**) and lup-20(29)-ene-2 α ,3 α ,11 α -triol (**3**), in addition to fatty acids, were identified. Among these, the two lupane triterpenes are reported here for the first time from *M. acanthophylla*. Furthermore, the compound **3** is described for the first time in the literature.

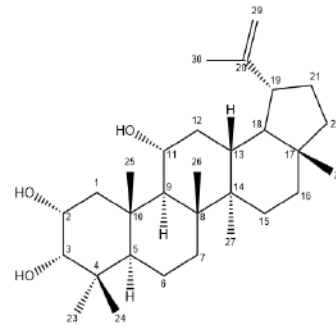
Figure 1: Chemical structure of compounds **1–3**.



friedelan-3 β -ol (**1**)



11 α -hydroxylup-20(29)-en-3-one (**2**)



lup-20(29)-ene-2 α ,3 α ,11 α -triol (**3**)

Keywords: Celastraceae; phytochemical study; pentacyclic triterpenes; lupanes.

References: 1) BIRAL, L. et al. Systematics of New World *Maytenus* (Celastraceae) and a New Delimitation of the Genus. *Systematic Botany*, 42, 680–693, 2017. 2)

Acknowledgments: CAPES, CNPq and FAPEMIG





ANTI-AGING, ANTIGLYCANT, ANTIPHOTOMUTAGENIC AND PHOTOPROTECTIVE POTENTIAL OF JURUBATIBA SANDBANK (RJ) PLANTS.

Leilane Falcão de Freitas^{1*}, Victor de Azevedo Neres¹, Alessandra da Silva Correia¹, Carla Monteiro Leal¹, Patrícia H. B. de Moura¹, Raiane Rosales Diniz³, Michelle Frazão Muzitano², Maria Isabel Sampaio dos Santos¹, Ivana C. R. Leal¹ falcao85@ufrj.br

¹Laboratório de Produtos Naturais e Ensaio Biológicos (LaProNEB), Faculdade de Farmácia, Universidade Federal do Rio de Janeiro; ²Laboratório de Produtos Bioativos (LPBio), Instituto de Ciências Farmacêuticas, Centro Multidisciplinar UFRJ – Macaé; ³Instituto de Ciências Farmacêuticas, Centro Multidisciplinar UFRJ – Macaé, Rio de Janeiro, Brazil

Skin aging may be associated with factors as senescence, sun exposure and high-sugar diet. Prolonged skin exposure to UV rays can increase the production of reactive oxygen species, damaging biomolecules, resulting in wrinkles. Several plant extracts have anti-aging properties, with emphasis on those rich in phenolics, due to their antioxidant and metalloenzyme-inhibiting capabilities. Therefore, this work aimed to investigate extracts from Jurubatiba Sandbank species, as follows: *Ocotea notata* (**ON**), *Humiria balsamifera* (**HB**), *Tapirira guianensis* (**TG**) and *Tocoyena bullata* (**TB**), regarding their chemical profile BY UHPLC-DAD-MS/MS. In addition, there were investigated the anti-aging, antiglycant, photoprotection and antiphotomutagenic potentials of the extracts in *in vitro* models. The antioxidant capacity was evaluated by the ABTS, DPPH, and FRAP methodologies. Enzyme inhibition has been analyzed with the enzymes tyrosinase, collagenase and elastase, and the antiglycant activity, by fluorimetry (adapted BSA-glucose model). Photoprotective and antiphotomutagenic activities were evaluated by irradiating *S. cerevisiae yno1* strain with simulated sunlight. Among the antioxidant assays, **ON** stood out for presenting free radical scavenging capacity by the ABTS ($EC_{50} = 2.62 \pm 1.21 \mu\text{g/mL}$) and DPPH ($EC_{50} = 8.23 \pm 1.55 \mu\text{g/mL}$) radicals scavenging capacities compared to the standard rutin ($EC_{50} = 4.65 \pm 0.61 \mu\text{g/mL}$ and $EC_{50} = 6.90 \pm 1.07 \mu\text{g/mL}$, respectively). The **ON** extract presented 63.88% inhibition activity of tyrosinase at $20 \mu\text{g/mL}$, showing to be promised in comparison to the kojic acid ($20 \mu\text{g/mL}$), with 93.48% inhibition. For the antiglycation assay, the four species showed promising results, with emphasis on **ON** (84.97%, at 0,5% after 28 days incubation). In addition, **ON** showed the presence of the flavonoid procianidin type B (m/z 577) as major metabolite, which are already recognized for their antioxidant capacity, among other minor compounds such as avicularin (m/z 433). *In vitro* assay with *S. cerevisiae yno1* strain showed that **ON** increased the LD37 from 2.5 kJ UVB (control) to 4.0 kJ UVB (treatment), demonstrating its photoprotective potential. Additionally, in the CanR mutant assay, **ON** reduced photomutagenicity by 2.4-fold (1469 vs. 3878 mutants), confirming its antiphotomutagenic activity. The results are promising, with emphasis on **ON**, which potential antioxidant, antiglycation, antiphotomutagenic and photoprotective effects. The extracts will also be investigated for activity against elastase and collagenase for future development of topical formulations.



Keywords: *Anti-aging, Photoprotection, Antiphotomutagenic, Antiglycants, Natural Products, Restinga de Jurubatiba, Ocotea notata.*

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Sociedade Brasileira de Química
Divisão de Produtos Naturais





**COMPARATIVE METABOLOMIC ANALYSIS OF SECONDARY METABOLITES
PRODUCED BY ENTOMOPATHOGENIC FUNGI**

Ana Livia Vezzoso^{1*}, Fabiola Almeida García¹, Marília Elias Gallon¹, Norberto Peoporine Lopes¹, Barbara Matos do Prado², Tatiana Magalhães², Lucas von Zuben²

analivia2442@usp.br

1-NPPNS, Faculdade de Ciências Farmacêuticas de Ribeirão Preto da Universidade de São Paulo (FCFRP-USP), Av. do Café, s/n, Ribeirão Preto, SP, 14040-903, Brazil. 2-Decoy Tecnologia em Controle de Pragas S.A., Av. Dra Nadir Aguiar, 1805, prédio 2, sala 301, Jd. Dr. Paulo Gomes Romeo, Ribeirão Preto, SP, 14056-440, Brazil.

Entomopathogenic fungi, microorganisms that infect and seriously disable or kill insects, are widely recognized for producing bioactive secondary metabolites with significant biotechnological potential. In this study, we investigated the chemical profiles of three entomopathogenic fungi, *Beauveria bassiana*, *Metarhizium anisopliae*, and *Purpureocillium lilacinum*, by analyzing the production of intracellular and extracellular metabolites using liquid cultivation in Potato Dextrose Broth (PDB). Intracellular metabolites were extracted from fungal biomass using a methanol:water (4:1, v:v) solution, while extracellular metabolites were isolated from the culture supernatant by liquid-liquid partitioning with ethyl acetate. Metabolomic analysis was conducted via liquid chromatography-tandem mass spectrometry (LC-MS/MS), following by data processing in the software MzMine and molecular networking analysis performed in the Global Natural Products Social Molecular Networking platform (GNPS). Results revealed distinct metabolomic signatures across species and extraction types. *Metarhizium anisopliae* was characterized by destruxins (A, B, E1, B1), known for insecticidal and immunosuppressive properties. *Beauveria bassiana* displayed a profile dominated by beauvericin, alkaloid derivatives, and diketopiperazines. *Purpureocillium lilacinum* exhibited significant biological activities, according to the literature. Extracellular extracts showed greater chemical diversity than intracellular extracts, suggesting secretion as the primary route for metabolite release. These findings highlight the metabolic diversity of entomopathogenic fungi and the effectiveness of LC-MS/MS and molecular networking for profiling secondary metabolites, providing a foundation for further studies on purification, structural elucidation, and bioactivity for biotechnological applications.

Keywords: *Beauveria bassiana*, *Metarhizium anisopliae*, *Purpureocillium lilacinum*, LC-MS/MS, molecular networking, natural products





CONSERVATION STRATEGY FOR *Macrosiphonia velame* (APOCYNACEAE)

Joanna Conde Maynié^{1,2*}, Valéria Sieiro Conde Correa¹, Juliana da Silva Coppede²

joanna.maynie@sou.unaerp.edu.br

1-Reserva EcoCerrado Brasil, Rod MG 262, Araxá, MG, km 715, Brazil, 2-Universidade de Ribeirão Preto, Pós-graduação em Biotecnologia, UNAERP, Av. Costabile Romano, 2201, 14096-380, Ribeirão Preto, SP, Brazil.

Subshrub species of the Cerrado are underrepresented in seed collection due to limited fruiting and anemochoric dispersal, which hinders propagule acquisition and compromises ecological restoration by restricting the recovery of the herbaceous-subshrub layer, crucial to the biome's resilience. *Macrosiphonia velame* (white velame) exemplifies this gap: a perennial species with erect stems measuring 25 to 40 cm, covered by a woolly indumentum and tuberous roots, used ethnopharmacologically in the treatment of dermatoses, gastrointestinal disorders, and rheumatic and infectious conditions (syphilis), highlighting its potential as a source of bioactive metabolites. For this species, there are no agronomic cultivation protocols or optimized propagation methods, in addition to its rare occurrence in the field, as indicated by ethnobotanical surveys according to Campos et al. (2010). This scenario is exacerbated by the loss of approximately 51% of the Cerrado's native vegetation, jeopardizing the goals established in the Paris Agreement. Policies such as the Participatory Climate Plan (2025) and the PPCerrado (2023) provide a regulatory framework, but effective conservation requires strategies. In this study, the conservation approach involved a biotechnological strategy, the *in vitro* introduction of *M. velame*. Seed collection was carried out and registered in SisGen under the code AB63A0D. Two hundred eighty of these seeds were sequentially disinfested with cercobin (0.5%), sodium hypochlorite (0.5%), autoclaved water at 82°C, and hydrogen peroxide (0.6V/L) and subsequently grown in MS/2 medium. After the emergence of the first pair of post-cotyledonary leaves, the seedlings were acclimated in a greenhouse using a 1:1:1 substrate (Carolina:soil:sand) with daily irrigation. One hundred twenty two seeds (43,57%) germinated, and six seedlings with the truth first pairs of leaves (2,14%) were submitted to acclimatization. This six plantlets were successfully acclimated (100%). This work aligns with the 2030 Agenda objectives, contributing to climate change mitigation, biodiversity conservation, water and food security, resilience to natural disasters, and the supply of bioactive compounds for pharmaceutical development.

Keywords: biotechnology, hydrogen peroxide, *in vitro* culture, velame





**PHYTOCHEMICAL STUDY OF THE HEXANE/ETHYL ETHER
EXTRACT OF *Maytenus quadrangulata* (CELASTRACEAE) ROOTS**

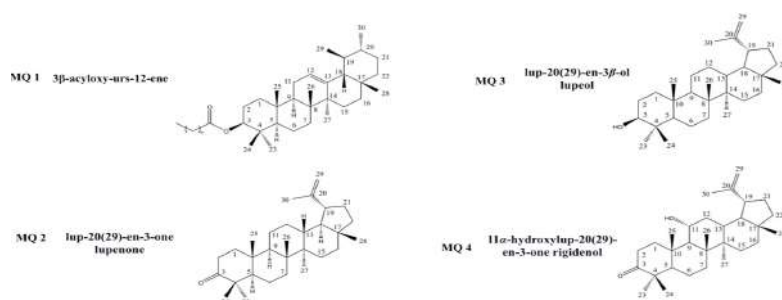
Fernanda C. Álvares^{1*}, Hiago O. Esteves¹, Mariana G. Aguiar¹, Grasiely F. Sousa¹,
Lucienir P. Duarte¹

fernandacamposalvares@gmail.com

1- Departamento de Química, Instituto de Ciência Exatas, UFMG.

The genus *Maytenus*, one of the largest within the Celastraceae family, is widely recognized for its chemical diversity and pharmacological potential, particularly due to the occurrence of pentacyclic triterpenes with remarkable biological activities.¹ *Maytenus quadrangulata*, a Brazilian species native to the Atlantic Forest and Caatinga biomes, popularly known as “espinho-de-deus”, has been the subject of phytochemical studies that revealed triterpenes with cytotoxic and antiviral activities²; however, it remains underexplored regarding the chemical composition of its roots. In this context, the present study reports the phytochemical investigation of the hexane/ethyl ether (1:1) root extract of *M. quadrangulata*. Successive column chromatography (CC) and some preparative layer chromatography (PLC) led to the isolation of four pentacyclic triterpenes: 3 β -acyloxy-urs-12-ene (**MQ 1**), an ursane skeleton compound with reported antioxidant and antimicrobial properties; lup-20(29)-en-3-one (lupenone, **MQ 2**), a lupane skeleton triterpene with anti-inflammatory, antiviral and anticancer activities, described for the first time as a constituent of this species; lup-20(29)-en-3 β -ol (lupeol, **MQ 3**), a triterpene known for its anti-inflammatory and antioxidant properties; and 11 α -hydroxylup-20(29)-en-3-one (rigidenol, **MQ 4**), with previously reported antimicrobial activity. The structural characterization of these compounds was achieved by ¹H and ¹³C NMR analyses. This study highlights the chemical richness of *M. quadrangulata* roots and reinforces the relevance of Celastraceae species as a promising source of bioactive molecules with potential applications in drug discovery.

Figure 1: Chemical structure of compounds **MQ 1– MQ 4**



Keywords: Triterpenes, Celastraceae, *Maytenus quadrangulata*, Pentacyclic terpenes.

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Prospecting antimicrobial molecules from marine bacteria of Northeastern Brazil

Anne Natália Almeida de Oliveira^{1*}, Magalie Robert^{2*}, Elthon Gois Ferreira^{3*}, Leticia Costa Lotufo³, Sylvie Chevalier², Renata Mendonça Araujo¹

annenatalia213@gmail.com

¹Universidade Federal do Rio Grande do Norte, Laboratório de Isolamento e Síntese de Compostos Orgânicos, Instituto de Química, 59078-970, Natal RN.

²CBSA (Laboratory of Bacterial Communication and Anti-infectious Strategies) da Universidade de Rouen/ França

³Laboratório de Farmacologia de Produtos Naturais Marinhos – ICB/USP

The search for new molecules to combat multidrug-resistant bacteria of the ESKAPE group is a global priority, as highlighted by the WHO. Natural products, especially those produced by *Streptomyces* species, remain among the most promising sources of new antibiotics. The Brazilian marine environment offers a unique opportunity to accelerate the discovery of innovative antimicrobial agents. In this study, we explored acetate extracts from *Streptomyces* strains (BRA 679, BRA 732, and BRA 720) from the MICROMARIN database, aiming to advance dereplication studies and to understand possible antimicrobial mechanisms of action against *Pseudomonas aeruginosa*, a pathogen with high resistance and biofilm-forming capacity. For this purpose, extracts at a concentration of 10 mg/mL were tested for biofilm formation and biofilm dispersion, as referenced by Monroe et al., 2014. For pyocyanin quantification, the method described by Saha et al., 2023 was applied. The results obtained from these three approaches demonstrated the promising potential of the evaluated extracts, providing a comprehensive view of their effects on bacterial viability as well as on factors related to virulence and infection persistence. The extracts showing the best results (BRA 679 and BRA 732) were further analyzed by MALDI-TOF, where a laser irradiates the sample, causing ionization, and the m/z is calculated from the time of flight. In this analysis, HCCA and DHB matrices were used, forming positive ions $[M+H]^+$, which allowed the identification of biomolecules. For strain BRA 679 (HCCA), characteristic peaks of seco-surugamide B (m/z 974.66) and fungicin C (m/z 711.15) were detected, while for strain BRA 732 (HCCA), surugamide A (m/z 911.62) and O-benzyl-surugamide F (m/z 1247.76) were observed. These compounds have been previously reported in the literature for their antimicrobial, cytotoxic, and antifungal activities. In addition, characteristic peaks of cyclic peptides were observed in both strains, a class well known for their high antimicrobial activity due to diverse mechanisms of action. These findings highlight the potential of this material as a promising source of antimicrobial molecules for addressing infections caused by multidrug-resistant strains.

Acknowledgments: PPGQ, CAPES, LISCO-UFRN, LBGM-UFRN, CEMMO-USP/Ribeirão Preto, CBSA, and LAFARMAR.

Keywords: “SKAPE”, “Antimicrobial Resistance”, “Marine bacteria”, “*Streptomyces*”, “MALDI”.

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Chemical diversity and antimicrobial activity of endophytic fungi associated with *Geissospermum* sp.

João Victor Do Nascimento^{3*}, Jacqueline S. Cruz², Kaio Murilo Monteiro Espíndola¹, Gabriel Pires Makhoul³, Matheus Gabriel Gomes Martin⁴, Lidilhone Hamerski¹

kaioespindola@hotmail.com

1-Instituto de Pesquisas de Produtos Naturais Walter Mors - Universidade Federal do Rio de Janeiro-IPPN/UFRJ. 2. Seção de Engenharia Química - Instituto Militar de Engenharia. 3 - Faculdade De Farmácia - Universidade Federal do Rio de Janeiro - FF/UFRJ. 4- Instituto de Química, Universidade do Estado do Rio de Janeiro (UERJ), Rio de Janeiro, Brasil.

The search for novel bioactive compounds has positioned the bioprospecting of endophytic fungi as a strategic field, due to the ability of these microorganisms to synthesize metabolites of biotechnological and pharmacological relevance. Therefore, the flora of the Atlantic Forest represents a rich reservoir of bioactive substances, with the genus *Geissospermum* notable for its traditional medicinal applications and chemical profile, which includes indole and bis-indole alkaloids and derivatives such as flavopereirine and geissosquizoline, compounds associated with antifungal, antileishmanial, and anticancer activities. Consequently, endophytic fungi associated with *Geissospermum* constitute a promising source for the discovery of bioactive molecules with high therapeutic potential. This study aimed to isolate and characterize the endophytic microbiota of *Geissospermum* and to evaluate the chemical profiles and biological activities of the obtained extracts. Leaves and stems of *Geissospermum* spp. were surface-sterilized and inoculated on various culture media for 15 days, followed by successive subculturing to obtain pure colonies. For extract production, the isolates were cultivated in potato dextrose broth under constant agitation at room temperature for 14 days, and metabolites were recovered through liquid-liquid extraction with ethyl acetate. HPLC analyses of the extracts revealed distinct chromatographic profiles, reflecting the chemical diversity of these strains. Notably, four isolates exhibited antimicrobial activity against *Staphylococcus aureus*. The authors would like to thank the funding bodies CAPES, CNPq, and FAPERJ.

Keywords: *Fungos endofíticos; Geissospermum; Bioprospecção; Compostos bioativos; HPLC; Atividade antimicrobiana*





METABOLIC AND BIOLOGICAL POTENTIAL OF PSEUDOALTEROMONAS SP. EXPLORED THROUGH THE OSMAC STRATEGY

Caroline Evangelista Nogueira dos Santos^{1*}, Jacqueline Santos Cruz², Fabiano Lopes Thompson³, Lidilhone Hamerski¹

caroline.evangelista@hotmail.com

1-Instituto de Pesquisas de Produtos Naturais Walter Mors, UFRJ, Av. Carlos Chagas Filho, 373, Cidade Universitária, RJ, Brazil. 2-Seção de Engenharia Química, IME, Praça Gen. Tibúrcio, 80, Urca, RJ, Brazil. 3-Instituto de Biologia, UFRJ, Av. Carlos Chagas Filho, 373, Cidade Universitária, RJ, Brazil.

Pseudoalteromonas is a genus of marine bacteria studied for their production of secondary metabolites, including alkaloids, polyketides, and peptides, which exhibit antifungal, antibacterial, and algicidal activities. Genomic studies suggest that certain microorganisms possess a greater potential for metabolite production due to the presence of biosynthetic gene clusters that remain unexpressed under standard laboratory cultivation conditions. New methods have been developed to activate these silent genes, aiming to fully harness their metabolic potential for the discovery of novel natural products. Strategies employed include modifying cultivation conditions such as culture medium composition, temperature, pH, co-cultivation, and the use of chemical elicitors. The present work aimed to investigate and modulate the secondary metabolite profile of strains of the marine bacterium *Pseudoalteromonas* sp., isolated from the invasive coral *Tubastraea coccinea*, correlating the induced chemical variations with the antibacterial potential. The metabolic potential of strain BCS15 was investigated through cultivation in two different media supplemented with chemical elicitors, aiming to induce the production of novel metabolites. Chromatographic profile analyses of the extracts revealed variations in metabolite production by this strain under different elicitor conditions. Extracts from *Pseudoalteromonas* sp. strains cultivated in two different culture media with added elicitors were evaluated for antibacterial activity. Notable activity was observed against methicillin-resistant *Staphylococcus aureus* (MRSA) and *Klebsiella pneumoniae*. The authors thank their institutions for support and acknowledge the financial support provided by CNPq and FAPERJ.

Keywords: *Tubastraea coccinea*, OSMAC, chemical elicitors, antibacterial activity.





INFLUENCE OF CLIMATIC PARAMETERS ON THE CHEMICAL COMPOSITION OF *Siparuna guianensis* ESSENTIAL OIL

Mayane dos Santos Souza^{1*}, *Luana de Sousa Peixoto Barros*², *Carlene Quaresma Fonseca*¹,
*Eduarda Karine Barbosa Melo*², *Joyce Kelly da Silva*² and *Pablo Luis Baia Figueiredo*^{1,2}.

mayanesouza098@gmail.com

1-UEPA, Tv. Dr. Enéas Pinheiro, 2626 - Marco, Belém - PA, 66095-015, Brazil. 2- UFPA, R. Augusto Corrêa, 01 - Guamá, 66075-110 Belém, PA, Brazil.

Siparuna guianensis Aubl. (Siparunaceae), popularly known as capitú, is a small tree widely distributed in the Amazon region. Traditional communities use their leaves to treat migraines, fevers, respiratory syndromes, and inflammatory processes [1]. This study aims to evaluate the influence of climatic parameters on the chemical composition of *S. guianensis* essential oil (SgEO). The leaves were collected in the municipality of Bragança, state of Pará, Brazil, during the dry (November-December) and rainy (March-April) seasons. The essential oil was obtained by hydrodistillation for 3 h. The chemical composition was determined by gas chromatography-mass spectrometry [2]. The botanical material was registered in accordance with Brazilian legislation for the protection of biodiversity (SISGEN AF7AC26). The SgEO yield varied from 0.5% (November 2024) to 1.4% (April 2025) with an average of 0.8 ± 0.4 throughout the study. According to INMET, between July and December 2024 (dry season), sunshine was high (208.4–262 h), accompanied by low precipitation. This period also recorded the highest average maximum temperatures (up to 35.3 °C) and a gradual decrease in relative humidity, which ranged from 85.4% (July) to 71.7% (November). In December, the transition to the rainy season began, marked by increased precipitation and a recovery in humidity levels [3]. The main classes among the 104 constituents identified were oxygenated sesquiterpenes (62.8-88.4%), followed by sesquiterpene hydrocarbons (3.9-26.7%). Spathulenol stood out as the majority, ranging from 14.3% in the rainy season to 42.0% in the dry season. Other constituents, although in smaller proportions, were the oxygenated sesquiterpenes germacrene B (1.5-6.1%), cyclocolorenone (0.8-40.8%) and β -Muurolo-4,10(14)-dien-1-ol (0.4-8.4%). Thus, the chemical composition of the essential oil of *Siparuna guianensis* varied according to seasonality, with higher yield in the rainy season and emphasis on spathulenol. The climatic differences between the dry and wet periods directly influenced the production of volatile constituents.

Keywords: volatiles, capitú, environmental factors

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ANIBA ROSIODORA DUCKE (LAURACEAE) ESSENTIAL OILS ANALYSIS FROM LEAVES AND STEMS SPROUTS

Érick Max Mourão Monteiro de Aguiar^{1*}, Gloria Cecilia Macia Ruiz², Carolina dos Reis Farias³, Caroline Schmaedeck Lara², Márcio Vinicius da Silva Gomes³, Paulo de Tarso Barbosa Sampaio², Monica Costa Padilha³, Valdir Florêncio da Veiga Junior¹

mourao.erick@hotmail.com

1-ABC-NP, Departamento de Química, IME, Praça Gen. Tibúrcio, 80 - Urca, Rio de Janeiro, RJ, 22290-270, Brazil. 2-Instituto Nacional de Pesquisas da Amazônia, Av. André Araújo, 2936, Aleixo, CEP 69060-001, Manaus – AM, Brazil. 3- Laboratório Brasileiro de Controle de Dopagem, Instituto de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ 21941-909, Brasil.

The rosewood essential oil (REO) is produced from the trunk of the trees of the endangered species *Aniba rosiodora*, globally traded as CITES, due to linalool content, the most abundant molecule in this oil. The alternative and sustainable approach to produce the linalool rich essential oil is to extract from leaves (ROLEO) and stems sprouts (ROSEO). At the present study, samples from leaves and stems sprouts from 91 trees were extracted and the 182 essential oils were analysed by GC-MS (single-quadrupole ISQ LT MS, with a DB-5ms column). The trees collected at Maués, Amazonas State, vary in age, girth, total tree height, and height. As expected, linalool was the predominant constituent in REO, approximately three times greater concentration than the sum of all other substances, varying at $50.3\% \pm 6.7$ and $41.8\% \pm 5.2$, to ROLEO and ROSEO, respectively. The following molecules were also detected in smaller quantities: cis-linalool oxide, trans-linalool oxide, alpha-terpineol, eudesma-4(14),11-diene, alpha-selinene, spathulenol, benzyl benzoate, and eucalyptol. Using Principal Component Analysis (PCA), plant part, tree age and the concentrations of each substance were considered as variables, and a correlation matrix was then calculated. A relationship between REO yield and age was not observed. By graphing the data using the first two principal components, which represent 65% of the data variance, it was possible to recognize that the samples tend to cluster into two distinct regions, highlighting the difference in chemical composition between leaves and stems. ROLEO were more associated with minoritarian monoterpenes (cis/trans-linalool oxide, and alpha-terpineol), while ROSEO were associated with minoritarian sesquiterpenes: alpha-selinene, eudesma-4(14),11-diene, and spathulenol. ROLEO aging between 18-34 years showed higher concentration of linalool. At ROSEO, youngest trees (7-17 years) showed a lower concentration of linalool and 18-34 year trees showed higher amount of cis/trans-linalool oxide. The compounds eucalyptol and benzyl benzoate, although less abundant, proved to be good markers for better discriminating between the leaves and stems groups. Gas chromatographic analysis was performed using linalool and linalool oxides standard curves, allowing the identification and quantification of these substances together with many other monoterpenes and also sesquiterpenes.

Keywords: *Aniba rosiodora*, Linalool, Chemometrics, Essential Oils.





Annotation of Bioactive Compounds from *Lippia organoides* Kunth by UHPLC-HRMS/MS with Cosmetic Potential

Joyce L. Vieira¹, Romário P. da Costa¹, Adriana P. M. G. Macedo¹, Lorena R. F. de Sousa¹, Quezia B. Cass², Richele P. Severino^{1*}

*richeleps@ufcat.edu.br

1-Instituto de Química, Universidade Federal de Catalão, Catalão, GO, 75704-020, Brazil. 2-Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP, 13565-905, Brazil.

In recent years, the market for natural ingredients applied in cosmetics has shown significant growth, reaching approximately USD 642 million in 2022, with projections to achieve USD 1.1 billion by 2030.¹ This scenario has driven research in bioinnovation, particularly in the prospecting of bioactive compounds for use in cosmetic formulations. In this context, the Brazilian Cerrado stands out for its vast biodiversity, still little explored in terms of chemical composition and biological activities, in addition to being a territory rich in traditional knowledge. Many of its plant species have been used medicinally for generations, including *Lippia organoides* Kunth, popularly known as “alecrim-pimenta.” Recognized by the Brazilian Ministry of Health as a medicinal plant, this species is employed in the treatment of skin conditions, infections, and as an antiseptic in mouth rinses.³ Previous studies have already reported the presence of compounds of great interest for cosmetic applications. Therefore, this study aimed to investigate the ethanolic extract of *L. organoides* to annotate bioactive compounds with potential application in cosmetics through ultra-high-performance liquid chromatography coupled with high-resolution mass spectrometry (UHPLC-HRMS/MS), associated with dereplication tools such as GNPS and SIRIUS platforms. This approach enabled the annotation of several metabolites, including 5,7-dihydroxycoumarin, eriodictyol, glycosylated eriodictyol, luteolin, quercetin, glycosylated quercetin, phlorizin, phloretin, naringenin, taxifolin, acteoside, glycosylated apigenin, scutellarein 4'-methyl ether and cirsimaritin. In addition to chemical characterization, biological assays were performed to evaluate the inhibitory activity of the extract and its fractions against elastase and tyrosinase, enzymes respectively involved in skin aging and hyperpigmentation. The results indicated that both the ethanolic extract and the dichloromethane fraction exhibited significant activity against tyrosinase, with inhibition rates of 60% and 89% at 100 µg/mL, respectively. These findings reinforce the potential of *L. organoides* as a source of bioactive compounds for the development of phytocosmetics.

Keywords: *Lippia organoides*, dereplication, tyrosinase, phytocosmetics.

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β -Carboline Alkaloids from *Galianthe thalictroides* Leaves: Uncovering a Novel Indole-Monoterpene-Flavan-3-ol Subclass

Pedro Becker Kerber*¹, Wilson Hino Kato Jr¹, Júlia Freire de Araújo¹, Ana Camila Micheletti², Fernanda Rodrigues Garcez¹, Walmir Silva Garcez¹, Nidia Cristiane Yoshida¹, Patrícia de Oliveira Figueiredo¹

pedro.beckerkerber@gmail.com

1- PRONABio, Instituto de Química, INQUI, UFMS, Av. Sen. Filinto Müller, 1555, Campo Grande, MS, Brazil. 2 - SINTMOL, Instituto de Química, INQUI, UFMS, Av. Sen. Filinto Müller, 1555, Campo Grande, MS, Brazil.

Galianthe thalictroides (Rubiaceae) is a South American shrub with a restricted distribution and a traditional use of root decoctions in folk medicine for cancer treatment in Brazil. Ethnopharmacological relevance has guided phytochemical research on this species, with root investigations previously leading to the discovery of β -carboline alkaloids and Rubiaceae-type cyclopeptides exhibiting potent in vitro cytotoxic activity. Phytochemical exploration of the leaves (unpublished data) revealed remarkable chemical diversity, with the isolation of eleven β -carboline alkaloids. Among them, a series of indole-monoterpene β -carbolines was identified, as well as novel hybrid molecules in which a flavan-3-ol (epicatechin) moiety is integrated into the monoterpene framework. This unprecedented arrangement constitutes a new subclass of β -carboline alkaloids, never previously described in the literature, significantly expanding the structural landscape of this alkaloid family. In addition to structural novelty, selected leaf-derived β -carbolines exhibited antibacterial activity. One compound showed strong inhibitory effects against *Staphylococcus aureus*, including resistant strains, moderate effects against *Enterococcus faecalis*, *Escherichia coli*, and vancomycin-resistant *E. faecium*, as well as synergistic or additive interactions with ampicillin. Other β -carbolines displayed moderate activity across multiple resistant strains. Furthermore, additional β -carboline alkaloids and other secondary metabolites remain under structural elucidation. Their chemical diversity, together with the unprecedented β -carboline-flavan-3-ol hybrids, provides a strong rationale for future anticancer investigations, aiming to validate their cytotoxic potential and explore pharmacological applications. In summary, *G. thalictroides* emerges as a rich source of novel β -carboline alkaloids, some with antibacterial activity and others with promising structural features for cytotoxicity, thereby expanding phytochemical knowledge and offering new avenues for the discovery of bioactive natural products within Rubiaceae.

Keywords: *Galianthe thalictroides*; alkaloids; β -carboline alkaloids; NMR





BIOTRANSFORMATION OF EPOXYISOPHORONE BY *ASPERGILLUS WELWITSCHIAE*

Lucas B. Filizzola^{1*}, Lucas P. Dutra^{1*}, Aristóteles Goes Neto^{2*}, Diogo M. Vidal^{1*}

lucasbauer926@gmail.com

¹Departamento de química UFMG; ²Instituto de ciências biológicas, UFMG

Biotransformation is a sustainable alternative for obtaining products with economic interest, once affordable reagents, such as isophorone and epoxyisophorone, may be employed to produce complex compounds, which are present in cosmetic, pharmaceutical and food industry. Fungi from *Aspergillus* genus are notorious microorganisms capable of performing such processes in a regio- and stereoselective manner. *A. niger*, for example, is a commonly strain employed in these biotransformation experiments. *A. welwitschiae* is a close related species to *A. niger*, which has never been exploited as biocatalyst. Thus, in this work epoxyisophorone was biotransformed by this fungus. The strain was pre-fermented in six 250 mL Erlenmeyers flasks filled with 100 mL of malt extract (30g/L). It was added 4 mL of a 25 mg/mL of epoxyisophorone DMSO solution in one sterile (positive control) and five inoculated media. To one of the inoculated media it was added 4 mL of DMSO (negative control). These cultures were fermented for more 96 h in the same conditions described above. After the fermentation period 1 mL of each media were extracted with 3x500 μ L of ethyl acetate for GC-MS analysis. Using the authentic hydrocarbons C10 until C26 pattern and comparing the mass spectrogram and retention index time on the literature it was possible to identified 3 peaks relating respectively to cyclohexanone 5-methyl-2-1-methylethyl (1a) with R_T 11,10 min, Cyclohex-2-en-1-one, 2-hydroxy-, 3,5,5-trimethyl R_T 11,75 min (1b) and ciclohexanone 3,3,5-trimethyl R_T 14,60 min (1c). Searching on WILEY7, FFNSC and NIST147 to compare the mass spectrum, it was observed 84% similarity for the compound 1a, 99% for 1b and 88% for 1c. The Retention index was also calculated, 1125 (a), 1152 (1b) and 1291 (1c), on NIST webbook it was found 1128, 1149.8 and 1285, respectively. Among this peak it was observed other 5 peaks relating to possible products wich, with the analysis method and database available, was not possible to identify.

Keywords: Biotransformation, epoxyisophorone, sustainable, regio and stereo reactions





Metabolomic Profiling of *Ternstroemia brasiliensis* from Jurubatiba Sandbank Phytophysionomies (Rio de Janeiro, Brazil) and Evaluation of its Antioxidant Potential

Gabrielle Lavor de Queiroz^{1*}, Beatriz Bastos Santos¹, Alessandra da Silva Correia¹, Leilane Falcão de Freitas¹, Stella Martins de Castro¹, Diego Rodrigues², Anderson da Rocha Gripp², Rodrigo Lemes², Henriette Uthe³, Jörg Ziegler³, Ludger A. Wessjohann³, Maria Sandra Ramos Queiroz⁴, Carla Monteiro Leal¹, Ivana Correa Ramos Leal¹
gabrielleqfarma@gmail.com

1-LaProNEB, Faculdade de Farmácia, UFRJ, Av. Carlos Chagas, 373, RJ, Brazil. 2-NUPEM, Instituto de Biodiversidade e Sustentabilidade, UFRJ, Avenida São José do Barreto, 764, RJ, Brazil. 3-IPB, MetaCom, Leibniz Institute of Plant Biochemistry, Weinberg 3 06120 Halle (Saale) 4-UNESA, R. Gen. Alfredo Bruno Gomes Martins, RJ, Brazil.

Jurubatiba Sandbank National Park (PARNA Jurubatiba), located in the northern region of the state of Rio de Janeiro, is a protected area that harbors xeromorphic plant species distributed across different phytophysionomies. *Ternstroemia brasiliensis* (Pentaphylacaceae), commonly known as “pinta-noiva” can be found in different phytophysionomic formations of the PARNA Jurubatiba, such as Clusia Open Shrub Formation (COSF) and Ericacea Open Shrub Formation (EOSF), commonly exposed to high temperatures, low rainfall, sandy soil, among other. Phytochemical studies of species from the genus *Ternstroemia* have reported the isolation of oleanane- and ursane-type triterpenes, triterpenoid saponins and *O*-glycosylated flavonoids. Biopharmacological investigations of the genus have demonstrated notable antioxidant activity. Therefore, the present study aims to carry out an untargeted metabolomic analysis of *T. brasiliensis* extracts obtained from different phytophysionomies, in different seasons, and to evaluate their antioxidant potential. Leaves of *T. brasiliensis* (n= 14; COSF and EOSF) were collected in the summer (-S) and autumn (-A) seasons and stored at -80°C. The dry and crushed material was extracted with MeOH:H₂O (8:2). The analyses were performed in an Agilent 1290 infinity II HPLC system coupled to a timsTOF Bruker® with ESI source, in the positive ionization mode. Data processing was performed in MetaboScape®, and the data analysis in the Sirius 5.8, Metlgel, GNPS2, and Metaboanalyst 6.0. The extracts were subjected to the DPPH antioxidant assay in order to evaluate their capacity to capture and neutralize the 1,1-diphenyl-2-picrylhydrazyl radical, using rutin as standard. *O*- and *C*-glycoside flavonoids were annotated in *T. brasiliensis* at COS and EOS formations, in both seasons. The *C*-glycoside flavonoids is being reported for the first time for this species. An unsupervised principal component analysis (PCA) enabled the assessment and grouping of samples based on the variance in their chemical profiles. The preliminary evaluation of antioxidant potential using the DPPH method showed promising results for summer extracts, from distinct phytophysionomies. Among the extracts of *T. brasiliensis*, specimens collected at EOSF-S showed EC₅₀ values at 6.01 µg/mL, compared to 1.45 µg/mL for rutin. The antioxidant assays for COSF-S are currently underway. Through this study it was possible to detect flavonoids as the compounds, and antioxidant potential of the *T. brasiliensis*.

Keywords: Antioxidants; Jurubatiba Sandbank; phytophysionomies; *Ternstroemia brasiliensis*; Untargeted Metabolomics.





CYTOTOXIC EFFECT OF CAROTENOIDS ON GASTRIC CANCER CELLS VIA A POTENTIAL PRO-OXIDANT MECHANISM

Sergio Gonzalez-Lopez^{1*}, Lina M. Trujillo Chacon¹, Edison Osorio¹.

sergio.gonzalez3@udea.edu.co

¹ Grupo de Investigación en Sustancias Bioactivas GISB, Facultad de Ciencias Farmacéuticas y Alimentarias, Universidad de Antioquia, Calle 70 No. 52-21, Medellín 0500100, Colombia.

Carotenoids are dietary compounds widely recognized for their antioxidant properties. However, under specific conditions, they may act as pro-oxidants, increasing intracellular reactive oxygen species (ROS) and triggering cytotoxic effects. This dual behavior has sparked growing interest in their potential application in cancer treatment. Nonetheless, the relationship between their pro-oxidant potential and cytotoxicity in gastric cancer remains unclear. This study aims to evaluate the cytotoxic effect of food-relevant carotenoids on a gastric adenocarcinoma cell line (AGS) through a three-phase approach.

In the first phase, cytotoxicity was assessed using the MTT assay in AGS and human keratinocytes (HaCaT) treated with five dietary carotenoids: β -carotene, astaxanthin, lutein, zeaxanthin, and fucoxanthin. Fucoxanthin and β -carotene showed the most promising results, with IC₅₀ values of $13.92 \pm 2.97 \mu\text{M}$ and $60.35 \pm 1.84 \mu\text{M}$ in AGS cells, respectively, and markedly lower IC₅₀ in HaCaT cells. This suggests differential sensitivity between tumor and non-tumor models. AGS and HaCaT were selected due to their relevance as gastric cancer and non-tumor epithelial models in toxicological and pharmacological screening.

The second phase focused on intracellular ROS quantification using the H₂DCFDA fluorescent probe. Contrary to expectations, a reduction in ROS levels was observed in AGS cells under all treatments. However, this may reflect the loss of viable, metabolically active cells rather than a true antioxidant effect. Since the ROS signal was not normalized to live cell count, current efforts aim to normalize fluorescence values to viability data to better interpret these results. Each treatment was tested at multiple concentrations and timepoints to evaluate both immediate and delayed oxidative responses.

The third phase, in progress, will apply NMR-based metabolomics to elucidate metabolic disruptions induced by the most active carotenoid. These findings may guide future research and support the rational use of dietary carotenoids as potential adjuvants in gastric cancer therapy.

Keywords: Carotenoids; Gastric cancer; Pro-oxidant activity; Reactive oxygen species (ROS).





BIOPROSPECTING OF CAPSICUM SPP. IN COLOMBIA: INTEGRATING BROMATOLOGICAL TRAITS AND TARGETED METABOLOMICS

Esteban Castaño Llanos^{*1, 2}, Daniel Pardo-Rodriguez³, Juan C. Henao-Rojas¹, Leidy P. Moreno Caicedo⁵, Mónica P. Cala³ and Guillermo Montoya^{2, 4}

¹ Centro de Investigación La Selva, Agrosavia. Km 7 Vía Rionegro – Las Palmas, Sector Llanogrande, Rionegro, Antioquia 054048, Colombia. ² Facultad de Ingeniería, Diseño y Ciencias Aplicadas. Escuela de Ciencias Aplicadas e Industria Sostenible, Departamento de Ciencias Farmacéuticas y Químicas, Universidad Icesi. Cali, Valle del Cauca 760031, Colombia. ³ Metabolomics Core Facility—MetCore, Vice-Presidency for Research, Universidad de los Andes, Bogotá 110111, Colombia. ⁴ BioInc. Center for Biomass Valorization Research, Universidad Icesi. Cali, Valle del Cauca 760031, Colombia. ⁵ Corporación Colombiana de Investigación Agropecuaria – Agrosavia. Centro de Investigación Palmira. Palmira - Valle del Cauca, Colombia
*escalla99@hotmail.com

The genus *Capsicum* comprises five widely cultivated and consumed species worldwide, valued not only for their sensory attributes like pungency, aroma, and color, but also for their remarkable phytochemical profiles. In recent years, *Capsicum* fruits have attracted growing interest as functional foods due to their richness in bioactive compounds such as polyphenols, flavonoids, carotenoids, and lipids, which are associated with antioxidant, anti-inflammatory, and metabolic regulatory effects. Significant diversity in the biochemical and functional composition of *Capsicum spp.* has been documented, largely influenced by genetic, environmental, and agronomic factors. This variability highlights their potential for applications across the food industry, nutraceutical development, and preventive health products. This study characterized 25 genotypes of *Capsicum spp.* from the Agrosavia Colombian germplasm bank, evaluating their bromatological traits (ash content, crude lipids, crude protein, crude fiber) and functional properties (β -carotene, capsaicinoids, FRAP, DPPH, and TPC), alongside a targeted flavonoid and polyphenol profiling by LC-ESI(-)-QqQ. The results revealed a clear species differentiation among *C. baccatum*, *C. chinense*, and *C. annuum* based on 13 metabolites, with ferulic acid, vanillic acid, and *p*-coumaric acid being the most discriminant. Bromatological and functional potential analyses indicated that *C. annuum* excelled in β -carotene, protein, Na and Fe content, while *C. chinense* exhibited the highest antioxidant activity and lipid content. This work identified a set of promising genotypes with desirable traits for the chili industry, enabling the selection and prioritization of materials for breeding programs and the sustainable exploitation of chili pepper biodiversity in Colombia. These findings provide a scientific basis for both the conservation and the industrial application of *Capsicum* genetic resources. The authors thank the support from Icesi University, Agrosavia and the financial support of Ministry of Science, Technology, and Innovation of Colombian Government. Grants 451-2021, and 435-2021.

Keywords: *Capsicum spp.*, bioprospecting, germplasm bank, metabolomics.





POSTER SESSION ABSTRACT

Session
Biological and Pharmacological
Activity of Natural Products



ANTI-*Helicobacter pylori* AND ANTICANCER PROPERTIES OF *Persea americana* SEED

Dalila Nickel Loose^{1*}, Amanda Cavalcante Gonzaga Nunes¹, Ricardo Machado Kuster²,
Rodrigo Rezende Kitagawa¹, Lorena Carnielli Queiroz¹, Rita de Cássia Ribeiro Gonçalves¹.

dalilaloose@gmail.com

1-Graduate Program in Pharmaceutical Sciences (PPGCFAR), Federal University of Espírito Santo (UFES), Vitória, ES, Brazil. 2-Graduate Program in Chemistry (PPGQUI), Federal University of Espírito Santo (UFES), Vitória, ES, Brazil.

Helicobacter pylori is a gram negative bacteria whose prevalence is over 40%, being the major cause of gastric cancer. Nowadays, incidence of side effects and the high cost of these drugs contribute to poor compliance and therapeutic failure, which is associated with the emergence of resistant strains. In the search for novel therapies, natural products such as avocado seed (*Persea americana*) have historical relevance to treat gastric disorders, and its constituents have great bioactive potential. Therefore, this study aimed to evaluate the anti-*H. pylori* and anti-gastric adenocarcinoma activities of avocado seed extract. The hydroalcoholic extract (70% ethylic alcohol) was prepared by 7 days maceration of previously dried and grounded avocado seeds. The result solution was filtered and the solvents were eliminated by rotary evaporation and lyophilization to obtain the crude extract. Anti-*H. pylori* activity of the extract was determined by the broth microdilution method with resazurin using ATCC 43504 or clinical strains (Parecer 6.114.766 - CEP/Ufes) in brucella broth. Cytotoxicity assays followed the MTT method in AGS (adenocarcinoma) and L929 (fibroblasts) cells, using cisplatin as standard drug. Chemical characterization performed by high resolution mass spectrometry revealed the presence of *Laureaceae* acetogenins, such as avocadene and avocadyne. During the antibacterial test with, the extract showed inhibitory activity at 64 µg/mL and bactericidal activity at 128 µg/mL, a good result for crude extracts. These values were similar in three clinical strains, including in amoxicillin resistant ones. Antitumoral activity on AGS cells had an IC₅₀ of 12,16 ± 0,6222 µg/ml, near to cisplatin (11,39 ± 0,3305 µg/ml). Nevertheless, in L929 cell avocado seed achieved higher values (110.93 ± 7.1728 µg/ml) compared to cisplatin (5.79 ± 0.2558 µg/ml). These results indicate that avocado seed compounds have been more specific to cancer cells, with a selectivity index of 6,78 compared to 0,5 of cisplatin. Hence, avocado seed compounds have both anti-*H. pylori* and anticancer activity with low toxicity to healthy cells *in vitro*, but its mechanism of action stands in need of elucidation by further studies.

Keywords: *Helicobacter pylori*, *Persea americana*, Anticancer, Antimicrobial.





NEUROPROTECTIVE PROPERTIES OF A 20-HYDROXYECDYSONE-RICH EXTRACT FROM PFAFFIA GLOMERATA (SPRENG.) PEDERSEN ROOTS IN A RESERPINE-INDUCED FIBROMYALGIA MODEL

Tamara Marques da Silva^{1*}, Ana Cláudia Gontijo Couto¹, Giovanna Praes Alvarenga Paula¹, Rodrigo Rodrigues Franco², Foued Salmen Espindola², Caroline Martins Mota³, Tiago Wilson Patriarca Mineo³, Cássia Regina da Silva¹

tamara_marques_silva@hotmail.com

1- Analgesia and Inflammation Research Group - GPANI; Laboratory of Biochemistry and animal toxins - LABITOX, Post-Graduate Program of Genetic and Biochemistry, Institute of Biotechnology, Federal University of Uberlândia, 38408-100, Uberlândia (MG), Brazil. 2-Laboratory of Biochemistry and Molecular Biology (LABIBI), Institute of Biotechnology, UFU. 3- Laboratory of Applied Immunology and Parasitology, Institute of Biomedical Sciences, UFU.

Fibromyalgia (FM) is the third most common musculoskeletal condition, affecting approximately 3% of the global population. It is characterized by widespread chronic pain and is often associated with comorbidities such as anxiety and depression. Medicinal plants are considered valuable resources for the treatment of chronic diseases due to their bioactive compounds, which may help reduce adverse effects. The roots of *Pfaffia glomerata* (PG) have been traditionally used for their antioxidant properties in the management of chronic conditions. Therefore, the present study aimed to evaluate the therapeutic effects of the dichloromethane fraction obtained from PG roots on pain, anxiety, depression, oxidative stress and inflammatory markers in an experimental model of FM. Male C57BL/6 mice were used and subjected to a reserpine (RE)-induced FM model, administered once daily for three consecutive days. Following the final RE administration, the animals were treated with saline (vehicle), the PG fraction, or pregabalin (positive control). Mechanical nociception and anxiety- and depression-like behaviors were assessed. Treatment with the PG fraction significantly reduced pain from day 1 to day 9 ($p < 0.001$) following model induction. Moreover, a 69% protective effect against anxiety-like behavior was observed, along with a 29% reduction in depression-like behavior. These findings indicate that treatment with the PG fraction is effective in reducing pain and exerts a protective effect against anxiety- and depression-like behaviors. Mechanical nociception was assessed using Von Frey filaments, while anxiety- and depression-like behaviors were evaluated through the elevated plus maze, open field, and forced swim test. Treatment with the PG fraction significantly reduced pain in animals from day 1 to day 9 following model induction ($p < 0.001$). Additionally, it provided a 69% protective effect against anxiety-like behavior and a 29% reduction in depression-like behavior. Furthermore, the treatment reduced levels of hydrogen peroxide and pro-inflammatory cytokines. These findings demonstrated that the PG root fraction is effective in alleviating pain and exhibits protective effects on anxiety- and depression-related behavioral parameters. The authors thank the support from their institutions and the financial support of FAPEMIG and CAPES.

Keywords: pain, anxiety, depression, natural products, oxidative stress





**THERAPEUTIC AND PROTECTIVE POTENTIAL OF *Monteverdia ilicifolia* IN
TYLOXAPOL-INDUCED HYPERLIPIDEMIC MICE**

Raquel Toledo Dohler^{*1}; Tarcisio Paiva Mendonça^{1,2}; Matheus
Cesar Rodrigues Garcia^{1,2}; Ana Luiza Silva Borges^{1,2}; Vinícius
Prado Bittar^{1,2}; Sandra Gabriela Klein³; Murilo Vieira da Silva^{3,4};
Foued Salmen Espíndola^{1, 2, 3,4}
raqueltolledohler@gmail.com

¹ Instituto de Biotecnologia/ Laboratório de Bioquímica e Biologia Molecular; ² Laboratório de Biotecnologia em Modelos Experimentais – Universidade Federal de Uberlândia, Uberlândia, MG 38400-902, Brazil. Programas de Pós-Graduação em ³Ciências da Saúde, Faculdade de Medicina, Ciências Veterinária, Faculdade de Veterinária ⁴Biologia Celular e Estrutural Aplicada, Instituto de Ciências Biomédicas, UFU, Uberlândia, MG, Brazil.

Maytenus ilicifolia, native to South America, is a medicinal plant traditionally used for its gastroprotective properties, notoriously rich in phenolic compounds. Previous studies from our laboratory (DOI: 10.1016/j.biopha.2021.112049; 10.3390/foods12112097) have demonstrated that fractions rich in polyphenols have beneficial effects in models of acute dyslipidemia. In the present study, the effects of different concentrations of the crude extract of the plant on cholesterol and triglyceride levels in C57BL/6 mice with Tyloxapol-induced hyperlipidemia were evaluated. C57BL/6 mice were divided into seven experimental groups with n = 6 animals each: Group 1 (N) normolipidemic (negative control: without Tyloxapol, without extract); Group 2 (NT) normolipidemic treated with 400 mg/kg EE-MI (toxicity group: extract 400 mg/kg); Group 3 (H) hyperlipidemic treated with salines solution; Group 4 (HS) hyperlipidemic treated with simvastatin; Group 5 (H100) hyperlipidemic treated with EE-MI 100 mg/kg; Group 6 (H200) hyperlipidemic treated with EE-MI 200 mg/kg; Group 7 (H400) hyperlipidemic treated with EE-MI 400 mg/kg. Hyperlipidemia was induced by intraperitoneal administration of Tyloxapol every 48 hours for 21 days. The treated groups received doses of 100, 200 or 400 mg/kg of extract by oral gavage. Serum levels of total cholesterol and triglycerides were monitored, measured with Labtest® kits. The groups treated with plant extract showed a significant reduction in triglyceride and total cholesterol levels compared to the hyperlipidemic group, with more expressive responses at doses of 100 mg/kg and 200 mg/kg. The crude extract of *Maytenus ilicifolia* demonstrated promising therapeutic potential in modulating lipid parameters associated with hyperlipidemia. The results suggest significant lipid-lowering activity, especially at doses of 100 and 200 mg/kg, reinforcing the therapeutic potential of the plant as a source of new natural agents against metabolic disorders. Acknowledgements: CAPES, CNPq, FAPEMIG

Keywords: *Maytenus ilicifolia*; Phenolic compounds; Tyloxapol; Hypolipidemic activity; Espinheira-Santa





ALLELOPATHIC ACTIVITY OF LECTINS FROM *Bauhinia holophylla* (FABACEAE:CERCIDOIDEAE)

Maria Fernanda de Oliveira Silva*, Lucas Santos Azevedo, Ludmila Maria Gonçalves Godói de Camargos, Luciana Alves Rodrigues dos Santos Lima e Ana Hortência Fonsêca Castro

mariafoliveira013@aluno.ufsj.edu.br

Universidade Federal de São João del-Rei, Campus Centro-Oeste, Av. Sebastião Gonçalves Coelho, 400 – Chanandour, Divinópolis, MG, 35501-296, Brazil

Plant bioactive compounds can be obtained from plant tissue culture and more specifically through callus culture, which allows the preservation of the species. *Bauhinia holophylla* is a woody species from the Cerrado widely distributed in Brazil. This species contains different bioactive compounds, and lectins have received special attention due to their broad potential against microorganisms, insects, tumor cells and as allelochemicals. This study aimed to assess the allelopathic potential of lectins found in *B. holophylla* callus. Calli were induced from leaf explants of *B. holophylla* in Wood Plant Medium (WPM) supplemented with 4.44 μM 6-benzylaminopurine added with 30 g L⁻¹ sucrose and solidified with 7 g L⁻¹ agar. The explants were incubated in the presence of light, at 27 °C and 16-h photoperiod for 60 days. Lectins were extracted from fresh callus using sodium chloride (0.9%). The extract was used to confirm the presence of lectin by hemagglutinating activity using human blood. The allelopathic potential was assessed by the effect of lectins on the germination (G), germination speed index (GSI) and elongation of the radicle and epicotyl of *Allium cepa* (onion), a monocotyledonous and *Lactuca sativa* (lettuce), an eudicotyledonous at concentrations of 250, 500, 750 and 1000 $\mu\text{g/mL}$. MES buffer solution and glyphosate/atrazine were used as negative and positive controls, respectively. For onion seeds there was a decrease in the percentage of G and in the GSI in the presence of the lectin extract at a concentration of 750 $\mu\text{g/mL}$, when compared to the atrazine ($p < 0.05$). Lectin extract did not affect the G and GSI of lettuce seeds. Lectin extract reduced the elongation of the onion radicle and epicotyl at concentrations of 250, 750 and 1000 $\mu\text{g/mL}$, with the lowest concentration being the most effective with a 32% reduction ($p < 0.05$). Lectin extract at 250 $\mu\text{g/mL}$ increased the elongation of the epicotyl in lettuce (17%) and no changes were observed in radicle elongation when compared with the controls. These results suggest a possible allelopathic activity of lectin from *B. holophylla* callus, especially on monocotyledonous species. The authors thank the support from UFSJ, CNPq and FAPEMIG (APQ-00861-22 and APQ 00000-23). This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001.

Keywords: allelochemicals, pata-de-vaca, lectin, medicinal plant, Cerrado.





SEARCH FOR NEW PLANT HORMONES AND BIOHERBICIDES: INFLUENCE OF SMILAX FLUMINENSIS EXTRACT AND FRACTIONS ON SEED GERMINATION AND SEEDLING DEVELOPMENT OF MONO AND EUDICOTYLEDONOUS SPECIES

Lucas Santos Azevedo¹, Ana Hortência Fonsêca Castro¹, Katyuze de Souza Farias², Vanessa Samúdio Santos Zanuncio², Denise Brentan Silva², **Luciana Alves Rodrigues dos Santos Lima^{1*}**

luarsantos@ufsj.edu.br

1-Campus Centro-Oeste Dona Lindu, UFSJ, Rua Sebastião Gonçalves Coelho, 400, Chanadour Divinópolis, MG, 35501-296, Brazil. 2-LaPNEM, FACFAN, UFMS, Avenida Costa e Silva, s/n, Bairro Universitário, Campo Grande, MS, 79070-900, Brazil.

With the increase in the world population, there is also a growing demand for food production. Thus, substances are used to increase agricultural production, and synthetic agrochemicals are used to control weeds in crops, but these can be highly toxic and can promote both physiological and biochemical changes in plants. Studies involving seed germination have been used to evaluate the biological activity of natural products with hormonal and/or herbicidal actions, which act by interfering with germination and/or development during the culture of important agricultural species. The species *Smilax fluminensis* Steud. (Smilacaceae), popularly known as “cipó-quina” and “ijuapecá guasu”, originates from Brazil and has several uses in folk medicine and indigenous peoples, with various proven biological activities. The aim of this study was to assess the influence of *S. fluminensis* extract and fractions on seed germination and seedling development of mono and eudicotyledonous species. Ethyl esters and phytol were characterized as the major compounds found in hexane fraction. In the polar samples, the main compounds annotated were kaempferol, luteolin and quercetin derivatives, and saponins. The ethanol extract (EE) and hexane (HEXF), dichloromethane (DCMF) and hydroethanol (HIDF) fractions increased the *in vitro* germination of *Allium cepa* seeds compared to controls. Ethyl acetate fraction (EACF) inhibited seed germination and seedling development. In general, the fractions inhibited the germination of *Nicotiana tabacum* seeds and reduced the seedlings development, mainly at 750 µg/mL and 1000 µg/mL, compared to the controls. Thus, this study suggests that the extract and fractions of *S. fluminensis* exhibited an effect more similar to plant hormones on *A. cepa* (monocotyledonous) and bioherbicide on *N. tabacum* (eudicotyledonous), and may therefore play an important role in sustainable agriculture.

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Keywords: *Smilax fluminensis*, allelopathy, natural agrochemicals, *in vitro* germination.





EVALUATION OF TOTAL PHENOL CONTENT AND ANTIOXIDANT ACTIVITY BY THE FRAP METHOD OF *BIDENS* SPP. LEAVES

Iasmin Fernandes Emediato^{1*}, Thaís Paula Rodrigues Gonçalves¹, Luciana Alves Rodrigues dos Santos Lima¹

iaemediato@gmail.com

1-LAFIT, Laboratório de Fitoquímica, UFSJ, Campus Centro-Oeste Dona Lindu, Rua Sebastião Gonçalves Coelho, 400, Divinópolis, Minas Gerais, 35501-296

The species *Bidens* spp., belonging to the family Asteraceae, is a plant typical of the Central-West, Southeast, and South regions of Brazil, popularly known as carrapicho-de-pontas, coambi, erva-picão, fura-capá, goambu, picão, picão-do-campo, and picão-preto. *Bidens* spp. is used in folk medicine as an ocular antiseptic and for treating canker sores and sore throats. Several plants used in traditional medicine are being evaluated for their biological activities. In this context, the objective of this study was to determine the content of total phenolic compounds and evaluate the antioxidant activity by ferric reducing antioxidant power (FRAP) of the extract and fractions of the leaves of *Bidens* spp. The extract (EE) was prepared from the leaves by turboextraction with 70% ethanol and subsequently partitioned with dichloromethane and ethyl acetate, obtaining the dichloromethane (DCM), ethyl acetate (EA) and hydroethanol (HE) fractions. The quantification of the total phenolic compound content was performed using the Folin-Ciocalteu reagent¹ and the antioxidant activity was determined by the FRAP assay². EE, and DCM, EA and HE fractions presented total phenolic compound contents of 62.83 µg GAE (gallic acid equivalents)/mg, 166.00 µg GAE/mg, 268.97 µg GAE/mg and 31.67 µg GAE/mg, respectively. All samples showed antioxidant activity by the FRAP method. The DCM and EA fractions were the most active, with EC₅₀ values of 2.11 and 0.85 µg/mL, respectively, with activity similar to that of BHT (methyl-2,6-di-t-butyl-phenol), which showed EC₅₀ of 0.57 µg/mL. A positive correlation was observed between the total phenolic compound content and antioxidant activity, suggesting that phenolic compounds contribute significantly to the antioxidant capacity. The data obtained encourage the performance of other tests to confirm the observed results and also to evaluate other biological activities of the leaves of *Bidens* spp.

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Keywords: *Bidens*, antioxidant, FRAP, fractions.

¹Food Research International, 60, 246-254, 2014. <https://doi.org/10.1016/j.foodres.2013.09.010>

²Food Research International, 156, 111145, 2022. <https://doi.org/10.1016/j.foodres.2022.111145>





TOTAL PHENOLIC CONTENT AND ANTIOXIDANT ACTIVITY OF THE EXTRACT AND FRACTIONS FROM THE PERICARP OF *TECOMA STANS*

Neide Aparecida da Silva^{1*}, Luana Cristina Diniz Santos¹, Iasmin Fernandes Emediato¹, André Vítor Caetano¹, Mairon César Coimbra¹, Luciana Alves Rodrigues dos Santos Lima¹

neideapsilva@yahoo.com.br

1-LAFIT, Laboratório de Fitoquímica, UFSJ, Campus Centro-Oeste Dona Lindu, Rua Sebastião Gonçalves Coelho, 400, Divinópolis, Minas Gerais, 35501-296, Brazil.

The increasing use of synthetic antioxidants in the food and cosmetic industries, associated with undesirable effects, has driven the search for natural and sustainable alternatives. Antioxidants play a crucial role in the efficacy of plants as medicines and in combating chronic diseases. These antioxidants are incorporated into our diet through compounds found in plants, in a practical and direct way. *Tecoma stans* (Bignoniaceae), a species introduced in Brazil for ornamental purposes, is widely recognized in traditional medicine for its antidiabetic, anti-inflammatory and antioxidant properties. However, the pharmacological potential of its pericarp remains poorly investigated. Therefore, this study aimed to evaluate the total phenolic content and antioxidant activity of the methanol extract (ME) and its fractions obtained from the pericarp of *T. stans*. Phenolic compounds were quantified using the Folin-Ciocalteu reagent, with results expressed in gallic acid equivalents (GAE), while antioxidant activity was evaluated through the ferric reducing antioxidant power (FRAP) assay. The dichloromethane (DCM) fraction showed the highest phenolic content 113.81 µg GAE/mg, followed by the ethyl acetate (EA) and hydromethanol (HM) fractions and ME, with 100.26, 78.72 and 74.19 µg GAE/mg, respectively. The total phenolic compound content quantified in the samples was directly proportional to the antioxidant capacity by the FRAP method, confirming a positive correlation between total phenolics and the reduction of ferric ions. The EC₅₀ values were 4.83, 17.72, 9.93 and 31.43 µg/mL, respectively, for DCM, EA, HM and ME. The results highlight the pericarp of *Tecoma stans* as a promising natural source of antioxidant compounds, with potential applications in pharmaceutical and phytotherapeutic formulations, in addition to highlighting the importance of investigating underutilized plant species in the search for bioactive molecules, contributing to the development of natural, safe and sustainable therapeutic strategies.

The authors thank the support from UFSJ and the financial support of CAPES, FAPEMIG and CNPq. This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001.

Keywords: *Tecoma stans*; phenolic compounds; antioxidants; FRAP; phytochemistry.





INFLUENCE OF PHENOLICS' IN THE GREEN SYNTHESIS OF SILVER NANOREMEDIATORS USING LEUCENA LEAVES' AQUEOUS EXTRACT

Karina Aparecida Neves Martins^{1*}, Christopher Santos Silva¹, Iasmin Fernandes Emediato¹, Clascídia Aparecida Furtado², Danilo Roberto Carvalho Ferreira², Luciana Alves Rodrigues dos Santos Lima¹, Flávia Cristina Policarpo Tonelli¹, Giullya Amaral Cordeiro Lembrança¹, Fernanda Maria Policarpo Tonelli¹

karinabioquimicaufs@gmail.com

1-Campus Centro Oeste, Universidade Federal de São João del Rei, Divinópolis, MG, 35501-296, Brazil. 2-Centro de Desenvolvimento da Tecnologia Nuclear, Belo Horizonte, MG, 31270-010, Brazil.

Phenolic compounds (PCs) are useful to generate metallic nanoparticles (NPs), reducing metal ions, capping and enhancing the yield. These NPs can present useful properties such as remediating the pollution caused by organic synthetic dyes. These environmental contaminants are commonly toxic to living beings. Methylene blue (MB), for example, largely applied in textile industry, can cause cyanosis and tissue necrosis in humans. The aim of the present study was to investigate if the variation in the concentration of PCs can influence the efficiency of promoting remediation of MB's pollution by silver NPs synthesized using an extract containing these natural products. As the vegetal source of PCs the leaves of the invasive species *Leucaena leucocephala* (Leucena) (PAMG herbarium n° 58919) were used. They were collected (20°8'7" S and 44°53'49" W), cleaned, dried and submitted to extraction (10g/100 mL of deionized water, 30 min., 80 °C). The extract had its PCs' dosage assessed through Folin-Ciocalteu method and was then added to a 1 mM aqueous solution of AgNO₃ at different proportions v/v: 1:1, 3:1, 6:1, 9:1. The mixtures were kept under agitation for 1 hour. The reaction products were washed, dried and had their nanoremediation capacity tested against MB (10mg/L). This assay was performed in 96-well plates, in triplicate, to test 5 different concentrations of NPs. The triplicates pipetted were (1) water; (2) MB; (3) NPs 1000 ppm in water; (4) NPs 1000 ppm and MB; (5) NPs 500 ppm in water; (6) NPs 500 ppm and MB; (7) NPs 250 ppm in water; (8) NPs 250 ppm and MB; (9) NPs 125 ppm in water; (10) NPs 125 ppm and MB; (11) NPs 62.5 ppm in water; and (12) NPs 62.5 ppm and MB. The absorbance was measured each 30 min for 2.5 h at 665 nm, and the results were analyzed (two-way ANOVA/Tukey's post-test). The PCs dosage of the crude extract was 383.95 ± 0.17mg/g of vegetal material. The maximum percentages of remediation (NPs 1000 ppm) were: 55.5% (1:1), 64.61% (3:1), 77.79% (6:1) and 100% (9:1). Therefore, the PCs' dosage influences in the efficiency of MB's remediation by NPs, enhance their performance.

Keywords: *Leucena leucocephala*, phenolics, Folin-Ciocalteu method, green synthesis, silver nanoparticles, nanoremediation





INHIBITORY POTENTIAL OF DAN SHEN ROOT FRACTIONS ON PAI-1: VIRTUAL, CHEMICAL AND BIOLOGICAL APPROACHES

Roney Vander dos Santos^{1,2}, Kaio Eduardo Buglio³, Luan Rabelo³, Augusto de Souza Silva^{1,3}, Ivan Mazoni⁴, João Ernesto de Carvalho^{1,3}, Ana Lucia Tasca Gois Ruiz^{1,3}, Mary Ann Foglio^{1,3}, Ljubica Tasic^{2,5}

r095969@dac.unicamp.br

1 - School of Pharmaceutical Science, University of Campinas, Campinas, SP, Brazil; 2 - Laboratory of Biological Chemistry, Institute of Chemistry, University of Campinas, Campinas, SP, Brazil; 3 - Laboratory of Phytochemistry, Pharmacology and Experimental Toxicology, School of Pharmaceutical Science, University of Campinas, Campinas, SP, Brazil; 4 - Research Group in Scientific Computing, Information Engineering and Automation, Embrapa Digital Agriculture, Campinas - SP, Brazil; 5 - Institute of Chemistry, University of Campinas, Campinas, SP, Brazil.

Plasminogen activator inhibitor-1 (PAI-1) is the main physiological inhibitor of fibrinolysis playing a key role in thrombosis, cancer progression, and inflammation. Modulating the activity of this target represents a promising approach for the development of new antithrombotic agents. This study aims to investigate the inhibitory effects of natural compounds from Dan Shen, *Salvia miltiorrhiza*, on PAI-1 using *in silico*, chemical, and biological approaches. Four plant root fractions were evaluated: an aqueous extract rich in phenolic acids, a tanshinone IIA-rich fraction, a cryptotanshinone-rich fraction, and isotanshinone V, obtained by hydrolysis of cryptotanshinone. Compounds were extracted and fractionated using liquid-liquid partitioning, followed by purification with chromatographic techniques. Chemical characterization was performed using HPLC (DAD, $\lambda = 365$ nm) and TLC. Molecular docking studies were conducted to evaluate the affinity of the compounds against PAI-1. Thereafter, *in vitro* assays were carried out using human tumor cell lines to assess cytotoxicity and functional effects on fibrinolysis, complemented by colorimetric assays with recombinant PAI-1. Preliminary results suggest that tanshinone IIA and isotanshinone V have high affinity for the reactive center loop of PAI-1 exhibiting promising inhibitory effects in biological assays. The aqueous fraction also showed moderate activity. These findings highlight the potential of *S. miltiorrhiza*-derived compounds as natural scaffolds for the development of indirect fibrinolytic agents targeting PAI-1.

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Keywords: PAI-1 inhibition; *Salvia miltiorrhiza*; fibrinolysis





***TOTAL PHENOLIC CONTENTS OF ALKALINE AQUEOUS EXTRACT OF
CALLISTEMON VIMINALIS***

Julia Eduarda de Oliveira Neves^{1*}, Fernanda Braz Aguiar¹, Mairon C. Coimbra¹, Tiago S. Gontijo¹, Rosimeire C. Barcelos¹, Juliana C. S. A. Bastos¹
(juliana.almeida@ufsj.edu.br)

Laboratório de Farmacognosia, Universidade Federal de São João Del Rei, campus CCO Dona Lindu, R. Sebastião Gonçalves Coelho, 400 - Chanadour, Divinópolis - MG, 35501-296

The *Melaleuca* genus is renowned for its fungicidal, bactericidal, anti-inflammatory, and antioxidant properties. *Callistemon viminalis*, a species within this genus native to Australia, is widely used for ornamental purposes in the city of Divinópolis. Its extracts are rich in phenolic compounds, tannins, terpenes, and flavonoids, which are primarily responsible for its biological activities. These compounds can be selectively extracted depending on solvent polarity: polar solvents are effective for flavonoids and phenolic compounds, while nonpolar solvents are better suited for terpenes and tannins. Given that water is a polar solvent, this study aimed to evaluate the efficiency of aqueous extraction of phenolic compounds from *C. viminalis* using water alkalized with sodium hydroxide at pH 8, 10, and 12. The extracts were freeze-dried, pulverized, and subsequently solubilized in ethanol. Total phenolic content was determined using the Folin–Ciocalteu method, following Bonoli et al. (2004) with modifications. Stock solutions (5 mg/mL) were prepared in ethanol (P.A.), and phenolics were quantified using a standard curve of gallic acid (18.75 to 600 µg/mL), expressed as gallic acid equivalents (mg GAE/g sample). Reaction mixtures contained 10 µL of diluted Folin–Ciocalteu reagent (1:10) and 40 µL of a 2% sodium carbonate solution, incubated at room temperature for one hour, protected from light. Absorbance was measured at 650 nm using an ELISA reader (Molecular Devices). The phenolic content measured was 138.79 ± 34 mg/g at pH 8, 110.89 ± 12 mg/g at pH 10, and 69.57 ± 7.6 mg/g at pH 12. One-way ANOVA followed by Tukey's post-hoc test revealed a statistically significant reduction between pH 8 and pH 12, while no significant difference was observed between pH 8 and pH 10. These results suggest that higher alkalinity reduces the aqueous extraction efficiency of phenolic compounds from *C. viminalis*.

Keywords: *Callistemon viminalis*, Phenolic compounds, Alkaline extraction, Folin_Ciocalteu method, pH influence, Aqueous solvents.





**IN VITRO AND IN VIVO ANTI-INFLAMMATORY POTENTIAL OF THE
ENDOPEROXIDE SESQUITERPENE 3,6-EPIDIOXI-BISABOLA-1,10-
DIENE-(EDBD) FROM *DRYMIS BRASILIENSIS*.**

Bruno Antonio Ferreira^{1*}; Taís de Campos Lima²; Isabella Silva Cassimiro²; Danielle Reis Napolitano²; Eric Umehara¹; **Felipe da Silva Sales¹**; João Henrique Ghilardi Lago¹; Fernanda de Assis Araújo³.

felipe.sales@ufabc.edu.br

1- Centro de Ciências Naturais e Humanas - Universidade Federal do ABC, São Paulo. Brasil. 2 - Departamento de Fisiologia, Instituto de Ciências Biomédicas – Universidade Federal de Uberlândia, Minas Gerais, Brasil. 3 - Laboratório de Fisiologia – Universidade Federal de São João del-Rei - Campus Centro-Oeste Dona Lindu, Minas Gerais, Brazil.

Plants of the genus *Drimys* (Winteraceae), including *D. brasiliensis*, are rich sources of specialized metabolites, such as sesquiterpenes with anti-inflammatory activity. The aim of this study was to evaluate the *in vitro* and *in vivo* anti-inflammatory potential of the endoperoxide sesquiterpene 3,6-epidioxi-bisabola-1,10-diene (EDBD), obtained from the hexanic extract of *Drimys brasiliensis* branches. Using Raw 264.7 macrophages, we evaluated the cytotoxicity of this sesquiterpene through the MTT assay, as well as its ability to inhibit the production of nitric oxide after stimulating the cells with LPS and zymosan (Griess method). The *in vivo* tests consisted of using the sponge implant model in C57BL/6 mice (CEUA/UFU - protocol number 23117.042533/2024-32). A sponge disc was aseptically implanted in the back of each of the 40 mice used in this stage of the study. The animals were treated daily with intraimplant injections containing 0.1, 1 or 10 µg of EDBD, solubilized in 10 µL of 0.5% DMSO solution, or with the vehicle alone (control group). On the 9th day after surgery, the animals were euthanized and the implants were collected, weighed and processed for biochemical analysis. Neutrophil and macrophage infiltrates near the sponge implants were indirectly assessed by measuring the activity of the enzymes myeloperoxidase (MPO) and N-acetyl-β-D-glucosaminidase (NAG), respectively. Our results showed low cytotoxicity associated with EDBD treatment (IC₅₀ ≈ 200 µg/mL) and the compound's ability to inhibit nitric oxide production in stimulated macrophages. In the *in vivo* tests, the activities of MPO and NAG enzymes were reduced in the animals that receiving daily injections containing 1 or 10 µg of the sesquiterpene. Our results showed the anti-inflammatory potential of this compound both *in vitro* and *in vivo*. The authors thank the support from their institutions and the financial support of CNPq (152604/2024-3), CAPES (finance code 001), FAPEMIG and FAPESP.

Keywords: natural products; sesquiterpenes; inflammation; chronic inflammation; sponge model.





**THE TRAJECTORY OF SCIENTIFIC PUBLICATIONS ON MULUNGU AND ITS
MEDICINAL PROPERTIES THROUGH A BIBLIOMETRIC APPROACH**

Bernardo C. de Oliveira^{1*}, Marcela N. Cabral¹, Rosimeire C. Barcelos¹, Juliana C. A.
Bastos¹, Tiago S. Gontijo¹

bernardo29slash@gmail.com

1- Federal University of São João del-Rei (UFSJ), Campus Centro-Oeste Dona Lindu, Divinópolis,
MG, 35.501-296, Brazil.

Interest in research related to the therapeutic use of medicinal plants has grown considerably in recent decades, driven by the search for safe and effective alternatives to conventional drugs. In this context, *Erythrina mulungu*, commonly known as *mulungu*, a species native to Brazil and widely used in traditional medicine, stands out for its pharmacological potential. This study presents a bibliometric analysis of publications related to the medicinal uses of *Erythrina mulungu*, aiming to assess the annual volume of publications on the topic, identify the main authors and institutions, analyze the collaboration network among researchers, and verify patents filed on the subject.

For this purpose, the Bibliometrix package in R software was used. Data were obtained through a thematic search (considering title, keywords, and abstract) carried out in the *Web of Science* and *Scopus* scientific databases (n = 271). The data collection was conducted on April 2, 2025, and included publications indexed between the years 1941 and 2025.

The temporal analysis indicated a significant increase in publications starting in 2001, peaking in 2014 (24 articles). Over 75% of the studies were published in the last 15 years, indicating a recent growth in scientific interest in the species. The Journal of Ethnopharmacology and the Brazilian Journal of Pharmacognosy led in the number of publications, followed by journals such as *Revista Árvore*, *Ciência Florestal*, and *Bioscience Journal*.

The predominance of preclinical studies and the concentration of articles in specialized journals pointed to a field in expansion. Brazil stands out as the main scientific contributor on the subject, reflecting its rich biodiversity and investment in research on medicinal plants. The results highlighted the importance of further clinical and multidisciplinary investigations to consolidate the safe and effective therapeutic use of *Erythrina mulungu*.

The authors thank UFSJ, CAPES, CNPq, and FAPEMIG for their support.

Keywords: *Erythrina mulungu*, medicinal plants, bibliometrics, ethnopharmacology, natural products





**METABOLOMICS AND ANTI-INFLAMMATORY PROPERTIES EVALUATION OF
CYRTOCYMURA SCORPIOIDES**

Paulo R. S. da Silva¹, Lara P. D M. Costa¹, Daniele de Oliveira Silva¹, Paula P. O. Salem¹,
Michael Murgu², Danielle F. Dias¹, Marisi G. Soares¹, Daniela A. Chagas de Paula¹

paulo.santos@sou.unifal-mg.edu.br

1-Institute of Chemistry, Federal University of Alfenas, 37130-001, Alfenas, MG, Brazil.

2-Waters Corporation, 06455-020, Barueri, SP, Brazil.

The species *Cyrtocymura scorpioides* (Lam.) H. Rob. (Asteraceae), popularly known as “Piracá,” “Capixingui,” “enxuga,” or “erva-de-São Simão,” is widely used in traditional medicine. Its use has been reported for anti-inflammatory, antitumor, and other purposes¹. However, there are no in-depth studies on the chemical composition of this species, nor scientific evidence regarding its anti-inflammatory properties. Metabolomic analyses were conducted using analytical techniques such as ultra-high-performance liquid chromatography coupled with high-resolution mass spectrometry, which enables a comprehensive analysis of the chemical composition of samples. Metabolomic analysis, when combined with chemometric and pharmacological studies, have simplified the identification of secondary metabolites². The anti-inflammatory effects were evaluated *ex vivo* in human blood samples, with an emphasis on the analysis of the COX and LOX pathways, targeting Prostaglandin E₂ (from COX) and leukotriene B₄ (from LOX). The chemical characterization was performed by UHPLC-ESI-HRMS in positive mode with DIA acquisition, followed by data processing using the MZmine 4 software and subsequent annotation using *in house* databases and online platforms. The stem micro extract and the hexane fraction exhibited the most effective inhibition of inflammatory mediators, with approximately 25% inhibition of prostaglandin E₂ (PGE₂) observed for both samples, and 22% inhibition of leukotriene B₄ (LTB₄) for the micro extract, compared to the negative control. Twenty-four compounds were annotated according to confidence level 2 of the Metabolomics Standards Initiative (MSI), with a predominance of flavonoids and sesquiterpene lactones³.

Keywords: Metabolomics, PGE₂, LTB₄, *Cyrtocymura*

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ASSESSMENT OF THE ANTI-INFLAMMATORY POTENTIAL OF *IXORA BREVIFOLIA BENTH*

Eduardo Choi Junior^{1*}, Daniele de Oliveira Silva¹, Lara P. D' M. Costa¹, Paulo R. S. da Silva¹, Paula P. O. Salem¹, Michael Murgu², Daniela A. Chagas de Paula¹, Danielle F. Dias¹, Marisi G. Soares¹

eduardo.choi@sou.unifal-mg.edu.br

1-Institute of Chemistry, Federal University of Alfenas, 37130-001, Alfenas, MG, Brazil.

2-Waters Corporation, 06455-020, Barueri, SP, Brazil.

Ixora brevifolia Benth. is an endemic Brazilian species belonging to the Rubiaceae family, known for its specialized metabolites, particularly indole alkaloids¹. The genus *Ixora*, which comprises approximately 400 species, is widely used in traditional medicine due to its pharmacological properties, including anti-inflammatory activity². Prostaglandin E₂ (PGE₂) and leukotriene B₄ (LTB₄) are key inflammatory mediators produced by the COX and LOX enzymes, respectively. Although non-steroidal anti-inflammatory drugs (NSAIDs) inhibit COX, their lack of effect on LOX can lead to increased leukotriene production, which is associated with various adverse effects³. Given the limitations of NSAIDs and the scarcity of information regarding the metabolites of *I. brevifolia*, the present study aimed to evaluate the anti-inflammatory potential of this species. Leaves of *I. brevifolia* were collected from the Atlantic Forest in the municipality of Alfenas (MG, Brazil), and subsequently dried, ground, and extracted using ethanol:water (7:3, v/v). The crude extract was partitioned to yield hexane (Ixh), ethyl acetate (Ixac), chloroform (Ixcl), and hydroalcoholic (Ixhd) fractions. Anti-inflammatory activity was assessed through an ex vivo assay measuring the levels of PGE₂ and LTB₄. The crude extract showed a yield of 14.0%, while the fractions ranged from 0.40% to 42.9%. The extract moderately inhibited the production of PGE₂ (34.9%) and LTB₄ (34.8%), with statistically significant differences compared to the negative control ($p \leq 0.05$). Future investigations will include the screening of the obtained fractions to identify the most bioactive one, guiding further bioactivity-directed isolation. Additionally, the chemical profile of the extract will be investigated through metabolomic analyses to further elucidate the species chemical composition.

Keywords: Rubiaceae, COX, LOX, Ex vivo assay.

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CHEMICAL PROFILE AND EVALUATION OF THE ANTI-INFLAMMATORY AND ANTIUROLITHIC ACTIVITY OF SOLANUM CERNUUM

Lara P. D M. Costa^{1*}, Daniele de Oliveira Silva¹, Paula P. O. Salem¹, Paulo R. S. da Silva¹, Michael Murgu², Daniela A. Chagas de Paula¹, Danielle F. Dias¹, Marisi G. Soares¹

lara.costa@sou.unifal-mg.edu.br

1-Institute of Chemistry, Federal University of Alfenas, 37130-001, Alfenas, MG, Brazil.

2-Waters Corporation, 06455-020, Barueri, SP, Brazil.

Solanum cernuum (Solanaceae), endemic to Brazil, is traditionally used to treat urinary disorders, mainly as a diuretic¹. Nephrolithiasis, or kidney stone disease, involves the formation of calcium oxalate (CaOx) crystals and is often linked to low fluid intake and poor diet. Its pathogenesis includes inflammatory processes mediated by arachidonic acid and prostaglandin E₂ (PGE₂), associated with hypercalciuria and hyperoxaluria². Considering the reported efficacy of *Solanum* species and the need for multi-target therapies, this study evaluated an infusion of *S. cernuum* for antiurolithiatic activity, anti-inflammatory effects on COX and LOX pathways, and chemical composition by UHPLC-ESI-HRMS. The infusion was prepared with dried leaves in boiling distilled water (1:20, w/v). Antiurolithiatic activity was tested in urine containing CaOx crystals (0.5–1.5 mg/mL), compared to positive controls (sodium citrate and Cystone®) and a negative control². Anti-inflammatory effects were investigated *ex vivo* in human blood, focusing on PGE₂ and leukotriene B₄ (LTB₄). Chemical profiling was performed by UHPLC-ESI-HRMS in positive mode with DIA acquisition, followed by data processing using MZmine 3 and annotation via internal and online databases. The infusion (yield 10.3%) significantly inhibited CaOx crystal formation (86.6% at the highest concentration; IC₅₀ = 0.47 mg/mL) and reduced inflammatory mediators by 39.8% (LTB₄) and 74.8% (PGE₂). Nineteen compounds were annotated according to Metabolomics Standards Initiative (MSI)³ confidence level 2, with flavonoids predominating. These compounds are recognized for pain relief, inflammation modulation, and CaOx crystal dissolution, potentially explaining the observed bioactivity^{2,4}. This is the first report of the antiurolithiatic potential of *S. cernuum*, demonstrating its effects on CaOx crystal reduction and inhibition of inflammatory mediators.

Keywords: Calcium oxalate, PGE₂, LTB₄, Flavonoids

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ETHYL ACETATE AND HYDROALCHOLIC EXTRACTS: AN ANALYSIS OF THE PHOTOPROTECTIVE POTENTIAL AND PHENOLIC COMPOUND CONTENT OF THE MELALEUCA VIMINALIS SPECIES

Marcela Nogueira Cabral^{1*}, Fernanda Braz Aguiar¹, Mairon César Coimbra¹, Juliana Cristina dos Santos Almeida Batos¹

marcelanogueiracabral0@gmail.com

1-Laboratório de Farmacognosia, Universidade Federal de São João del-Rei campus Centro-Oeste Dona Lindu, Divinópolis, Minas Gerais, 35501-296, Brazil.

The purpose of this study was to analyze the relationship between the amount of phenolic compounds and the photoprotective capacity of extracts obtained through ultrasound-assisted extraction (UAE) from *Melaleuca viminalis* leaves. To achieve this goal, plant material was collected in the city of Divinópolis, MG, where 100 g of selected leaves were cut, dried in an oven at 40 °C, and subsequently ground before undergoing the extraction process. The following solvents were used for extraction: 1–ethyl acetate, 2–ethanol:water (8:2), 3–ethanol:water (7:3), and 4–ethanol:water (1:1). Phenolic compounds were quantified using the Folin-Ciocalteu method^[1], employing gallic acid as a standard at concentrations of 600, 300, 150, 75, 37.5, and 18.75 µg/mL. The extract obtained with ethyl acetate (1) showed the highest level of phenolic compounds (70.5 ± 2.357 GAE/g), while the ethanol:water (1:1) extract (4) presented the lowest value (15.5 ± 1.179 GAE/g), followed by the ethanol:water (8:2) extract (2) (20.92 ± 1.768 GAE/g). Due to the statistically significant differences observed among most extracts, the photoprotective potential was assessed using the modified Mansur method^[2], with samples of each extract at 0.2 mg/mL in methanol:water (8:2) analyzed in a spectrophotometer within the UVB range (290 to 320 nm), with readings every 5 nm. Although the ethyl acetate extract (1) contained the highest phenolic content, it did not achieve the highest sun protection factor (SPF), which was obtained by the ethanol:water (1:1) extract (4) – SPF 42, followed by the ethanol:water (7:3) extract (3) – SPF 37.75. Therefore, no direct correlation was found between the amount of phenolic compounds and the SPF of the *M. viminalis* extracts. However, all extracts complied with the ANVISA regulations, which require a minimum SPF of 6 for a substance to be considered photoprotective. Thus, all the extracts proved to be promising options for developing products with photoprotective effects.

Keywords: *Callistemon viminalis*, leaves, UVB ray

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**ANALYSIS OF THE RELATIONSHIP BETWEEN PHENOLIC COMPOUNDS AND
PHOTOPROTECTIVE POTENTIAL OF ULTRASOUND EXTRACTS OF THE
SPECIES MELALEUCA VIMINALIS**

Fernanda Braz Aguiar^{1*}, *Marcela Nogueira Cabral¹*, *Mairon César Coimbra¹*, *Tiago
Silveira Gontijo¹*, *Rosimeire Coura Barcelos¹*, *Juliana Cristina dos Santos Almeida Batos¹*

nanda-brazaguiar@hotmail.com

1-Laboratório de Farmacognosia, Universidade Federal de São João del-Rei *campus* Centro-Oeste
Dona Lindu, R. Sebastião Gonçalves Coelho, 400, Divinópolis, Minas Gerais, 35501-296, Brazil.

This study aimed to evaluate the relationship between the phenolic compounds content and the photoprotective potential of ultrasound-assisted extracts^[1] from *Melaleuca viminalis* leaves. Plant material was collected in Divinópolis, Minas Gerais (MG), in which samples of 100 g of pre-selected leaves were cut, oven-dried at 40 °C, and pulverized to then be subjected to the ultrasound-assisted extraction. The selected solvents were water (EUA), 96°GL ethanol (EUE), methanol (EUM), and ethyl acetate (EUAc). The quantification of phenolic compounds was carried out using the Folin- Ciocalteu method^[2] using gallic acid as the standard at concentrations of 600, 300, 150, 75, 37.5 and 18.75 µg/mL. Due to the statistically significant difference among most extracts using ANOVA one-way and Tukey, their photoprotective potential was evaluated using the modified Mansur method^[3]. Each extract was prepared at 0.2 mg/mL in a methanol:water (8:2) solution and analyzed by a UV spectrophotometer in the UVB range (290 to 320 nm) at 5 nm intervals. Among the extracts, EUA had the lowest phenolic content (17.167 ± 2.205 GAE/g), while EUAc had the highest (70.5 ± 2.357 GAE/g), followed by EUM (34.944 ± 1.925 GAE/g). Even though EUAc had the highest phenolic content, it did not yield the highest sun protection factor (SPF). The highest SPF was observed for EUE (SPF 35), followed by EUM (SPF 33,9). Thus, a direct correlation between the phenolic content and the sun protection factor of these extracts of *M. viminalis* species was not observed. Nevertheless, all extracts fit the ANVISA legislation, which requires a minimum SPF of 6 to qualify as a photoprotective agent. Therefore, all extracts demonstrated potential as viable ingredients in photoprotective formulations.

Keywords: *Callistemon viminalis*, leaves, UVB rays

Acknowledgements: FAPEMIG, CAPES, CNPq, GCUB, UFSJ.

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GOLD NANORODS SYNTHESIZED USING ANALYTICAL AND COMMERCIAL RUTIN: EFFECTS ON SURFACE PLASMON RESONANCE

Lucas Henrique Faria Santos^{1*}, Kennedy Batista Gonçalves², Tiago Silveira Contijo¹, Juliana Cristina dos Santos Almeida Bastos¹, Livia Siman Gomes², Rosimeire Coura Barcelos¹

lucashenriquefs3@gmail.com

¹Federal University of São João del-Rei (UFSJ), Campus Centro-Oeste Dona Lindu, Divinópolis, MG, Brazil – 35.501-296; ²Nanomaterials and Graphene Technology Center, Federal University of Minas Gerais, BH/MG – 31.310-260.

Gold nanorods (AuNRs) have been widely applied in biomedicine, sensing, and electronics due to their unique physicochemical properties, such as high colloidal stability and tuneable optical absorption via aspect ratio modulation [1]. Several chemical synthesis strategies employ reducing and stabilizing agents to ensure colloidal stability and enable the functionalization of AuNRs for therapeutic and diagnostic purposes [2]. In this context, rutin, a natural flavonoid widely found in plants, exhibits antioxidant properties and can act as a reducing agent in the synthesis. In this study, we reported a comparison between AuNRs synthesized in seedless syntheses mediated by rutin samples purchased from Aldrich and from a compounding pharmacy. Chloroauric acid (0.1 mol/L), silver nitrate (0.025 mol/L), and rutin (0.055 mol/L) were sequentially added to a CTAB solution (0.055 mol/L) under continuous stirring. Subsequently, a NaBH₄ solution (4.5 mmol/L) was added. Finally, the reaction mixture was heated to 70 °C and incubated for 4 h. The characterization of AuNRs was performed using UV-Vis spectroscopy. The nanorods obtained by analytical and commercial purity rutin exhibited localized Surface Plasmon Resonance (LSPR) at 718 nm and 802 nm, respectively. These results demonstrate that the degree of purity of the reducing agent significantly influenced the optical properties of AuNRs. The observed change in LSPR highlighted the importance of selection and possible purification of reducing agents to achieve specific nanostructural characteristics. Studies are underway to optimize the synthesis and purification parameters of commercially available rutin, a cheaper reagent, aiming to increase control over nanorod morphology and plasmonic behavior.

Keywords: Gold nanorods; Seedless synthesis; Rutin.

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OPTIMIZATION OF THE EXTRACTION PROCESS OF *ERYTHRINA MULUNGU* PEELS RICH WITH PHENOLIC COMPOUNDS

Aline Luísa de Faria¹, Fernanda Braz Aguiar¹, Mairon César Coimbra¹, Tiago Silveira Gontijo¹, Rosimeire Coura Barcelos¹, Juliana Cristina S A Bastos^{1*}

*juliana.almeida@ufsj.edu.br

1-Federal University of São João del Rei, 400, Divinópolis, Minas Gerais, 35501-296, Brazil .

This study aimed to optimize the extraction process from the powder of the bark of the species *Erythrina mulungu* for the production of extracts rich in phenolic compounds. The selected extraction processes were ultrasound-assisted extraction, maceration in electromagnetic agitation, and continuous extraction in a reflux system. The extracting solvents used were: ethanol 96GL; methanol; ethanol:water (8:2); ethanol:water (7:3); ethyl acetate; ethanol: ethyl acetate (1:1). In 10.0 g of the acquired plant material, 100 mL of the extracting solvent was added and the extraction was carried out at room temperature for 40 minutes. Afterwards, the extracts were centrifuged, filtered, evaporated in a rotary evaporator at 40°C and finally placed in an oven at 40°C for complete drying. To determine the content of total phenolic compounds, the Folin-Ciocalteu method was used, in which gallic acid at 1 mg/ mL in methanol was used as a standard at concentrations of 300, 150, 75, 37.5, 18.75, 9.375, 4.69 µg/ mL and the extracts were tested at a concentration of 2 mg/ mL in methanol, of which 150 µL aliquots were transferred to a 96-well plate and 40 µL of a 4% sodium carbonate solution and 10 µL of a Folin reagent solution were added. Ciocalteu 10%. Afterwards, the plate was incubated in the dark for 1 hour and the absorbance was read in a microplate reader at 650 nm. All analyses were performed in quadruplicate and the results were expressed in EAG (gallic acid equivalents) per gram of sample and submitted to analysis of variance (ANOVA- One way) followed by the Tukey test, with p value <0.5. The correlation coefficient presented a value of 0.995 and the equation of the straight line of $x = (y - 0.6537) / (0.0036)$. The extracts that presented the highest content of phenolic compounds were the one in ethanol:water (8:2) by the extractive method of maceration in electromagnetic agitation with 314.81 ± 0.107 EAG/g; the extract in ethanol:water (8:2) by the extraction method in a reflux system with 262.79 ± 0.208 EAG/g and the ethanolic extract obtained by maceration in an ultrasound bath with 252.44 ± 0.259 EAG/g. The extracts that presented the greatest statistical significance when compared to each other were Ethanol: Ethyl Acetate (1:1) by the extractive method in a reflux system with Ethanol : Water (7:3) obtained by maceration in electromagnetic agitation.

Keywords: compounds, bark, mulungu, phenolics

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**IMPACT OF EXTRACTION PARAMETERS ON THE PHOTOPROTECTIVE
POTENCIAL OF *Melaleuca viminalis* LEAF EXTRACTS**

Pedro Henrique de O. S. Xavier¹; Gabriel M. de Freitas¹; **Nicolas G. T. e Castro¹**; Fernanda B. Aguiar¹; Rosimeire C. Barcelos¹; Juliana Cristina dos S. A. Bastos^{1*}

juliana.almeida@ufs.j.edu.br

1- Federal University of São João del-Rei, Street Sebastião Gonçalves Coelho 400, Divinópolis, MG, 35501-296.

Sunscreens often contain organic and inorganic compounds, the latter associated with adverse effects such as allergies and allergies. In view of this, low-toxicity natural active ingredients have emerged as safer alternatives (Bhattacharjee et al., 2021). Furthermore, due to growing concern about the environmental impact of cosmetics, the use of less toxic solvents and more sustainable and efficient processes has become a global priority (NEVES et al., 2020). *Melaleuca viminalis*, from the Myrtaceae family, is rich in phenolic compounds with antioxidants, anti-inflammatory, antibacterial, antitumor and photoprotective properties (Bhagat et al., 2017). In this context, this study evaluated the photoprotective potential of *M. viminalis* leaf extracts.

10 g of dried and ground plant material were added to 100 mL of three different solvents (ethanol, methanol, and ethyl acetate). Ultrasound-assisted extraction was performed for 30, 60, and 90 minutes, in triplicate. Subsequently, the photoprotective potential was evaluated by the modified Mansur method, using ethanolic solutions 0.02 mg/mL of each extract. Absorbance readings were performed in quadruplicate using a microplate reader, with 5 nm intervals within the UVB radiation range (290–320 nm). The ethanolic extracts exhibited the highest Sun Protection Factor (SPF), followed by those extracted with methanol and ethyl acetate. The extraction time positively influenced the photoprotective potential of the methanolic extracts, whose SPF values were 9.77, 10.39 and 11.41 for the extractions at 30, 60 and 90 minutes, respectively. However, for the extracts obtained with ethyl acetate there was no significant variation in SPF (5.47, 5.67 and 5.94 for 30, 60 and 90 minutes of extraction, respectively). These results confirmed the photoprotective potential of *M. viminalis*, as well as the importance of the solvent and extraction's time in the search for effective, safe and environmentally friendly photoprotective agents.

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Keywords: Photoprotection, Sunscreens, Extracts, *Melaleuca viminalis*.





**METABOLOMICS REVEALS THE IMPACT OF SEASONAL VARIATION ON THE
CHEMICAL PROFILE AND ANTI-INFLAMMATORY ACTIVITY OF OCOTEA
ODORIFERA (VELL.) ROHWER ESSENTIAL OILS**

Renato Almeida Oliveira¹, Rodrigo Moreira da Silva¹, Albert Katchborian-Neto^{1,3}, Miller Santos Ferreira¹, Paula Pio de Oliveira Salem¹, João Henrique Glilardi Lago², Karen de Jesus Nicacio², Danielle Ferreira Dias¹, Marisi Gomes Soares¹ and Daniela Aparecida Chagas-Paula^{1*}

renato.oliveira@sou.unifal.edu.mg.br

1-Institute of Chemistry, Federal University of Alfenas, 37130-001, Alfenas, Minas Gerais, Brazil; 2-Department of Chemistry, Federal University of Mato Grosso, 14040-901, Cuiabá, Mato Grosso, Brazil; 2- Center of Natural Sciences and Humanities, Federal University of ABC, Santo Andre, São Paulo, Brazil;

Ocotea odorifera, commonly known as sassafras or canela-sassafras, has long been used in Brazilian traditional medicine to treat ailments such as edema, gastrointestinal disorders, arthritis, syphilis, and fever. Beyond its ethnopharmacological significance, the species has demonstrated scientifically validated antioxidant, antimicrobial, antimutagenic, and more recently, anti-inflammatory properties¹. In this study, a metabolomics-driven approach was employed to investigate, for the first time, how seasonal variation shapes both the chemical composition and the anti-inflammatory activity of *O. odorifera* essential oils. Leaves were collected monthly over one year, and essential oils were extracted via hydrodistillation. Gas Chromatography-Mass Spectrometry (GC-MS) analysis revealed pronounced seasonal shifts in composition, with safrole consistently dominant yet variable in concentration levels (55-80%), alongside less abundant constituents such as camphor (4-9%), followed by bicyclogermacrene (2-7%). The essential oils were assessed using an *ex vivo* anti-inflammatory assay, measuring prostaglandin E₂ (PGE₂) levels in lipopolysaccharide-stimulated human whole blood. Ultra-Performance Liquid Chromatography coupled with Tandem Mass Spectrometry (UPLC-MS/MS) was employed to determine PGE₂ inhibition levels. Untargeted metabolomics demonstrated that oils harvested in autumn and spring exhibited fluctuations in the chemical composition, which favored greater PGE₂ inhibition levels compared to those samples from summer. However, the OPLS-DA model revealed β -pinene, limonene, and sabinene as statistically significant variables, all negatively correlated with increased anti-inflammatory activity (VIP > 1; $p < 0.05$; $q < 0.05$). While 4-terpineol and α -cadinol also exhibited high variance important in projection (VIP) scores, and positive correlation, indicating potential biological relevance. However, they did not reach statistical significance threshold, likely due to the limited sample size. These findings highlight how seasonal variations influence the specialized metabolism and anti-inflammatory properties of *O. odorifera* essential oils, providing valuable insights into their therapeutic potential.

Keywords: *Ocotea odorifera*, Canela-sassafras, seasonal variation, GC-MS, UPLC-MS/MS, Prostaglandin E₂.



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Metabolomics, Anti-inflammatory and Antitumoral Activity of the Endophytic Fungi from *Ocotea* ssp. (Lauraceae).

Chronic inflammation within the tumor microenvironment plays a pivotal role in cancer progression and therapeutic resistance. In this study, endophytic fungi isolated from *Ocotea odorifera* and *O. diospyrofolia* were evaluated for their anti-inflammatory and antitumor properties, alongside compound dereplication via UPLC/HRMS analysis. Ethyl acetate extracts of these endophytes were assessed through *ex vivo* and *in vitro* assays, revealing that several isolates, particularly those from *O. diospyrofolia*, effectively reduced pro-inflammatory mediators (PGE2 and LTB4) and decreased melanoma cell viability. One extract, derived from *Lasiodiplodia* sp., demonstrated potent antiproliferative activity against the SK-MEL-147 melanoma cell line, with an IC₅₀ of 9.01 µg/mL, surpassing the efficacy of the reference drug Temozolomide. Cell cycle analysis revealed an increased SubG1 population, accompanied by a reduction in the G0/G1, S, and G2/M populations. Mechanistic investigations further indicated the induction of apoptosis, as evidenced by Annexin V assay and Caspase-3 immunofluorescence, along with disruption of the microtubule network. Additionally, there was a dual inhibition of the COX and LOX inflammatory pathways. Importantly, the extract exhibited low cytotoxicity toward normal fibroblast cultures and significantly suppressed clonogenic potential at subtoxic concentrations. Collectively, these findings highlight the fungal-derived metabolites as inflammation and apoptosis modulators, supporting the further exploration of *Lasiodiplodia* sp. as a potential candidate for the treatment of metastatic melanoma, a malignancy with high lethality and limited therapeutic options.

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Keywords: *Ocotea*, metabolomics, cancer, inflammation, endophytic fungi.





ANTIMICROBIAL PROSPECTION OF CHITOSAN BIOFILMS WITH ETHANOLIC EXTRACT FROM *Libidibia ferrea* STEM

Luís Filipe Gomes Santos^{1*}, Aiane Nascimento Santana¹, Marcos Malta³, Lourdes Cardoso de Souza Neta¹, Sandra Aparecida Alexandre Lucas², Rodrigo Lassarote Lavall², Luciano da Silva Pinto⁴, Arnaud Victor dos Santos¹, Madson de Godoi Pereira¹

luisfilipeg21@gmail.com

1-Departamento de Ciências Exatas e da Terra, Universidade do Estado da Bahia, R. Silveira Martins, 2555, 41150-00, Salvador, BA, Brazil. 2-Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Av. Antônio Carlos, 6627, 31270-901 Belo Horizonte, MG, Brazil. 3-Universidade Federal da Bahia, Av. Milton Santos – Salvador – BA, 40170-110, Brazil. 4-University of São Paulo Av. Prof. Lineu Prestes, 580 – São Paulo – SP, Brazil

The aqueous and alcoholic extracts of the fruit of *Libidibia ferrea* (Fabaceae family) are used in traditional medicine as antibacterial, antifungal, and wound healing agent. The antibacterial and antifungal prospecting of the aqueous (EAQ) and ethanolic (EET) extracts of the fruit of *L. ferrea*, as well as their biofilms produced based on chitosan, was developed against eight strains of microorganisms. The crude aqueous (EAQ) and ethanolic (EET) extracts of the fruits were antibacterial against *Staphylococcus epidermidis* (MIC = 15.63 $\mu\text{g mL}^{-1}$, for both; MBC = 500 $\mu\text{g mL}^{-1}$, only for EET), *Bacillus subtilis* and *B. cereus* (MICs = 1000 $\mu\text{g mL}^{-1}$). Regarding the fungicidal effect, only EET was active against *Candida albicans* [MIC = 15.6 $\mu\text{g mL}^{-1}$; MFC = 31.25 $\mu\text{g mL}^{-1}$). The FQEET 30% biofilm was more active against *Micrococcus luteus*, among all microorganisms tested, with values of growth inhibition zone (ZI) = 2.05 mm, by agar diffusion method. The biofilms of the aqueous extract of chitosan, FQEAQ, and the ethanolic extract (FQEET) showed ZIs in the range of 1.06 mm to 2.56 mm for *M. luteus*, *S. aureus*, and *S. epidermidis*, respectively. The chitosan biofilm (100%) did not exhibit an inhibitory effect against the tested microorganisms. Thus, the antimicrobial activity presented by the biofilms was due to the compounds present in the extracts, which are mainly phenolic derivatives [total phenolic (TP): EAQ: 327.95 $\pm$ 14.61 $\mu\text{g mg}^{-1}$ EAG; (TP): EET: (292.06 $\pm$ 24.35 $\mu\text{g mg}^{-1}$ EAG)] e [total tannins (TT): EAQ: 227.74 $\pm$ 17.43 $\mu\text{g mg}^{-1}$ of EAT; EEt = 189.49 $\pm$ 20.92 $\mu\text{g mg}^{-1}$ of EAT]. This study has resulted in the production of antimicrobial biofilms from chitosan extracts of the fruit of *L. ferrea*, with long-term potential for use in the treatment of antimicrobial infections in skin wounds. Acknowledgments: FAPESB, UNEB, PGQA, UFBA, UFMG, CAPES.

Keywords: Antibacterial, Antifungal, Composite





ANTIMICROBIAL PROSPECTING OF THE ETHANOLIC EXTRACT OF THE FRUIT *Libidibia ferrea* AND ITS FRACTIONS

Maria Clara Silva Sacramento^{1*}, Aiane Nascimento Santana¹, Júlia Oliveira Tanajura Mendes¹, Helena Carla Magalhães dos Reis¹, Giovanna Regina Gonzalez de Santana Wojnar¹, Livia Dantas Silva Bizerra¹, Luís Filipe Gomes Santos¹, Robert Agapito Cardoso¹, Madson de Godoi Pereira¹, Suzimone de Jesus Correia Torquato¹, Luciano da Silva Pinto², Lourdes Cardoso de Souza Neta¹

mariasacramento@uneb.br

1-Departamento de Ciências Exatas e da Terra, Universidade do Estado da Bahia, R. Silveira Martins, 2555, Cabula, 41150-00, Salvador, Bahia, Brazil. 2- Food Research Center (FoRC), Department of Food and Experimental Nutrition Faculty of Pharmaceutical Sciences – University of São Paulo, Av. Prof. Lineu Prestes, 580 – Bloco 14 05508-900 São Paulo, São Paulo, Brazil,

Extracts from the fruit and stem of *Libidibia ferrea* (Fabaceae) show several biological activities, such as antibacterial, antifungal, antioxidant, and wound healing. Given this, the prospection of the ethanolic extract of the fruit of *L. ferrea* and its fractions was investigated against microorganisms of the genera *Bacillus sp*, *Escherichia sp*, *Pseudomonas sp*, *Salmonella sp*, *Staphylococcus sp*, and *Candida sp*, by broth microdilution method. The ethanolic extract of the fruit (EEtFr) was fractionated by silica gel column chromatography, yielding 17 fractions (FEtFr1 – FEtFr17), which were eluted with a polarity gradient. The fractions showed antimicrobial activity only for the bacteria *Staphylococcus aureus* and *Bacillus cereus*. FEtFr1 and FEtFr9 were the most active, among all tested, against *S. aureus*, with bacteriostatic (MICs 62.50 $\mu\text{g mL}^{-1}$ and 125.0 $\mu\text{g mL}^{-1}$, respectively) and bactericidal (MBC = 125 $\mu\text{g mL}^{-1}$ and MBC = 500 $\mu\text{g mL}^{-1}$, respectively) effects. The fractions FEtFr5-7, FEtFr1-10, and FEtFr13 were also bactericidal for *S. aureus* (MICs = 250 $\mu\text{g mL}^{-1}$ for all and MBC values ranging from = 250 $\mu\text{g mL}^{-1}$ to 500 $\mu\text{g mL}^{-1}$). Regarding *B. cereus*, the fractions FEtFr1–5, FEtFr7, FEtFr9-10, FEtFr12-15 were bacteriostatic (MIC value range = 250 $\mu\text{g mL}^{-1}$ to 500 $\mu\text{g mL}^{-1}$; MBC = 500 $\mu\text{g mL}^{-1}$ for the bactericidal ones). Additionally, ¹H NMR data from the fruit extract and fractions confirm the presence of phenolic compounds. However, the study of the chemical profile of the extracts and fractions by HPLC-MS is under analysis. The results suggest that the antibacterial fractions may contribute to the discovery of new antimicrobial agents in the long term. Acknowledgments: UNEB, FAPESB, CAPES, UFBA, USP.

Keywords: Antibacterial, Phenolic compounds, Fabaceae





PHYTOCHEMICAL CHARACTERIZATION, ANTINOCICEPTIVE POTENTIAL, AND SAFETY ASSESSMENT OF CHAMAECRISTA DIPHYLLA (L.) GREENE

José Diogo Evangelista Reis^{1*}, Brenda Costa da Conceição², Eloise Karoline Serrão Cardoso², Lucas Villar Pedrosa da Silva Pantoja², Monique Silva Kussler², Renata Garcia Nogueira², Luanna Melo Pereira Fernandes³, Jofre Jacob da Silva Freitas³, Washington Luiz Assunção Pereira⁴, Ana Paula França Rodrigues¹, Consuelo Yumiko Yoshioka e Silva¹, Cristiane Socorro Ferraz Maia², Eneas Andrade Fontes-Junior², Paulo Wender Portal Gomes¹, Milton Nascimento da Silva¹

reis.diogo190@gmail.com

¹Amazon Integrated Metabolomics Center (CIMAZON), Exact and Natural Sciences Institute, Federal University of Pará, Belém 66075110, PA, Brazil.

²Laboratory of Pharmacology of Inflammation and Behavioral (LAFICO), Health Science Institute, Federal University of Pará, Belém 66075110, PA, Brazil.

³Department of Physiological and Morphological Sciences, Health and Biologic Science Center, State University of Pará, 66087-662 Belém, PA, Brazil.

⁴Animal Pathology Laboratory, Amazon Federal Rural University, Belém 66077830, PA, Brazil.

The Amazon is rich in plant biodiversity, with several species used in traditional medicine, such as *Chamaecrista diphylla* (L.) Greene, a small herb used for therapeutic purposes in treating ulcers, wounds, and constipation, has an abundance of phenolic compounds. Therefore, this study investigated the phytochemical profile of the aqueous extract of *C. diphylla*, its acute oral toxicity, antinociceptive potential, and the possible pathways involved in this activity. Manual inspection of each mirror plot between experimental mass spectra and reference available in the GNPS libraries allowed the annotation of 23 compounds. The analyzed *C. diphylla* aerial parts infusion mainly contains twelve flavonoids, including flavones, anthocyanins, flava-3-ols and flavonols. Furthermore, eight organic acids and three terpenes were also annotated. For toxicity studies, rats were treated with a limiting dose (2000 mg/kg) of aerial parts extract, followed by an evaluation of the occurrence of deaths or hippocratic, behavioral, biochemical, anatomical or histopathological signs of intoxication. Antinociceptive activity was evaluated in male mice using the writhing test with acetic acid and the pathways were investigated using opioid, cholinergic and adrenergic antagonists and K⁺ channel blockers. The extract showed low acute oral toxicity and dose-dependent antinociceptive activity, possibly related to adrenergic and cholinergic pathway modulation.

Keywords: *Chamaecrista diphylla*, acute toxicity, antinociceptive, folk medicine, phytochemistry.





CHEMICAL PROFILE AND EVALUATION OF THE ANTIOXIDANT AND ANTI-*Helicobacter pylori* ACTIVITIES OF *Eugenia astringens* (MYRTACEAE)

Deanne Fiorio*, Dalila Nikel Loose, Rita de Cássia Ribeiro, Claudia Masrouah Jamal

deanne.fiorio@edu.ufes.br

Department of Pharmaceutical Sciences, Health Sciences Center, Federal University of Espírito Santo, Vitória, ES, 29040-091, Brazil

The Myrtaceae family is one of the largest and most diverse families of plant species found in Brazil. Among them, *Eugenia astringens* is traditionally used in folk medicine for its anti-inflammatory, antidiabetic and gastric disorder-relieving properties. Therefore, the aim of this study was to evaluate the chemical profile as well as the antioxidant and anti-*Helicobacter pylori* activities of *E. astringens*. The leaf extract was prepared by maceration using methanol as the solvent. Chemical characterization was carried out using Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI(-/+)-FT-ICR MS). Antioxidant activity was determined by DPPH and ABTS assays using spectrometric methods. The determination of Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) followed the guidelines of the Clinical and Laboratory Standards Institute (CLSI, M7-A10 standard, 2015). Through mass spectrometry analysis (ESI(-/+)-FT-ICR MS) of the extract, six flavonoids were identified: quercetin, quercitrin, myricitrin, myricetin, luteolin and tricetin; as well as seven terpenes: selinene, sitosterol, amyrine, taraxerol, betulinic acid, corosolic acid and maslinic acid. *E. astringens* exhibited antioxidant activity with IC₅₀ values of 11.173 µg/mL in the DPPH assay and 23.865 µg/mL in the ABTS assay. The MIC and MBC values were both 128 µg/mL. Results below 1000 µg/mL are considered active against *H. pylori*, which is the standard adopted in screening studies for substances with antimicrobial potential. Based on the results obtained, it can be concluded that both the antioxidant activity and the MIC and MBC values against *H. pylori* are significant and may be associated with the presence of terpenes and phenolic compounds in its chemical composition. Thus, these findings demonstrate consistency between the biological activities traditionally reported by the population for *E. astringens* and the results obtained in this study.

Keywords: *Eugenia astringens*, mass spectrometry, antioxidant, *Helicobacter pylori*.





***EFFECT OF AQUEOUS AND ETHANOLIC EXTRACTS OF
PLECTRANTHUS BARBATUS ON HYPERURICEMIA***

Ana Carolina Silva^{1*}, Isabela Fernanda Souza¹, Rafaela Cunha Matosinhos¹, Andressa Magalhães Barbosa¹, Ana Clara da Silva¹, Aureliana de Fátima dos Reis Menezes¹, Dênia Antunes Saúde Guimarães¹

ana.silva5@aluno.ufop.edu.br

1- Laboratório de Pesquisa de Plantas Medicinais, Escola de Farmácia, Universidade Federal de Ouro Preto, Ouro Preto, Minas Gerais Brazil.

Hyperuricemia can lead to the development of gouty arthritis, which is highly prevalent in the global population. Gouty arthritis is an inflammatory disease caused by the deposition of monosodium urate crystals in joint, resulting from elevated blood uric acid (UA) levels. Conventional chronic gout treatment aims to reduce uricemia using medications such as allopurinol, benzbromarone, and probenecid. However, these medications are limited and have proven ineffective in treating 20% of hyperuricemic patients. *Plectranthus barbatus* (Brazilian boldo) is a medicinal plant widely used in traditional medicine for pain relief and inflammatory conditions. This study aimed to investigate the hypouricemic potential of aqueous and ethanolic extracts from *P. barbatus* leaves in a rat model of hyperuricemia. Hyperuricemia was experimentally induced in male Wistar rats by intraperitoneal (i.p.) administration of potassium oxonate and uric acid by gavage, except for the animals in the normal control group. The extracts were administered to animals (i.p.) at doses of 5, 15, 30, 60, 120 e 240 mg/kg. The treatments were compared to positive controls (allopurinol, probenecid and benzbromarone) and to a hyperuricemic control group (animals in this group were induced to hyperuricemia and treated with vehicle only). The results showed that both extracts significantly reduced serum UA levels at all evaluated doses ($p < 0,05$), compared to the hyperuricemic group (11,16 mg/dL). The ethanolic extract at doses of 15, 60, and 120 mg/kg and the aqueous extract at 5 mg/kg significantly increased urinary UA excretion. Additionally, both extracts significantly inhibited hepatic xanthine oxidase activity at all doses, suggesting the therapeutic potential of *P. barbatus* in managing hyperuricemia and reinforce the importance of studying medicinal plants as source of new hypouricemic agents. The authors thank the support from their institutions and the financial support of Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG), Universidade Federal de Ouro Preto (UFOP), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Financiadora de Estudos e Projetos (FINEP).

Keywords: Hyperuricemia, *Plectranthus*, gout, uric acid, uricosuric agents, xanthine oxidase





CHITOSAN BIOFILMS WITH ETHANOLIC EXTRACT OF *Libidibia ferrea* LEAVES: ANTIBACTERIAL POTENTIAL

Helena Carla Magalhães dos Reis^{1*}, Andreza S. de Jesus¹, Aiane N. Santana¹, Luis Filipe G. Santos¹, Maria Clara S. Sacramento¹, Caline G. Ferraz³, Vitor Hugo M.¹, Sandra Aparecida A. Lucas², Rodrigo L. Lavall², Isaac Matheus J. Silva³, Walter Nei L. Santos¹, Madson de G. Pereira¹, Lourdes C. de Souza Neta¹

hcarla01.hc@gmail.com

1-Departamento de Ciências Exatas e da Terra, Universidade do Estado da Bahia, R. Silveira Martins, 2555, Cabula, 41150-00, Salvador, Bahia, Brazil. 2-Universidade Federal de Minas Gerais, Belo Horizonte, Universidade do Estado de Minas Gerais, João Monlevade, Minas Gerais, 35930-314, Brazil. 3-Universidade Federal da Bahia, Av. Milton Santos - Ondina, Salvador - BA, 40170-110

Chitosan is widely used as a base for synthesizing biofilms with potential applications in food preservation and wound healing. Thus, combining medicinal plant extracts with chitosan to prepare biofilms is a strategy for discovering new antimicrobial materials. Given this context, were developed the synthesis and antimicrobial evaluation of biofilms from the ethanolic extract of *Libidibia ferrea* stem and its fractions in ethyl acetate and water. Antimicrobial assays were conducted against *Staphylococcus* sp, *Bacillus* sp, *Escherichia* sp, *Pseudomonas* sp, *Candida* sp by broth microdilution and agar diffusion methods. The chitosan film with the extract (FQEEt) and the crude extract (EEt) were active against *S. aureus*. [inhibition zone (IZ) of FQEEt = 1.41 ± 0.07 cm; IZ of crude EEt = 1.40 ± 0.1 cm]. However, the crude EEt also inhibited *B. cereus* [IZ = 1.40 ± 0.1 cm]. The chitosan films with fractions FFETOA and FFAQ inhibited *S. aureus* [IZ = 1.2 ± 0.1 cm] and *B. cereus* [IZ of FFETOA = FFAQ = 1 ± 0.1 cm]. The pure chitosan film (100%) showed no antimicrobial effect. In the broth microdilution tests, the FFAQ fraction was bacteriostatic against *S. aureus* [MIC = 500 $\mu\text{g mL}^{-1}$] and bactericidal for *B. cereus* [MIC = MBC = 250 $\mu\text{g mL}^{-1}$]. Meanwhile, the FFETOA fraction showed both effects for *S. aureus* [MIC = MBC = 500 $\mu\text{g mL}^{-1}$] and *B. cereus* [MIC = 125 $\mu\text{g mL}^{-1}$ and MBC = 250 $\mu\text{g mL}^{-1}$]. Tetracycline showed MIC = MBC $\leq 7,8 \mu\text{g mL}^{-1}$ for both bacteria. The results demonstrated that the antimicrobial activity of the biofilms was due to the incorporation of *L. ferrea* samples, highlighting the potential of these materials for long-term use as antimicrobial packaging and/or wound dressings. The authors would like to thank FAPESB, UNEB, PGQA, UFBA, UFMG, and CAPES for their financial and institutional support, which was essential for the development of this research.

Keywords: Biofilms, Antibacterial, Fabaceae



Activity-driven discovery of Brazilian biodiversity using native metabolomics

Gabriel Santos Arini^{1,2,3*}, Paolo Stincone¹, Tilman Schramm¹, Elthon Ferreira⁴, Iasmin Cartaxo Taveira⁵, João Vitor Ferreira², Luiz Mencucini², Paula Jimenez⁶, Leticia Lotufo⁴, Norberto Lopes⁷, Daniel Petras¹, Ricardo Roberto da Silva^{2,3,7}

gabriel.arini@usp.br

1-Functional Metabolomics Lab, Biochemistry Department, UC Riverside, Riverside, California, USA. 2-Computational Chemical Biology Lab, Department of BioMolecular Sciences, University of São Paulo, Ribeirão Preto, Brazil. 3- Department of Cell and Molecular Biology, University of São Paulo, Ribeirão Preto, Brazil. 4- Department of Pharmacology, University of São Paulo, São Paulo, Brazil. 5-Department of Biochemistry, University of São Paulo, Ribeirão Preto, Brazil. 6-Instituto do Mar, Federal University of São Paulo. 7-Faculty of Pharmaceutical Sciences, University of São Paulo, Ribeirão Preto, Brazil

Natural products are a valuable resource for discovering and developing new drugs. The main challenge in this process is identifying compounds that act on specific targets. One way to overcome this challenge is through targeted metabolomic screening. Native metabolomics, a mass spectrometry-based method, has emerged as a promising way to identify compounds in complex matrices that can interact with specific protein targets on a large scale. BR177, a marine actinomycete isolated off the Brazilian coast, showed promising results regarding the anti-tumor activity of its extracts. However, the targets and modulators of this activity have not yet been fully elucidated. Therefore, we hypothesized that one or more metabolites could act on proteases, thereby triggering the observed effect on tumor cells. To test this hypothesis, we used native metabolomics to evaluate the potential of bioactive compounds in the exometabolome of BRA177 on chymotrypsin, a model serine protease. Two metabolites, among 2,197 detected features, interacted with chymotrypsin. Based on their fragmentation spectra, we annotated both compounds as riboflavin, a pteridine, and a terpenoid derived from glucopyranosiduronic acid. Through docking, both compounds demonstrated binding capacity with the target protein in all described isomers of riboflavin and three of the five described isomers of the terpenoid derivative. These results demonstrate the potential of native metabolomics as a platform for the directed discovery of new bioactive candidates from complex matrices, with a focus on Brazilian diversity.

Keywords: Mass spectrometry; Guided-discovery approach; Native metabolomics





SYNERGISTIC ANTIMICROBIAL EFFECTS OF COFFEE GREEN EXTRACT AND OIL IN MICROEMULSIONS ENHANCED BY PHOTODYNAMIC THERAPY: A STRATEGY AGAINST ANTIBIOTIC RESISTANCE

Paulinne Moreira Lima^{1*}, Catarina Silva Guimarães¹, Caroline Vieira Gonçalves¹, Caio Cesar Pereira¹, Laryana Borges Garcia¹, Isabela Dias dos Santos¹, Jayne Ferreira da Silva Oliveira¹, Micaela Sousa Coutinho Silva¹, Mateus Freire Leite², André Luís Morais Ruela³, Gabriel Azevedo de Brito Damasceno¹, Denise Brentan da Silva⁴, Robson Amaro Augusto da Silva¹, Juliano Geraldo Amaral¹

paulinneml@ufba.br

1- Universidade Federal da Bahia, CAT- IMS, Rua Hormindo Barros, 58, Candeias, Vitória da Conquista, 45029094, Bahia, Brazil. 2- Universidade Federal de Alfenas, Rua Gabriel Monteiro da Silva, Alfenas, Centro, 37130001, Minas Gerais, Brazil. 3- Universidade Federal de Ouro Preto, Morro do Cruzeiro, Bauxita, Ouro Preto, 35400000, Minas Gerais, Brazil 4 - Universidade Federal de Mato Grosso do Sul, Av. Costa e Silva, Universitário, 79002970, Campo Grande, Mato Grosso do Sul, Brazil.

Coffee, one of the main tropical crops, has Brazil as its leading global producer. Rich in chlorogenic acids, it exhibits antimicrobial activity and serves as a natural alternative against antibiotic resistance, a major public health issue. Another promising strategy is antimicrobial photodynamic therapy (aPDT), which uses photosensitizers, light, and oxygen to eliminate microorganisms. The green coffee oil was characterized using gas chromatography, and the green coffee extract using high-performance liquid chromatography, both coupled with mass spectrometry. Microemulsions were prepared by the spontaneous emulsification method, containing green coffee oil and extract, stabilized by surfactants. The antimicrobial potential of the developed microemulsion system and the green coffee extract was evaluated *in vitro* by PDT using high-intensity blue LED light against methicillin-resistant *Staphylococcus aureus* (ATCC 43300). The dispersed systems obtained presented droplet sizes of approximately 25 to 60 nm, PDI of 0.088 to 0.290, and zeta potential of approximately -12 to -25 mV, at different temperatures and stability tests. Furthermore, they exhibited Newtonian flow behavior with a viscosity of approximately 30 cP. In addition, they were effective in treating microorganisms at lower doses than previously reported in the literature, with a potentiated effect when combined with photodynamic therapy, acting at a minimum green coffee extract concentration of 250 $\mu\text{g} \cdot \text{mL}^{-1}$ and, when photoactivated, acting at 125 $\mu\text{g} \cdot \text{mL}^{-1}$, in addition to also showing activity without the incorporated extract. The developed microemulsions show potential as antimicrobial agents in the pharmaceutical industry, with antibacterial action enhanced by photodynamic effects. The study highlights the use of plant compounds, promoting the bioeconomy and benefiting family farming, due to the economic value of coffee in Brazil.

Keywords: Nanotechnology; Bioeconomy; Bioactive compounds; Pharmaceuticals; Natural products; Photosensitizer;





AFFINITY SELECTION MASS SPECTROMETRY FOR IDENTIFICATION OF ACETYLCHOLINESTERASE LIGANDS IN *STRYCHNOS PECKII*

Fernando Cassas^{1*}, Carla L.G. Santos², Felipe M. A. da Silva ², Quezia B Cass¹

fcassas@protonmail.com; qcass@ufscar.br

1- *Separare- Nucleo de Pesquisa em Cromatografia, Departamento de Química, Universidade Federal de São Carlos, (UFSCAR), São Carlos - SP, Brazil* 2- *Instituto de Química, Universidade Federal do Amazonas (UFAM), Manaus - AM, Brazil*

Strychnos species are recognized for biosynthesizing a wide range of alkaloids with proven activity on the central nervous system. *Strychnos peckii* is traditionally used as a component of *curare*, a preparation employed by Indigenous natives from northern Brazil for hunting and warfare. Due to its use in paralytic preparations, the aqueous extract of *S. peckii* was selected to search for acetylcholinesterase (AChE) ligands using affinity selection mass spectrometry (AS-MS), via enzyme immobilization on magnetic particles. Untargeted dereplication was initially carried out resulting in 46 annotated metabolites of which 33 were alkaloids¹. For the AS-MS assay, 200 µg of *ee*AChE was immobilized on 10 mg of amino-functionalized magnetic beads through Schiff's base, using glutaraldehyde as the linker.² Control samples were prepared under identical conditions, with enzyme inactivation achieved using 100% MeOH (t = 60 min). Choline formation was monitored to assess enzymatic activity. The four stages of the assay were modulated using galantamine as the standard ligand: incubation, separation, ligand dissociation, and ligand identification by LC-HRMS. An affinity ratio (AR) of 1.3 was determined for galantamine. The affinity selection assay was thus carried out under these modulated conditions. Dissociated ligands were analyzed by LC-HRMS, and the data were processed using MZmine for ion alignment, deconvolution, and peak area calculation. The metabolites with AR > 1.3 were identified as AChE ligands and annotated as: (1) *lyaloside* (3.73), (2) *10-hydroxygeissoschizol* (3.69), (3) *camptothecin derivative* (2.51); (4) *5-carboxy strictosidine* (2.05); (5) *corynantheol* (2.04); (6) *isodolichantoside* (1.90); (7) *derivative* (1.68); (8) *strictosidine* (1.66); (9) *corynantheidol* (1.63); (10) *desoxycordifoline* (1.57); (11) *kaempferol-3-O-rhamnoside* (1.36); (12) *kaempferol* (1.35); (13) *topotecan derivative* (1.29); (14) *harman-3-carboxylic acid* (1.27). Among them, compounds (1), (3), (7), (8), (10-12), and (14) have already been described as AChE ligands in the literature. The metabolites (4), (8), (10) and (11) have been isolated and are currently undergoing orthogonal assays for structural confirmation and biochemical characterization.

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Keywords: AChE ligands, Natural Products, *Strychnos* L., AS-MS





Antiproliferative and Anti-*H. pylori* Activities of Coumarin-Enriched Fractions from *Calophyllum brasiliense* Oil

Maurício Candal de Matos¹, Patricia Campos da Rocha Loss¹, Ricardo Machado Kuster^{2*}, Rodrigo Rezende Kitagawa¹, Rodrigo de Almeida Romagna¹, Ester da Silva Tonini¹

Mauricio.c.matos@edu.ufes.br

1- Departamento de ciências farmacêuticas, Universidade Federal do Espírito Santo, Vitória, Espírito Santo, 29043-213, Brazil 2- Departamento de química, Universidade Federal do Espírito Santo, Vitória, Espírito Santo, 29075-910, Brazil

The genus *Calophyllum* comprises approximately 200 species of tropical trees. In Brazil, the most representative species is *Calophyllum brasiliense* (guanandi). Pre-clinical studies have attributed several properties to extracts of *C. brasiliense*, with a notable emphasis on its antitumor activity, which is the focus of this research. Its main chemical constituents include xanthenes, coumarins, chromanones, flavonoids, and terpenoids. Evidence has demonstrated that chromanones isolated from guanandi exhibit activity against *Helicobacter pylori*, a bacterium considered a primary risk factor for gastric adenocarcinoma (GAC). This study aimed to fractionate the oil of *C. brasiliense* to obtain coumarin-enriched fractions and to evaluate their antiproliferative activity against gastric adenocarcinoma (GAC) cells and antibacterial activity against *Helicobacter pylori*. The sample, produced by the rural producer Rubens Szpilman, was subjected to a liquid-liquid partition, yielding hexanic and methanolic fractions. The methanolic fraction was purified by column chromatography (Sephadex LH-20) using methanol as the mobile phase, which generated four fractions. Following analysis by thin-layer chromatography, the first three fractions were combined and set aside, while fraction 4 was selected for structural elucidation by mass spectrometry and for biological assays of cytotoxicity (AGS and L929 cells) and antibacterial activity (*H. pylori*). The results indicated that fraction 4 exhibited an IC₅₀ of 41.25 ± 0.85 µL/mL against AGS cells, with a selectivity index of 1.58. The cisplatin control showed an IC₅₀ of 6.54 ± 0.78 µL/mL with a selectivity index of 1.02. For *H. pylori*, the Minimum Inhibitory Concentration (MIC) and Minimum Bactericidal Concentration (MBC) were both 8 µL/mL. The amoxicillin control presented an MIC of 0.0062 µL/mL and an MBC of 0.125 µL/mL. Analysis by (+)-ESI-FT-ICR mass spectrometry provided the exact molecular formula (C₂₂H₂₂NaO₅) for the molecular ion at m/z 425.13609 [M+H]⁺ and mass fragments at m/z 375 (M-CO) and 347 [(100%), M-C₄H₈], indicating the presence of 4-phenyldipyrancoumarins as the class of substances responsible for the observed biological activities.

Keywords: *Calophyllum brasiliense*, Coumarins, Chromanones, Gastric Adenocarcinoma, Mass Spectrometry.





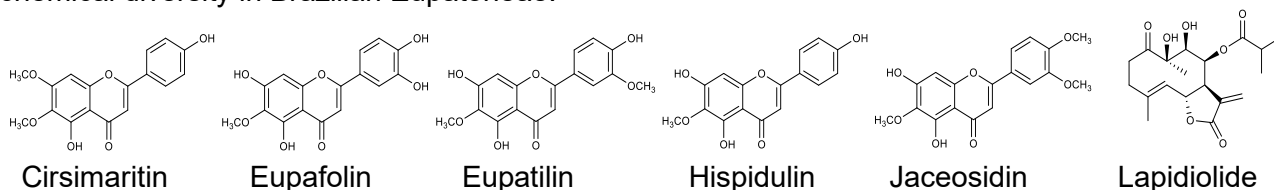
PHYTOCHEMISTRY AND CYTOTOXIC ACTIVITY OF *LAPIDIA APICIFOLIA* (EUPATORIEAE, ASTERACEAE)

Marcos Lorenzi Martins^{1*}, Simone Teixeira², Leticia Veras Costa-Lotufo², Nádia Roque^{3†},
Marcelo J. Pena Ferreira¹

marcos.lorenzi@usp.br

1- Instituto de Biociências, IB-USP, R. Matão, 277, São Paulo, SP, Brazil. 2- Instituto de Ciências Biomédicas, ICB-USP, Av. Prof. Lineu Prestes, 1524, São Paulo, SP, Brazil. 3- Instituto de Biologia, Universidade Federal da Bahia, UFBA, Salvador, BA, Brazil † (deceased).

The evolutionary success of Asteraceae is largely attributed to its chemical diversity and bioactive metabolites. Among its tribes, Eupatorieae stands out as one of the most derived, with rich species diversity and endemism in Brazil, yet its phytochemistry remains poorly understood. This study characterizes the leaf surface chemistry of *Lapidia apicifolia* Roque & S.C. Ferreira, a monospecific and endemic genus from Chapada Diamantina, Bahia, with no prior chemical or bioactivity data. Leaves of *L. apicifolia* (94.5 g) were twice immersed in dichloromethane for 30 s, yielding 16 g of surface extract after solvent evaporation. The extract was partitioned with methanol (MeOH) affording soluble and insoluble phases. The MeOH-insoluble phase was analyzed by GC-MS, identifying 18 compounds: five *n*-alkanes, seven fatty acids, three primary alcohols, two steroids, and one triterpene. The compounds of MeOH-soluble phase were analyzed and isolated by HPLC-UV (TAMAYOSE et al., 2019), leading to the NMR-based identification of five methoxylated flavones (cirsimaritin, eupafolin, eupatilin, hispidulin, and jaceosidin), and a new sesquiterpene lactone named lapidiolide. Both phases and the isolated compounds were evaluated for cytotoxic activity against two tumor cell lines: HCT-116 (human colorectal carcinoma) and MCF-7 (human breast carcinoma), at concentrations of 50 $\mu\text{g}\cdot\text{mL}^{-1}$ and 5 $\mu\text{g}\cdot\text{mL}^{-1}$. At 50 $\mu\text{g}\cdot\text{mL}^{-1}$, the MeOH-soluble phase inhibited HCT-116 and MCF-7 cells by $92.45 \pm 4.90\%$ and $84.92 \pm 2.93\%$, respectively, while lapidiolide showed $91.18 \pm 5.52\%$ and $86.17 \pm 7.44\%$ inhibition. IC_{50} values against HCT-116 were 3.51 (MeOH-soluble phase) and $15.87 \mu\text{g}\cdot\text{mL}^{-1}$ (lapidiolide); for MCF-7, only the MeOH-soluble phase showed a low IC_{50} ($4.78 \mu\text{g}\cdot\text{mL}^{-1}$). Although the results are promising, the cytotoxic activity remains less potent than that of the positive control. These results enhance our understanding of chemical diversity in Brazilian Eupatorieae.



Keywords: *Lapidia apicifolia*, Compositae, Sesquiterpene lactones, Cytotoxicity





MONTEVERDIA SALICIFOLIA REISSEK: A SOURCE OF METABOLITES WITH ANTIDIABETIC POTENTIAL

Cássia Gonçalves Magalhães^{1,2*}, Lucienir Pains Duarte², Maria Cecília Cardoso dos Santos³, Bruna Gonçalves Lopes³, Micheli Debiasi Alberton³

cgmagalhaes@uepg.br

1- Departamento de Química, SEXATAS, UEPG, Av. Carlos Cavalcanti, 4748, Ponta Grossa, PR, Brazil. 2- Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 3- Departamento de Ciências Farmacêuticas, CCS, FURB, Rua Antônio da Veiga, 140, Blumenau, SC, Brazil.

Diabetes mellitus is a multifactorial global health disorder that is rising at an alarming rate. One effective therapeutic approach for controlling hyperglycemia associated with type-2 diabetes is to target enzymes that catalyze starch and maltose hydrolysis in the intestine, such as α -glucosidase. Plant extracts are widely studied as potent candidates in the prevention and treatment of type 2 diabetes. *Monteverdia salicifolia* (syn. *Maytenus salicifolia*, Celastraceae) occurs in Southeast of Brazil. Its leaves are used in the traditional medicine for treatment of gastric ulcers and skin allergies. This species is a source of pentacyclic triterpenes, quinonemethides and flavonoids. In a continuation of the studies about the bioactive potential of *M. salicifolia*, this work aimed to evaluate the *in vitro* antiglycation activity and α -glucosidase inhibition of 4'-O-methylepigallocatechin and 16- β -hydroxypristimetin, previously isolated of this species, and its roots ethanolic extract. *In vitro* antiglycation activity by oxidative pathway was performed as described by Ramos *et al.* (2019) using glyoxal as substrate. Quercetin (1 mg mL⁻¹) was used as standard and DMSO as the negative control. Results were expressed as percentage of inhibition. The α -glucosidase inhibitory assay will be performed according to Kim, Wang, & Rhee, (2004). All the tests were performed in triplicate. The isolated compounds and the extract were able to inhibit effectively the enzyme as well as the glycation, showing a better performance than quercetin. These results support the traditional use of *Monteverdia species* in diabetes and stimulate the continuation of evaluation of the activity of these metabolites *in vivo* models. The authors thank the support from their institutions and the financial support of CAPES and CNPq.

Keywords: quinonemethides, catechins, *Monteverdia salicifolia*





Synthesis of new salicylic acid derivatives with potential bioactivity

Jennifer Blandon Pardo¹, Andre G. Tempone², Dayana Agnes Santos Ferreira², Karina Alacid Salles³, Sarah Christina Caldas Oliveira³, Laura P. R. Figueroa¹, Warley de Souza Borges^{1*}

laura.figueroa@edu.ufes.br

¹Center of Exact Sciences, Department of Chemistry, Universidade Federal do Espírito Santo, CEP 29075-910, Vitória, ES, Brazil

²Pathophysiology Laboratory, Butantan Institute, CEP 05503-900, São Paulo, SP, Brazil

³Institute of Biological Sciences, Department of Botany, Universidade de Brasília, CEP 70910-900, Brasília, DF, Brazil

The derivatization of natural products enables the generation of novel molecular entities through straightforward synthetic methodologies, providing an effective route for the incorporation of diverse functional groups. This strategy facilitates the development of compound libraries with significant structural diversity. Salicylic acid derivatives have been widely used in the treatment of several conditions, with acetylsalicylic acid being the most well-known example due to its extensive use as an anti-inflammatory agent. Other derivatives, such as methyl salicylate, salol, and salicylanilide, are recognized for their analgesic, antipyretic, antimicrobial, antiproliferative, and cytotoxic properties. In this work, a series of 27 ether derivatives of salicylic acid were synthesized using the Williamson ether synthesis, as modifications in the ether moiety can influence biological activity. Structural elucidation was performed using NMR spectroscopy. The phytotoxicity of all synthesized compounds was evaluated, revealing weak to moderate activity. Additionally, antibacterial activity was assessed against multidrug-resistant bacteria (ESKAPE); however, no significant activity was observed for any of the compounds up to 100 µM.

Keywords: salicylic acid, ether derivatives

Acknowledgments: CAPES, CNPq, FAPES, LabPetro.

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**CHEMICAL CHARACTERIZATION AND IN VITRO EVALUATION OF SOURSOP
(*Annona muricata*) SEED OIL ON FIBROBLAST PROLIFERATION AND NITRIC
OXIDE INHIBITION: A POTENTIAL BIOINPUT**

Maurília de Oliveira Souza^{1*}, Rodrigo de Almeida Romagna¹, Ester da Silva Tonini¹,
Rodrigo Rezende Kitagawa¹, Ricardo Machado Kuster¹, Janaina Cecília Oliveira Villanova²,
Cristiane dos Santos Giuberti¹.

*maurilia.souza@edu.ufes.br

*1-Programa de Pós-graduação em Ciências Farmacêuticas, Centro de Ciências da Saúde,
Universidade Federal do Espírito Santo, Vitória, ES, Brazil. 2-Programa de Pós-graduação em
Ciências Farmacêuticas, Centro de Ciências Exatas, Naturais e da Saúde, Universidade Federal do
Espírito Santo, Alegre, ES, Brazil.*

Soursop seed oil (SSO) is rich in fatty acids and acetogenins, which are associated with various pharmacological properties. This study aimed to determine the chemical composition of SSO, investigate its wound-healing potential using a scratch assay on L-929 fibroblast cells, and its ability to inhibit nitric oxide (NO) release in a cell-free system. The chemical composition was determined using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS), operated in positive ion mode. For the scratch assay, L-929 fibroblasts (1×10^5 cells/mL) were seeded in 24-well plates. After 24 h, a linear scratch was made, and cells were treated with SSO (6.25–100 $\mu\text{g/mL}$) in unsupplemented DMEM. Control wells received only the medium. After 24 h of incubation, wound areas were imaged and analyzed using an inverted microscope. The assay was performed in duplicate, and results were expressed as mean wound closure rates. In the NO inhibition assay, sodium nitroprusside (1.25 mM) was prepared in a phosphate buffer (0.1 M, pH 7.0). In 96-well plates, SSO (3.125–100 $\mu\text{g/mL}$) was incubated with NPS for 1 h under intense light. Griess reagent was added, and absorbance was measured at 540 nm. Gallic acid served as a positive control. FT-ICR MS revealed that SSO contains high levels of hydroxy stearic, palmitic, and stearic acids, and confirmed the occurrence of potent acetogenins, including squamocin, annonacinone, gonionenin, and montanacin. Notably, SSO achieved a near doubling of wound healing rate at 100 $\mu\text{g/mL}$ compared to the control ($p < 0.05$), indicating strong stimulation of fibroblast migration and/or proliferation. Furthermore, SSO significantly inhibited NO release, and this inhibitory effect was maintained even after substantial dilution (20 mg/mL), clearly demonstrating potent anti-inflammatory potential. Overall, these results strongly suggest that SSO holds considerable promise as a multifunctional ingredient for topical applications, warranting further investigation.

Keywords: Fatty acids, Vegetable fixed oils, Scratch assay, Wound healing, Nitric oxide inhibition, Acetogenins

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BIOACTIVE COMPOUNDS FROM MIMOSA TENUIFLORA: CHEMICAL PROFILING, CYTOTOXICITY AND ANTIPLASMODIAL EVALUATION

Lucas Tavares dos Santos^{1*}, Renato P. de Sousa¹, Claudia do Ó Pessoa², João Victor de M. Pereira², Pedro M. da Silva Costa², Fernando de P. Varotti³, Amanda L. da Fonseca³, Ana Claudia de S. Pinto³, Fernanda A. de Oliveira³, Bruno A. M. Sanchez⁴, Gerardo Magela Vieira Júnior¹

lucas.tavares2k18@gmail.com

1- Department of Chemistry, UFPI, Teresina, PI, 64049-550, Brazil. 2- Laboratory of Experimental Oncology, UFCE, Fortaleza, CE, 64023-275, Brazil. 3- Laboratory of Medicinal Biochemistry, UFSJ, São João del-Rei, MG, 35501-296, Brazil. 4- Laboratory of Immunopathology and Tropical Diseases, UFMT, Sinop, MT, 78550-728, Brazil.

Mimosa tenuiflora (Willd.) Poir., popularly known as "jurema preta," is a species of the Fabaceae family widely distributed in Northeast region of Brazil, particularly in the caatinga biome. In traditional medicine, its bark is used for treating burns and inflammations. The species' chemical composition includes flavonoids, phenoxychromones, indole alkaloids and saponins¹. Pharmacological studies have demonstrated its antinociceptive, antimicrobial, antioxidant, and wound-healing potential². This work aimed to conduct a phytochemical investigation of the aerial parts and stem bark of *M. tenuiflora*, along with the evaluation of its cytotoxic and antiplasmodial activities. The ethanolic extracts from the root bark (RBEE) and aerial parts (APEE) were obtained by exhaustive extraction (72h) at room temperature. Both extracts underwent liquid-liquid partitioning, yielding hexane (RB-H, AP-H) and ethyl acetate (RB-Ac, AP-Ac) fractions. The RB-Ac fraction was analyzed by UPLC-MS, which enabled the identification of six proanthocyanidins (**1–6**). Chromatographic fractionation of the AP-Ac fraction led to the isolation of six additional compounds: two flavones (**7** and **8**), one phenoxychromone (**9**), and three chalcones (**10–12**) (Fig. 1). Compound identification was achieved using 1D and 2D NMR (¹H and ¹³C), DI-ESI-IT/MSⁿ, and comparison with literature data. The *in vitro* cytotoxicity of the root bark fractions was assessed by the MTT assay³ against the HCT116 (colorectal carcinoma) and HL60 (leukemia) tumor cell lines. RB-H and RB-Ac fractions exhibited promising cytotoxic activity against HL60, with IC₅₀ values of 53.80 µg mL⁻¹ and 61.57 µg mL⁻¹, respectively, while showing no cytotoxicity toward the non-tumorigenic L929 murine fibroblast cell line (IC₅₀ > 250 µg mL⁻¹). Additionally, the antiplasmodial activity of the aerial parts was evaluated against chloroquine-resistant *P. falciparum* W2 strain using the SYBR Green I assay. The PA-H fraction exhibited the highest antimalarial potential, with an IC₅₀ value of 26.39 µg mL⁻¹. These findings underscore the chemical and pharmacological potential of *M. tenuiflora*, constituting the first report of *in vitro* antimalarial activity for this species. Furthermore, compound **8** is reported for the first time in the *Mimosa* genus.

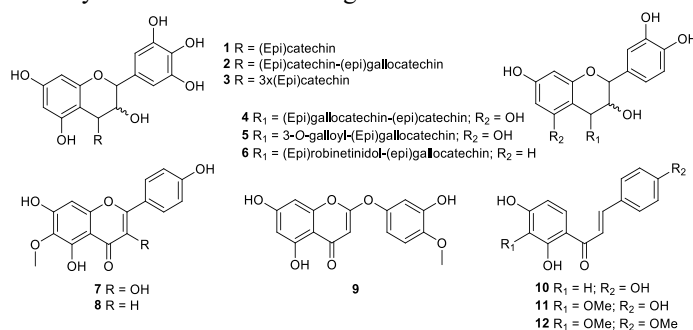


Fig 1. Chemical structures of the compounds identified in *M. tenuiflora*

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Keywords: *Mimosa tenuiflora*, proanthocyanidins, flavonoids, cytotoxicity, antiplasmodial activity



**MOLECULAR NETWORKING AS TOOL FOR DEREPLICATING COMPOUNDS
WITH ANTI-INFLAMMATORY POTENTIAL FROM *BACCHARIS TRIMERA***

Lorena R. F. de Sousa^{1*}, Wéldion G. Mesquita^{1*}, Richele P. Severino¹, Romário P. da Costa², Quezia B. Cass², Vanessa G. P. Severino³, Philipp Gabor⁴, Alexander Weng⁴

lorennarf@ufcat.edu.br

1-Instituto de Química, Universidade Federal de Catalão, Catalão, GO, 75704-020, Brazil. 2-Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP, 13565-905, Brazil. 3-Instituto de Química, Universidade Federal de Goiás, Goiânia, Goiás, 74690-900, Brazil. 4-Institute of Pharmacy, Freie Universität Berlin, 14195, Berlin, Germany

Baccharis trimera (Asteraceae), popular known as carqueja, is a medicinal plant widespread in Brazilian Cerrado with biological potential. This plant has been used in phytotherapy for stomach issues, but no usage of extract for skincare applications are known. Flavonoids, lactones and sesquiterpenes are chemical constituents previously known in the leaves of carqueja. In this view, this work aimed to investigate for anti-inflammatory potential of the leaves of this species and to dereplicate the active compounds for cosmetics application. Ethanolic solution of *B. trimera* (Sisgen A9D0265) was provided by Livealoe company and crude extract was obtained after removing the solvent in a rotatory evaporator. Fractionation was performed with hexane and ethyl acetate. THP-1 macrophage pro-inflammatory response assay was used to evaluate the ethanolic extract and fractions through the inhibition of pro-inflammatory cytokines (TNF- α , IL-1 β , IL-6). The crude extract was dereplicated using hyphenated technique of Liquid Chromatography coupled to High Resolution Mass Spectrometry (LC-HRMS) and ionization in positive ion mode. The MS/MS data were analyzed using Bruker Smart Formula 3D, Compound Crawler, DataAnalysis 4.0 software, and Molecular Networking (GNPS). Biological investigation revealed that crude extract strongly inhibits IL-6 cytokine while polar fraction inhibit IL-6 with less intensity and apolar fraction inhibited TNF- α . GNPS data treatment exhibited 452 nodes, 534 edges and 38 clusters, where 28 compounds were annotated by platform. Analysis of data comparing ion fragments with literature led to eleven compounds, terpenes, sesquiterpenes, fatty acid, hydroxycinnamic acid derivative, and flavonoids. Among the secondary metabolites annotated, seven compounds are known for anti-inflammatory potential, dihydroxy-dimethoxy-isoflavone, apigenin-6,8-di-C-hexoside, isokaempferide, eupatorine, isoschaftoside, aristolone, and linolenic acid. These results bring insights of anti-inflammatory properties of carqueja leaf extract and revealed several related active compounds, as a source of material that could be further investigated for cosmetic application.

Keywords: molecular networking, *Baccharis trimera*, anti-inflammatory potential





EVALUATION OF THE ANTIVIRAL POTENTIAL OF BRAZILIAN PROPOLIS AGAINST ZIKV

Anna Lívia Oliveira Santos^{1*}; Nagela Bernadelli Sousa Silva ¹; Júlia Amaral Vieira d'Almeida ², Natasha Marques Cassani ², Ana Carolina Gomes Jardim ²; Jairo Kenupp Bastos³; Carlos Henrique Gomes Martins¹

anna.livia@ufu.br

1-Laboratory of Antimicrobial Testing, Institute of Biomedical Sciences (ICBIM), Federal University of Uberlândia (UFU) Av. Maranhão - 1783, Uberlândia, MG, Brazil 2-Laboratory of Antiviral Research / Institute of Biomedical Sciences (ICBIM), Federal University of Uberlândia (UFU), 38405-318, Uberlândia, MG, Brazil 3- Faculty of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo (USP), 14040-903, Ribeirão Preto, SP, Brazil.

Neonatal infections represent a critical public health issue, given their association with neurological complications and increased risk of mortality. Among the viral agents of concern, Zika virus (ZIKV) stands out for its ability to cross the placental barrier and cause severe congenital disorders, raising global concern. Although it has significant clinical relevance and epidemiological impact, no vaccines or approved antiviral treatments are currently available. In this context, natural compounds such as Brazilian propolis extracts have attracted attention for their potential antiviral properties. Therefore, this study aimed to evaluate the cytotoxicity and antiviral activity of Brazilian Green Propolis from the Caatinga biome and Brazilian Propolis against ZIKV in an *in vitro* model. Vero E6 cells were treated with the extracts at concentrations of 2, 10 and 50 µg/mL and subjected to the MTT assay after 72 hours to assess cell viability. For the antiviral assay, cells were infected with the ZIKVPE243 strain (Donald et al., 2016) at multiplicity of infection (MOI) 0.005 for Green Propolis and MOI 0.01 for Red Propolis, in the presence or absence of the extracts at their highest non-cytotoxic concentration. After 72 hours, cells were fixed and analyzed by immunofluorescence to quantify infectious foci (FFU/mL) as previously described (Cassani et al., 2023). All treatments showed cell viability greater than 80%. In the antiviral assay, Green Propolis reduced ZIKV infection by 40.4%, while Red Propolis achieved a 33.5% inhibition, both at 10 µg/mL. These findings indicate that the evaluated propolis extracts exhibit low cytotoxicity and relevant antiviral activity against ZIKV, suggesting their potential as sources of new antiviral compounds.

Keywords: antiviral activity, Brazilian propolis extracts, cytotoxicity, Zika virus

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BURITI OIL MICROEMULSION: A NANOTECHNOLOGICAL APPROACH FOR NATURAL COSMETIC FORMULATIONS

Catarina Silva Guimarães^{1*}, Paulinne Moreira Lima¹, Caroline Vieira Gonçalves¹, Robson Amaro Augusto da Silva¹, Gabriel Azevedo de Brito Damasceno¹, Juliano Geraldo Amaral¹

*catarinasguimaraes@hotmail.com

¹Universidade Federal da Bahia, CAT- IMS, Rua Hormindo Barros, 58, Candeias, Vitória da Conquista, 45029094, Bahia, Brazil.

Buriti (*Mauritia flexuosa*) is a palm native to Latin America, widely distributed in the Amazon region. It has ecological importance as an indicator of water presence in poorly drained soils, and economic relevance due to its applications in the food, cosmetic, fuel, and folk medicine industries. Buriti oil exhibits reported biological activities, including moisturizing, photoprotective, antibacterial, and wound-healing effects. Nanotechnology, particularly microemulsions, has been employed to enhance the solubility, absorption, and stability of bioactive compounds, offering advantages such as nanometric droplet size and thermodynamic stability. This study aimed to develop and evaluate the stability of a buriti oil-based microemulsion with moisturizing and photoprotective potential. The oil was obtained by cold pressing. A pseudoternary phase diagram was constructed using PEG-40 Hydrogenated Castor Oil, Sorbitan Oleate, and Propylene Glycol as surfactants, buriti oil as the oil phase, and ultrapure water as the aqueous phase. The selected formulation underwent centrifugation, pH, rheology, preliminary stability (5 days at 45 °C), and accelerated stability (60 days at 4 °C, 25 °C, and 45 °C) tests. Macroscopic characteristics, droplet size, polydispersity index (PDI), zeta potential, and conductivity were evaluated. The formulation was transparent and fluid, with an initial droplet size of 66.48 nm, PDI approximately of 0.2, and zeta potential of |22.3| mV, remaining stable after centrifugation. The pH (5.82) was suitable for topical application, and rheology indicated a Newtonian fluid with low viscosity (30 cP). After accelerated stability testing, all parameters remained within the ideal range for microemulsions (<100 nm), with a slight droplet size increase at 45 °C (72.07 nm) and reduced zeta potential, but still far from zero, indicating stability. PDI and conductivity showed no significant changes, with low conductivity suggesting an oil-in-water microemulsion. The developed microemulsion displayed stable physicochemical characteristics, indicating its potential as a nanotechnological delivery system for buriti oil in cosmetic formulations.

Keywords: *Mauritia flexuosa*; Nanotechnology; Topical delivery; Natural products; Physicochemical stability.





PROSPECTING ANTIMICROBIAL METABOLITES FROM SOIL-DERIVED *Pseudomonas* sp.

Geovana Henrique Passos^{1*}, Ivan L. F. Migliorini¹, Weilan G. P. Melo², Claudia C. de Macedo¹, Amanda S. Hirata³, Letícia N. de Campos⁴, Letícia V. Costa-Lotufo³, Ilana L. B. C. Camargo⁴, Mônica T. Pupo¹

geovana.passos@usp.br

¹ School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, Brazil. ² State University of the Tocantina Region of Maranhão, Estreito, Brazil. ³ Institute of Biomedical Sciences, University of São Paulo, São Paulo, Brazil. ⁴ São Carlos Institute of Physics, University of São Paulo, São Carlos, Brazil.

The search for new compounds with antimicrobial properties has become increasingly important due to the rise of multidrug-resistant microorganisms. A promising source of these compounds is natural microbial products, especially those derived from soil, an ecosystem that harbors about 59% of life on Earth. In Brazil, soils are highly biodiverse, considering the diverse biomes distributed throughout its territory. In this context, the iCHIP (Isolation chip) technique is relevant for isolating and culturing microorganisms that are difficult to grow under laboratory conditions. Microorganisms were isolated from soil samples collected in the ecotone region between the Cerrado and the Atlantic Forest to prospect for compounds with antimicrobial activity from microorganisms isolated using the iCHIP technique. Among the strains selected based on antagonism tests against *Pseudomonas aeruginosa*, *Staphylococcus aureus*, and *Candida albicans*, the strain *Pseudomonas* sp. 3.2S2 stands out. After cultivation, extracts were obtained, fractionation techniques (SPE) were applied, and biological assays were performed to evaluate the activity against human pathogens, biofilm eradication, and cytotoxicity against cancer cells. For chemical profile analysis, metabolomics was used through the application of chromatographic methods (HPLC-DAD-ELSD and HPLC-MS/MS) and, for the dereplication process, the GNPS platform, in addition to the Dictionary of Natural Products and Natural Products Atlas databases. The MeOH 100% fraction obtained from *Pseudomonas* sp. 3.2S2 showed activity against *S. aureus* ATCC 25923 (MIC 128 µg/mL), *S. aureus* ATCC 29212 (MIC 256 µg/mL), and *Staphylococcus epidermidis* (MIC 64 µg/mL), as well as the ability to eradicate biofilm from *S. aureus* ATCC 25923 (63.3% ± 10.0). The major compound was isolated using preparative HPLC, and characterized as pseudopyronine B, based on NMR data. Spectroscopic (UV-Vis) and spectrometric data also confirmed the presence, in lower concentrations, of pseudopyronines A and C. The MIC of the isolated compound against *S. aureus* was 0.3906 µg/mL. In addition to the activity against *S. aureus* reported in this study, the literature also describes the action of pseudopyronines against other pathogens, reinforcing the potential of these metabolites as promising antimicrobial agents and highlighting the value of soil microorganisms in the production of bioactive compounds. The authors thank the support from their institutions and the financial support from FAPESP (grants 2023/12439-9; 2013/07600-3), CNPq (grant 404180/2019-1), and CAPES (Finance Code 001).

Keywords: antimicrobial activity, iCHIP, soil microorganisms, pseudopyronines





ISOLATION AND IDENTIFICATION OF METABOLITES FROM *Plectranthus barbatus* (LAMIACEAE) AND IN VITRO EVALUATION OF EXTRACTS AGAINST *Schistosoma mansoni*

Paloma Carolina de Lima Carvalho^{1,2*}, Júlia de Carvalho Silva¹, Everton Allan Ferreira¹, Thainá R. Teixeira³, Gilson Costa Macedo⁴, Josué de Moraes³, Ademar Alves da Silva Filho¹

palomacarolina147@gmail.com

¹Departamento de Ciências Farmacêuticas, Universidade Federal de Juiz de Fora, R. José Lourenço Kelmer s/n, Campus Universitário, Juiz de Fora, MG, 36036-900, Brazil.

²Graduate Program in Chemistry, Federal University of Juiz de Fora, R. José Lourenço Kelmer s/n, University Campus, Juiz de Fora, MG, 36036-900, Brazil.

³Núcleo de Pesquisa em Doenças Negligenciadas, Universidade Guarulhos, Guarulhos, SP, 07023-070, Brazil.

⁴ Department of Biochemistry, Biological Sciences Institute, Federal University of Juiz de Fora, Juiz de Fora - MG 36036-900, Brazil.

Schistosomiasis is a neglected tropical disease caused by flatworms of the genus *Schistosoma*, mainly *S. mansoni*, affects over 250 million people globally with significant socioeconomic impact, especially in Brazil. Praziquantel (PZQ) is the only drug currently available for treatment. However, the emerging resistance and ineffectiveness against juvenile worms of PZQ underscore the urgent need for new schistosomicidal drugs. This study investigated the schistosomicidal potential of extracts from *Plectranthus barbatus* and conducted a phytochemical investigation of these samples. Root and leaf extracts were obtained by maceration and evaluated for their in vitro activity against adult *S. mansoni* worms. Both extracts exhibited schistosomicidal activity, achieving 100% parasite mortality within 48 hours, with the root extract showing the highest activity. The extracts were characterized by HPLC-DAD and UHPLC-ESI-QTOF-MS. Chromatographic fractionation and spectroscopic analyses (MS, ¹H and ¹³C NMR) led to the isolation and identification of barbatusin (1), forskolin (2), and rosmarinic acid (3). Cytotoxicity showed low toxicity for the leaf extract, with 100% cell viability, even at the highest concentrations tested (up to 100 µg/mL). These results highlight the potential of *P. barbatus* as a promising source of active schistosomicidal metabolites. We thank UFJF, FAPEMIG, and CAPES for financial support, and CENTRALBIO-UFJF for assistance in conducting this research.

Keywords: Schistosomiasis, Natural Products, *Plectranthus barbatus*





***CHEMICAL COMPOSITION OF ESSENTIAL OILS FROM THE LEAVES, BARKS
AND HEARTWOOD OF OCOTEA ACIPHYLLA (LAURACEAE)***

Antonio Geilson Matias Monteiro^{1*}, Raimundo Carlos Pereira Junior², Waldireny Rocha
Gomes³, Hector Henrique Ferreira Koolen⁴

geilsontonho@gmail.com

1-Programa de pós-graduação em Química, (UFAM) Manaus-AM. 2-Centro de Estudos Superiores de Tefé da Universidade do Estado do Amazonas, UEA/Tefé, Amazonas, Brazil. 3-Faculdade de Ciências Farmacêutica, (UFAM), Manaus-AM, Brazil. 4 -Ciências Biológicas da Universidade do Estado do Amazonas, Manaus, Brazil.

Ocotea aciphylla (abacatirana), native to the Amazon and belonging to the Lauraceae family, is little studied regarding its chemical composition and therapeutic potential. In this work, essential oils (EOs) from leaves, bark, and heartwood were obtained by hydrodistillation (4 h) and characterized by gas chromatography-mass spectrometry (GC-MS). The leaves presented a yield of 0.70% and 58 peaks, with major constituents (E)-caryophyllene (17.53%), germacrene D (15.23%), viridiflorene (10.59%), and aromadendrene (7.32%), associated with antimicrobial and immunomodulatory activities (FRANCO et al., 2021). The bark showed a yield of 0.28% and 73 peaks, with emphasis on eremoligenol (9.09%), viridiflorol (7.50%), rosifoliol (5.59%), intermedeol (5.23%), α -terpineol (4.70%) and α -eudesmol (4.36%), compounds with anti-inflammatory, antimycobacterial and antioxidant properties (HACHILAFI et al., 2023). The heartwood showed a yield of 0.63% and 96 peaks, with the main ones being α -terpineol (3.80%), δ -cadinene (3.77%), elemol (3.15%), guaiol (4.28%), β -eudesmol (4.41%) and γ -eudesmol (12.02%). The latter exhibit activities such as neurogenic vasodilation, reduction of dural leakage, and hepatoprotection (KENDALL, 2017). The leaves showed greater diversity and concentration of secondary metabolites, possibly due to their defense function against biotic and abiotic factors, while the heartwood, which has a structural function, exhibited a similar chemical profile but with lower yield. The results highlight the potential of *O. aciphylla* as a source of bioactive compounds of pharmacological and industrial interest, reinforcing the importance of further studies, especially *in vivo*, to validate its efficacy and elucidate its mechanisms of action, contributing to the valorization and sustainable use of Amazonian biodiversity.

Keywords: *Ocotea aciphylla*, volatiles, GC-MS, *Ocotea*, Lauraceae





LIPOSOMAL FORMULATIONS CONTAINING SESQUITERPENE LACTONES AS A PROMISING STRATEGY AGAINST GOUT

Rafaela Cunha Matosinhos^{1*}, Frédéric Frézard², Sabrina Mendes Silva Araújo², Andressa Magalhães Barbosa¹, Isabela Fernanda de Souza¹, José Dias de Souza Filho³, Jacqueline de Souza⁴, Serena Nencini⁵, Sofia Passaponti⁵, Francesca Ietta⁵, Agnese Magnani⁶ & Dênia Antunes Saúde-Guimarães¹

rafaela.matosinhos@ufop.edu.br

1-Laboratório de Plantas Medicinais (LAPLAMED), Escola de Farmácia, UFOP, R. Nove, 27, Ouro Preto, MG, Brazil. 2- LabNano, Departamento de Fisiologia e Biofísica, ICB, UFMG, Av. Presidente Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 3 - Laboratório Multiusuário de Caracterização de Moléculas, Escola de Farmácia, UFOP, R. Nove, 27, Ouro Preto, MG, Brazil. 4 – LCQ, Escola de Farmácia, UFOP, R. Nove, 27, Ouro Preto, MG, Brazil. 5 - Dipartimento Scienze della Vita, UNISI, Via Aldo Moro, 2, Siena, Tuscany, Italy. 6 - Dipartimento di Biotecnologie, Chimica e Farmacia, UNISI, Via Aldo Moro, 2, Siena, Tuscany, Italy.

Eremantholide C (EREC) and goyazensolide (GOIA), isolated from *Lychnophora trichocarpa* and *Lychnophora passerina*, respectively, have shown potential for the treatment of gout. However, they exhibited low gastrointestinal stability and toxicity. In this study, the sesquiterpene lactones EREC and GOIA were incorporated into liposomal nanocarriers as a strategy to enhance their pharmacological activities while minimizing their inherent toxicity. Liposomes were prepared using soybean phosphatidylcholine and characterized by nanometric size (~110 nm), narrow polydispersity index (<0.1), and zeta potential (~-4.5 mV). Encapsulation efficiencies reached ~70% for EREC and ~80% for GOIA. Both liposomal formulations (LIPO + EREC and LIPO + GOIA) demonstrated good stability over 12 months and under simulated gastrointestinal conditions. *In vitro* studies using Caco-2 cells revealed increased viability by the sulforhodamine B assay (IC₅₀= 0.2798 µg/mL for LIPO + EREC, and an IC₅₀= 0.9645 µg/mL for LIPO + GOIA). *In vivo* assays showed a significant reduction in neutrophil migration (~72% for LIPO + EREC, and ~85% for LIPO + GOIA) and pro-inflammatory cytokines (IL-1β, IL-6, TNF-α) production (>60% for both formulations) in a murine gout model induced by monosodium urate crystals. These results support the potential of liposomal formulations containing sesquiterpene lactones as effective candidates for the treatment of gout. The authors thank the support from their institutions and the financial support of Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG), Universidade Federal de Ouro Preto (UFOP), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) and Financiadora de Estudos e Projetos (FINEP).

Keywords: Sesquiterpene lactones, eremantholide C, goyazensolide, *Lychnophora*, liposomes; gout.





***EFFECTS OF *Plectranthus amboinicus* EXTRACTS ON SERUM URIC ACID LEVELS
IN AN ANIMAL MODEL OF HYPERURICEMIA***

Ana Carolina Silva^{1*}, **Isabela Fernanda de Souza¹**, Andressa Magalhães Barbosa¹, Rafaela Cunha matosinho¹, Daniela Moraes e Souza¹, Maria Gabrielle Freire Martins¹,
Dênia Antunes Saúde Guimarães

saude@ufop.edu.br

1-Laboratorio de plantas medicinais (LAPLAMED), Escola de Farmácia, Universidade Federal de Ouro Preto - UFOP, rua nova nove, 27, Bauxita, Ouro Preto, MG, Brazil.

Hyperuricemia is characterized by increased blood uric acid levels above 6.8 mg/dL. This occurs due to increased production or decreased excretion of uric acid. Hyperuricemia, if left uncontrolled, can lead to the development of cardiovascular disease, kidney disease, and gout. There are few medications available to treat hyperuricemia, and a significant percentage of patients do not respond to treatment. Furthermore, these medications have adverse effects. Therefore, the search for new options for hyperuricemia therapy becomes relevant. This study investigated the effects of ethanolic and aqueous extracts of *Plectranthus amboinicus*, popularly known as "Brazilian boldo or boldinho", on biochemical and enzymatic parameters in an animal model of hyperuricemia induced by potassium oxonate injected intraperitoneal and administration of uric acid by gavage, in male Wistar rats. The experiments were conducted following protocol approved by the Animal Ethics Committee (CEUA-UFOP), under number 8876050723. After the induction of hyperuricemia, the animals were treated with different doses of the extracts (5, 15, 30, 60, 120, and 240 mg/kg). Urine was analyzed to quantify excreted uric acid over a five-hour period. Blood was collected to determine serum uric acid levels, and the liver was used for analyzing xanthine oxidase (XOD) enzyme activity. The action of this enzyme is responsible for the metabolism of uric acid for renal excretion, which consequently reduces serum uric acid levels. The extracts were evaluated for their ability to increase renal excretion and reduce serum uric acid levels, aiming to improve the clinical condition of patients with gout. A significant reduction in serum uric acid levels and inhibition of hepatic XOD activity were observed in all treated groups for both extracts, at all doses evaluated. Furthermore, treatment with the aqueous extract at doses of 60, 120, and 240 mg/kg significantly increased urinary uric acid excretion, while the ethanolic extract had no effect at any of the doses evaluated. The results indicated that the ethanolic extract of *P. amboinicus* showed an effect in reducing serum uric acid by inhibiting XOD. While the aqueous extract of *P. amboinicus* demonstrated therapeutic potential for the treatment of hyperuricemia, through inhibition of XOD and increased renal uric acid excretion. The authors thank the support from their institutions and the financial support of Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG), Universidade Federal de Ouro Preto (UFOP), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

Keywords: *Plectranthus amboinicus*, inflammation, arthropathy, gout, hyperuricemia.





IMPACT OF SEASONAL VARIATION ON THE CHEMICAL COMPOSITION AND BIOACTIVITIES OF *Spondias tuberosa*

Natasha Silva Mayrink^{*1}, Gabrielle Silva de Campos Lazzarini¹, Rodrigo Luiz Fabri¹

^{*}natymayrink@gmail.com

¹Laboratório de Produtos Naturais Bioativos, Departamento de Bioquímica, Instituto de Ciências Biológicas, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora, MG, Brasil.

The Brazilian semi-arid region harbors *Spondias tuberosa* L., a species traditionally used in folk medicine for various conditions, including diabetes and inflammatory disorders. Its leaves are rich in bioactive compounds such as alkaloids, phenolics, and triterpenes. Given its economic relevance, the fruits are processed industrially, generating residual biomass, including branches and leaves. The chemical composition and biological properties of plants are influenced by multiple factors, notably environmental conditions. This study aims to investigate the influence of seasonality on the chemical composition and biological activities of four extracts from *S. tuberosa*. Hydroethanolic leaf extracts (1:1) were obtained by maceration and labeled according to the collection season: summer (STHV), autumn (STHO), winter (STHI) and spring (STHP). Total phenolic content was determined using Folin–Ciocalteu, while flavonoid and terpenoid content was determined by colorimetric assays. STHI exhibited the highest phenolic content (150.50 ± 1.66 mg/g), whereas STHP presented the lowest (77.87 ± 6.28 mg/g), and all extracts differed statistically ($p < 0.05$), except STHV and STHO. STHP displayed the highest flavonoid content (52.07 ± 0.71 mg/g) and STHV the lowest (42.46 ± 1.81 mg/g). The highest terpenoid content was found in STHO (77.65 ± 3.40 mg/g) and the lowest in STHV (37.61 ± 4.27 mg/g), with significant differences from all other extracts. Antioxidant activity was evaluated through phosphomolybdenum assay, where the highest AAR%(rutin) was $56.98 \pm 3.96\%$ (STHI) and the lowest $35.48 \pm 4.17\%$ (STHV), with STHV and STHP being statistically similar. Wound healing activity was evaluated by scratch assay. At lower concentration (18.75 μ g/mL), after 24 h, STHP promoted the greatest wound closure ($99.20 \pm 1.26\%$), while STHV promoted the least ($91.17 \pm 3.12\%$). At the higher concentration (37.50 μ g/mL), STHO and STHI achieved complete closure, whereas STHV achieved $90.51 \pm 2.83\%$. STHV was statistically different from all extracts. The results indicate that all four extracts present significant variations in phytochemical composition and biological activity. For instance, STHI, with the highest contents, showed superior antioxidant activity, while STHV, with the lowest contents, exhibited the weakest antioxidant and wound-healing activities. These findings highlight the relevance of studying residues and underutilized parts, reinforce the importance of seasonal factors in phytopharmacological research, and support further investigations, as chemical characterization, anti-inflammatory and antimicrobial evaluations.

Keywords: Umbu, Caatinga, Seasonality, Hydroalcoholic, Sustainability





In vivo Leishmanicidal Activity of Beauvericin Produced by the Fungus *Aspergillus terreus* P63

Lívia C. S. Epifanio^{1*}, Virilânio A. de Oliveira Filho, Danilo C. Miguel², Roberto G. S. Berlinck¹

ciciliniivia@usp.br; rgsberlinck@iqsc.usp.br

1-Instituto de Química de São Carlos, USP - Av. Trabalhador São Carlense, 400 – 13566-590 – São Carlos, Brasil

2- Instituto de Biologia - UNICAMP - R. Monteiro Lobato, 255 - 13083-862 - Campinas.

Beauvericin is a bioactive cyclic hexadepsipeptide produced by the marine-derived fungus *Aspergillus terreus* P63, previously reported to exhibit potent antileishmanial activity *in vitro*. Leishmaniasis remains a neglected tropical disease with significant global health impact, and current treatments are limited by toxicity, drug resistance, and variable efficacy. The discovery of novel natural products with selective leishmanicidal activity is therefore a pressing need. This study aimed to re-isolate and purify beauvericin from *A. terreus* P63 using chromatographic methods, and to conduct preliminary *in vivo* assays to investigate its potential mechanism(s) of action. Solid-state fermentation was performed for 30 days, followed by methanolic extraction, sequential solvent partitioning, silica gel and Sephadex® LH-20 column chromatography, and final purification by HPLC-UV. Beauvericin was identified by HPLC-UV-MS, showing the [M+H]⁺ ion at m/z 784, consistent with literature data, and confirmed by ¹H NMR spectroscopy. The isolation procedure yielded over 300 mg of the pure compound. In preliminary *in vivo* assays against *Leishmania amazonensis* promastigotes, beauvericin induced approximately a 20% increase in lipid peroxidation compared to untreated controls, indicating a mild oxidative stress response. These findings suggest that oxidative membrane damage may contribute to its leishmanicidal mechanism, potentially leading to loss of parasite membrane integrity and cell death. The results demonstrate the successful isolation of beauvericin and provide mechanistic insights into its biological activity, reinforcing its potential as a promising lead compound for the development of innovative therapies against leishmaniasis. Further studies are underway to confirm these observations, to investigate the possible *in vivo* mechanism-of-action of beauvericin (possibly related to its ability to chelate metals and/or to promote the permeation of membrane cells) and to fully elucidate its therapeutic applicability. The authors gratefully acknowledge the support from their institutions and funding from FAPESP, CAPES and CNPq.

Keywords: *Chromatography, Aspergillus terreus* P63, beauvericin, leishmaniasis.





BIOPROSPECTING OF ETHANOLIC EXTRACTS FROM *Cupania emarginata* Cambess FRUITS FOR POTENTIAL ANTI- *Trypanosoma cruzi* ACTIVITY

Anna Maria Romano Silva^{1*}, Esther Maria Ferreira Lucas¹, Alisson Samuel Portes Caldeira², Tânia Maria de Almeida Alves²

annamaria.rs1204@gmail.com

1- Programa de Pós-Graduação em Tecnologias de Produtos e Processos, PPGTPP, CEFET-MG, Av. Amazonas, 5855, Belo Horizonte, MG, 30510-000, Brazil. 2-QPNB, Instituto René Rachou, FIOCRUZ-MINAS, Av. Augusto de Lima, 1715, Belo Horizonte, MG, 30190-002, Brazil.

Described in 1909 by Brazilian scientist Carlos Chagas, Chagas disease is a chronic infection caused by the protozoan *Trypanosoma cruzi*. Considered a neglected tropical disease, its occurrence is concentrated in Latin America, with insects known as “kissing bugs” (*Triatominae*) serving as the primary vectors of transmission. Although anti-*T. cruzi* therapeutic drugs exist, none currently provide a definitive cure for the chronic phase of trypanosomiasis. Given their therapeutic versatility, phytopharmaceuticals may offer an alternative for treatment of the disease. Despite the lack of studies on the potential trypanocidal activity of the species *Cupania emarginata* Cambess, popularly known as camboatá, previous research has reported the presence of bioactive cupanosides against *Trypanosoma brucei rhodesiense* in extracts of *Cupania cinerea*. Thus, considering that species of the same genus tend to produce similar classes of secondary metabolites, the present study proposes a biomonitoring chemical investigation aimed at bioprospecting an ethanolic extract of *C. emarginata* fruits with potential anti-*T. cruzi* activity. The methodology included fractionation of the crude extract by ultra high performance liquid chromatography (UHPLC) in a 96-well plate and *in vitro* evaluation of anti-*T. cruzi* activity of both the extract and its fractions. These fractions were also subjected to electrospray ionization mass spectrometry (ESI-MS/MS) to determine their chemical profiles. To achieve the isolation and structural elucidation of bioactive compounds, a semi-preparative fractionation was performed using high performance liquid chromatography (HPLC). The resulting fractions were then analyzed by UHPLC-ESI-MS/MS and nuclear magnetic resonance (NMR) to identify the most active substances. Preliminary results showed that the crude extract exhibited protozoan inhibition activity ($IC_{50} = 25.6 \pm 4.0 \mu\text{g/mL}$), and four collected fractions were bioactive, with protozoan growth inhibition percentages of 68.0%, 80.0%, 85.6%, and 86.9%, respectively. Chemical characterization of the crude extract led to the annotation of xanthotoxin, epicatechin, and a triterpenoid. The substances present in the active fractions are currently under analysis. Future perspectives include the isolation and characterization of these bioactive molecules to elucidate their chemical structures using UHPLC-ESI-MS/MS and NMR.

Keywords: *Cupania emarginata* Cambess, Phytopharmaceuticals, *Trypanosoma cruzi*





EVALUATION OF LIMONENE ENANTIOMERS AND TWO COPPER(II) COMPLEXES ON CELL VIABILITY AND PROLIFERATION

Bruna Eduarda Silva^{1*}, Robson Pontes¹, Josélia Cristina de Oliveira Moreira¹, Ademir dos Anjos², Ana Lucia Tasca Gois Ruiz¹

*b291188@dac.unicamp.br

1- Faculdade de Ciências Farmacêuticas, LAFTE_x, Rua Cândido Portinari, 200, Cidade Universitária Zeferino Vaz, Campinas, São Paulo, 13083-871, Brasil; 2-UEMS, Unidade Universitária de Naviraí, Naviraí, MS, 79950-000, Brasil.

Chronic exposure to UV radiation is strongly correlated with the development of skin tumors. In the search for new therapeutic options, nature is a rich source of inspiration, just as coordination compound chemistry has proven to be a strong ally in the new drugs development. One of the challenges in topical treatment of skin cancers is permeation. Limonene, present in many essential oils, is described as a skin permeation enhancer. This study investigated the effects of limonene enantiomers and two copper(II) complexes with the ligands N,N',N,N'-bis-[2-hydroxy-3,5-di-*tert*-butylbenzyl)(2-piridylmethyl)]-1,3-propanediamine (CuPPN) and N,N',N,N'-bis-[2-hydroxy-3,5-di-*tert*-butylbenzyl)(2-piridylmethyl)]-ethylenediamine (CuPEN) on the viability and proliferation of human melanoma (SK-MEL-28) and immortalized murine fibroblasts (3T3) cell lines, aiming to propose combinations between limonene and metallic complex. Both *S*-(-)-limonene and *R*-(+)-limonene did not affect the viability of SK-MEL-28 and 3T3 cells ($IC_{50} \geq 150 \mu\text{g/ml}$) while the CuPEN complex showed greater activity ($IC_{50} = 1.1 \mu\text{g/ml}$, for both 3T3 and SK-MEL-28) than CuPPN ($IC_{50} = 16.2$ and $27.5 \mu\text{g/ml}$, for 3T3 and SK-MEL-28 cells, respectively). In the clonogenic assay, both complexes showed irreversible antiproliferative effect with significant reduction in colony number (surviving fraction = 29 to 50%) in SK-MEL-28 cells, at concentrations of 1 to 2 $\mu\text{g/ml}$ for CuPEN and 7.5 to 30 $\mu\text{g/ml}$ for CuPPN. Despite the absence of selectivity in cytotoxic effect, in the clonogenic assay both complexes stimulated colony formation in immortalized murine fibroblasts 3T3. The results obtained so far indicate that the CuPEN complex is more potent than the CuPPN complex and that limonene stereoisomerism does not seem to interfere with the effect on cell viability. Future studies are being designed to verify how the combination of limonene, a skin permeation enhancer without cytotoxic effect, with CuPEN and CuPPN complexes will influence the antiproliferative action evidenced for these complexes.

Acknowledgments: CAPES, CNPq, FAEPEX/Unicamp.

Keywords: Limonene, Copper complexes, Melanoma, Clonogenic assay, Anticancer activity





CYTOTOXIC ACTIVITY OF BROWN PROPOLIS ON HUMAN TUMOR CELLS

*Karin Carla dos Santos Schmidt^{1*}, Fernanda Caroline Knob¹, Suelen dos Santos²,
Elisângela Düsmann³, Tatiane Luiza Cadorin Oldoni¹*

karinsschmidt@gmail.com

1-Programa de Pós-Graduação em Tecnologia de Processos Químicos e Bioquímicos (PPGTP-PB), Universidade Tecnológica Federal do Paraná (UTFPR) - Campus Pato Branco, Via do Conhecimento, s/n - Km 1, Fraron, Pato Branco, PR, 85503-390, Brazil. 2-Programa de Pós-Graduação em Química Aplicada (PPGQA), Universidade Estadual do Centro Oeste (UNICENTRO) - Campus CEDETEG, Alameda Élio Antonio Dalla Vecchia, 838, Vila Carli, Guarapuava, PR, 85040-167, Brazil. 3- Departamento de Química e Biologia, Universidade Tecnológica Federal do Paraná (UTFPR) – Campus Francisco Beltrão, Rua Gelindo João Folador, 2000, Novo Horizonte, Francisco Beltrão, PR, 85602-863, Brazil.

Propolis is a complex mixture produced by bees from plant exudates, wax, and salivary secretions, containing phenolic compounds, terpenes, and other secondary metabolites with recognized biological relevance. Its chemical composition varies according to botanical and geographical origin, directly influencing its activity profile. Sequential extraction processes using solvents with different polarities produce subfractions with distinct chemical constituents, enabling targeted evaluation of their biological effects. This study investigated the cytotoxic effect of four purified fractions of brown propolis collected in the southwest region of Paraná, Brazil. Fractions were obtained sequentially with hexane, dichloromethane, ethyl acetate, and acetone. Samples were evaluated *in vitro* on human hepatoblastoma cells (HepG2) using the MTT assay at concentrations of 5, 10, 50, 100, 200, 300, 400, 500, and 1000 µg/mL, with incubation times of 24, 48, and 72 h. The hexane fraction reduced cell viability at 300 and 400 µg/mL (48 and 72 h), 500 µg/mL (24, 48, and 72 h), and 1000 µg/mL (24 h). The dichloromethane fraction reduced viability starting at 5 µg/mL (48 h) and at all concentrations ≥400 µg/mL at all time points. The ethyl acetate fraction reduced viability from 50 µg/mL (72 h), with additional reductions at 500 µg/mL (24 and 72 h) and 1000 µg/mL (72 h). The acetone fraction reduced viability from 5 µg/mL (72 h) and at concentrations ≥50 µg/mL (48 and 72 h). The data indicates that the extraction solvent's polarity influences the brown propolis subfractions' cytotoxicity profile. Among the conditions evaluated, the acetone fraction showed the broadest range of concentrations associated with reduced cell viability. These results highlight the need for further chemical characterization and mechanistic studies to identify the compounds involved and assess their biological relevance.

Keywords: bioassay, cytotoxic activity, cell viability, brown propolis





EFFECT OF HANDROANTHUS IMPETIGINOSUS EXTRACT AND FRACTIONS ON SEED GERMINATION AND SEEDLING DEVELOPMENT OF NICOTIANA TABACUM

Luana Cristina Diniz Santos^{1*}, Ana Hortência Fonsêca Castro¹, Luciana Alves Rodrigues dos Santos Lima¹

luanadiniz.santos@gmail.com

¹Programa de Pós-Graduação em Biotecnologia, Universidade Federal de São João del-Rei, Divinópolis, MG, Brasil.

The increasing use of synthetic herbicides, exacerbated by a lack of regulation, poses serious environmental and human health risks. Therefore, natural alternatives, such as bioherbicides derived from secondary metabolites, are becoming increasingly attractive. The species *Handroanthus impetiginosus* (Mart. Ex Dc.) Mattos, known as purple ipê, is rich in compounds such as naphthoquinones, flavonoids, and tannins, and possesses diverse biological activities¹. This study evaluated the effect of *H. impetiginosus* extract and fractions on the *in vitro* germination of seeds and development of *Nicotiana tabacum* (tobacco) seedlings. The methanol extract was prepared from *Handroanthus impetiginosus* seeds using a Soxhlet apparatus. Liquid-liquid extraction of the plant extract fraction yielded dichloromethane (DCM), acetoethyl (ACT), and hydromethanol (HID) fractions. Tobacco seed disinfection was performed using an ethanol/sterile water solution (7:3, v/v) for 1 min and a 2% NaOCl solution in sterile water plus a drop of TWEEN® 20 for 30 min under mechanical pressure. In a laminar flow chamber, one seed was placed in 15 mL of Murashige and Skoog (MS) medium, and the extract and fractions were added. The controls were gibberellin (positive) and MS medium supplemented with DMSO 1% (negative). After inoculation, the seeds were kept in the growth room for 30 days². The parameters analyzed at the end of the test were germination, number of leaves, nodes and shoots, stem and root size for seedlings, and shoot and root dry weight. The results demonstrated an increase in the *in vitro* germination rate of *N. tabacum* seeds in the presence of EM and the HID fraction, and a reduction in the DCM fraction. The ACT fraction completely inhibited seed germination at higher concentrations. Samples of the extract and fractions of *H. impetiginosus* demonstrated an inhibitory effect on *Nicotiana tabacum* when compared to the positive control hormone gibberellin, with an action similar to that of bioherbicides.

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¹ Chemistry & Biodiversity, 0:e01126, 2025. <https://doi.org/10.1002/cbdv.202501126>

² Biocatalysis and Agricultural Biotechnology, 103523, 64 2025. <https://doi.org/10.1016/j.bcab.2025.103523>

Keywords: *Handroanthus impetiginosus*, *in vitro* germination *Nicotiana tabacum*, methanol extract.





PHYTOCHEMICAL PROFILE AND BIOACTIVITY OF *Lantana camara* LEAF EXTRACT

Gabrielle Silva de Campos Lazzarini^{*1}, Natasha Silva Mayrink¹, Ari Sérgio de Oliveira Lemos¹, Rodrigo Luiz Fabri¹

^{*}gabrielle.lazzarini@estudante.ufjf.br

¹Laboratório de Produtos Naturais Bioativos, Departamento de Bioquímica, Instituto de Ciências Biológicas, Universidade Federal de Juiz de Fora (UFJF), Juiz de Fora, MG, Brasil.

Lantana camara L. (Verbenaceae) is a plant widely utilized in traditional medicine for the treatment of wounds, inflammatory disorders, and microbial infections, largely attributed to its rich phytochemical composition, including flavonoids, phenolic acids, and triterpenes, which are known for their antioxidant and anti-inflammatory activities. Despite its ethnopharmacological relevance, scientific investigations into its pharmacological potential, especially in the context of inflammatory skin diseases, remain scarce and incomplete. This study aimed to evaluate the *in vitro* antioxidant and anti-inflammatory activities of a hydroalcoholic leaf extract of *L. camara* (LCHA) and characterize its phytochemical composition to support its potential therapeutic applications. Quantitative spectrophotometric assays revealed substantial levels of total phenolics, terpenes, and saponins in the extract. Advanced analytical characterization using UFLC-QTOF-MS identified key bioactive compounds such as lamiide, geniposide, pectolinarin, luteolin-7-O-glucoside, and rhamnocitrin-O-glucoside, many of which have been previously linked to anti-inflammatory and antioxidant effects. The biological activities of LCHA were assessed in peritoneal macrophages and L929 fibroblasts to evaluate cytotoxicity using MTT assay. Cell viability remained above 80% for all evaluated concentrations of LCHA in peritoneal macrophages, indicating no cytotoxicity effects on this cell line. In L929 fibroblasts, viability remained above 70% only up to a concentration of 150 µg/mL, suggesting a concentration-dependent reduction in cell viability, suggesting a concentration-dependent reduction in cell viability. The production of nitric oxide (NO) was indirectly evaluated by quantifying nitrites (NO₂⁻) using the Griess method and the extract exhibited potent inhibition of NO production, achieving complete suppression at the highest tested concentration (300 µg/mL). Also, LCHA significantly decreased lipid body accumulation by approximately 69% in activated macrophages. Antioxidant capacity was confirmed through multiple complementary assays, including DPPH radical scavenging, phosphomolybdenum reduction, the β-carotene/linoleic acid system, and intracellular reactive oxygen species (ROS) quantification, with LCHA reducing lipid peroxidation by 42% and ROS levels by 65% in stimulated macrophages. Collectively, these results corroborate the traditional use of *L. camara* and provide a mechanistic basis for its potential application as a plant-derived therapeutic agent targeting inflammatory skin conditions. The distinctive phytochemical composition and significant bioactivities identified herein underscore the relevance of further preclinical and translational studies aimed at developing standardized and effective formulations.

Keywords: *Lantana camara*, Phytochemistry, Anti-inflammatory, Antioxidant.





PHLOROGLUCINOLS FROM *Melaleuca viminalis*: DEREPLICATION, ISOLATION AND ANTIMICROBIAL ACTIVITY AGAINST METHICILLIN-RESISTANT *Staphylococcus aureus*

Ana Clara Lima Nunes Silva^{1*}, Beatriz Isabel Mota do Carmo¹, Simone dos Santos Grecco¹, Francisco Ozório Bessa Neto¹, Rodrigo Cayô da Silva¹, Marisi Gomes Soares², Miriam Uemi³, João Henrique Ghilardi Lago³, Patricia Sartorelli¹.

clara_nunes17@unifesp.br

¹Universidade Federal de São Paulo, Diadema – SP, Brazil. ²Universidade Federal de Alfenas, Alfenas – MG, Brazil. ³Universidade Federal do ABC, Santo André – SP, Brazil.

Staphylococcus aureus is a Gram-positive bacterium classified among the ESKAPE pathogens, recognized for its high prevalence in hospital settings and its increasing resistance to multiple drugs, particularly methicillin. This resilience is largely due to its efficient adaptive mechanisms against conventional antibiotic therapies. In this context, the search for alternative compounds capable of inhibiting its survival and pathogenicity is urgent. CEPID-ARIES has been dedicated to the discovery of natural products with potential to counteract microbial resistance¹. Among the plant species of interest, *Melaleuca viminalis* (Myrtaceae) stands out for its diverse classes of secondary metabolites, especially phloroglucinols—compounds with remarkable structural diversity, including bicyclic, tricyclic, and other frameworks—and relevant biological potential. Previous studies have reported antimicrobial activity of phloroglucinols isolated from *M. viminalis* against both Gram-positive and Gram-negative bacteria². Considering the increasing dissemination of resistant bacterial strains, this study aimed to perform the dereplication of compounds from the dichloromethane phase fraction by LC-MS/MS integrating the data obtained into the GNPS2 platform and to evaluate their antimicrobial activity against two *S. aureus* strains: ATCC Sa29213 (susceptible to several antimicrobials, including oxacillin) and MRSA Sa43300 (methicillin-resistant), followed by isolation via HPLC. GNPS2 analysis revealed a cluster with fragmentation patterns consistent with phloroglucinols. Subsequent isolation and characterization enabled the manual annotation of three compounds: 2,6-dihydroxy-4-methoxyisovalerophenone, Aspidinol C, and Pulverulentone. In antimicrobial assays, the fraction exhibited inhibition zones of 10.6 mm (Sa29213) and 16.8 mm (Sa43300). The Minimum Inhibitory Concentration values were >64 µg/mL for the sensitive strain and 32 µg/mL for the resistant strain. These findings highlight the promising antimicrobial potential of phloroglucinols from this fraction, particularly against methicillin-resistant *S. aureus*, and underscore their relevance as candidates for future pharmacological investigations. In light of these results, the isolated compounds may be tested to assess their non-synergistic potential.

Keywords: Phloroglucinols, Dereplication, GNPS2, Antimicrobial Activity, *Staphylococcus aureus*.

¹CEPID-ARIES - Antimicrobial Resistance Institute of São Paulo (FAPESP 2021/10599-3) (<https://site.unifesp.br/cepidaries/>)

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PREUSSIA AFRICANA ENDOPHYTE AN ALTERNATIVE SOURCE FOR THE PRODUCTION OF ANTIFUNGAL METABOLITES

Hillary Ananda Gonçalves Aniceto^{1*}, Jaine Honorata Hortolan Luiz¹, Daniela Battaglia Hirata¹

hillary.aniceto@sou.unifal-mg.edu.br

1- Instituto de Química – Universidade Federal de Alfenas, UNIFAL, Rua Gabriel Monteiro da Silva 714, Alfenas, MG, 37130-000, Brazil.

Invasive fungal infections (IFIs) represent a major threat to global health, particularly in immunocompromised individuals. Treatment is hindered by the limited availability of antifungal drugs and the increasing prevalence of antifungal resistance (WHO, 2022), underscoring the urgent need for novel antifungal agents with both effective and reduced side effects (El-Sayed et al., 2024). In this context, the genus *Preussia* has emerged as a promising source of secondary metabolites with antimicrobial activity (Xu et al., 2019). This study aimed to optimize the cultivation conditions of *Preussia africana* endophyte, isolated from *Handroanthus impetiginosus*, in order to maximize the production of antifungal compounds against *Candida* species. A Central Composite Rotatable Design (CCRD) was employed to evaluate selected carbon sources and inoculum numbers. Ethyl acetate (AcOEt) and chloroform (CHCl₃) extracts were tested against *Candida albicans*, *C. glabrata*, and *C. tropicalis* by determining the Minimum Inhibitory Concentration (MIC). Toxicity was assessed in the *in vivo* *Galleria mellonella* model. The extracts showed higher activity against *C. albicans* and *C. glabrata*. CHCl₃ extracts obtained at the optimal point (OP) exhibited MIC values ranging from 25 to 100 µg/mL against *C. albicans*, whereas AcOEt extracts displayed MIC values from 50 to 100 µg/mL. Assays 10 and 12 (CHCl₃ extracts) also stood out for their antifungal activity against *C. glabrata* (MIC 25–50 µg/mL). AcOEt extracts from the OP demonstrated good activity against both *C. glabrata* and *C. albicans* (MIC 50–100 µg/mL), exhibiting fungicidal action at the same concentration against *C. albicans*. Notably, the most active extracts displayed low toxicity against *G. mellonella* at concentrations up to 800 µg/mL, resulting in high larval survival rates. In conclusion, optimization of *P. africana* cultivation proved to be an effective strategy for producing extracts with potent and selective antifungal activity, highlighting this endophyte as a promising source for the development of novel therapeutic agents.

Keywords: *Preussia africana*, antifungal activity, *Candida*, secondary metabolites, cultivation optimization.





NATURAL MODULATION OF MELANIN PRODUCTION: TYROSINASE INHIBITION BY *Stachys byzantina* K. KOCH

Victor Campana Leite^{1*}, Jéssica Pereira Silva¹, José Alisson da Silva Lima¹, Maria Luiza de Almeida Aquino Soares¹, Nicolas de Castro Campos Pinto¹

nicolas.pinto@ufjf.br

1-Laboratory of Bioactive Natural Products, Department of Biochemistry, Institute of Biological Sciences, Federal University of Juiz de Fora – UFJF, Rua José Lourenço Kelmer, s/n - São Pedro, Juiz de Fora - MG, 36036-900, Brazil.

Stachys byzantina is a plant species of medicinal interest due to its high content of phenols and remarkable antioxidant and anti-inflammatory activities. For this reason, *S. byzantina* presents potential applications in skin care, particularly for conditions associated with oxidative stress, inflammation, skin aging, and pigmentation diseases, including melasma and solar lentigines, which are particularly linked to increased tyrosinase activity. Previous studies from our group reported that the dichloromethane fraction (DF) obtained from the ethanolic extract of *S. byzantina* presents relevant tyrosinase inhibitory action. The present study aimed to fractionate DF in order to identify at least one compound responsible for this inhibition. *S. byzantina* aerial parts were collected at UFJF Faculty of Pharmacy Garden (SisGen A3DD429). A voucher was deposited in CESJF herbarium (no. 46598). The ethanolic extract was obtained by ultrasound-assisted extraction and subsequently fractionated (30 g) by liquid partition using organic solvents of increasing polarity, yielding DF (6.75 g). DF was further fractionated on a silica gel column, resulting in 29 fractions. Tyrosinase inhibitory activity was evaluated according to Khatib et al. (2005). Each fraction was incubated at 62.5 µg/mL with tyrosinase (250 U/mL) and L-tyrosine (2 nM), and the absorbance was monitored at 450 nm for 30 minutes. Fraction F12.2 was further analyzed by HPLC-UV due to its highest inhibitory activity (81.33 ± 2.62 %), using a C18 column. The mobile phase was 0-5 min: 5-15% methanol (95-85% water); 5.01-30 min: gradient 45-100% methanol (55-0% water). The injection volume was 20 µL, and the wavelength was set to 330 nm. The major peak was identified as apigenin (RT = 16.11 min) by comparing the retention time and co-elution with the standard (0.025 mg/mL). A standard curve was constructed ($R^2 = 0.9998$), and apigenin was quantified at 32.03 ± 4.17 mg/g. Apigenin is a flavonoid widely recognized for its tyrosinase inhibitory activity, as well as its antioxidant and anti-inflammatory properties, which may collectively contribute to reducing hyperpigmentation. These findings highlight the potential of this plant as a source of natural cosmetic products for modulating melanin production, and further encourage studies to identify additional bioactive compounds.

Keywords: Tyrosinase inhibition, Hyperpigmentation, *Stachys byzantina*, Apigenin, Dermatological applications.



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LARVICIDAL MICROEMULSION OF PEPPERMINT ESSENTIAL OIL TO *Aedes aegypti* CONTROL

Natasha Reynauld¹, Celda Miranda¹, Marcos Paulo Gomes Mol², Sérgio Caldas³, **Carolina Paula de Souza Moreira¹**

cpsmoreira@gmail.com

1-Serviço de Desenvolvimento Tecnológico Farmacêutico, Diretoria de Pesquisa e Desenvolvimento, FUNED, Rua Conde Pereira Carneiro, 80, Belo Horizonte, MG, 30510-010, Brazil. 2- Serviço de Ecotoxinologia, Diretoria de Pesquisa e Desenvolvimento, FUNED, Rua Conde Pereira Carneiro, 80, Belo Horizonte, MG, 30510-010, Brazil 3- Serviço de Pesquisa em Doenças Infecciosas, Diretoria de Pesquisa e Desenvolvimento, FUNED, Rua Conde Pereira Carneiro, 80, Belo Horizonte, MG, 30510-010, Brazil.

Aedes aegypti is the primary vector for diseases such as dengue, Zika, and chikungunya, which present significant public health challenges in various regions worldwide. The increasing resistance of mosquitoes to insecticides, along with the associated risks of their use, underscores the urgent need for safer and more effective alternatives for mosquito control. Essential oils (EOs) are emerging as promising natural solutions, particularly as larvicides. Microemulsions (MEs) are colloidal systems that are highly stable, cost-effective to produce, and easy to apply. They enhance the penetration and dispersion of biocidal active ingredients, thereby improving their effectiveness in complex environments. The objective of this study was to develop a ME based on peppermint (*Mentha piperita* L.) essential oil to complement existing *A. aegypti* control strategies. The EO was purchased commercially, and its chemical composition was analyzed using gas chromatography-mass spectrometry (GC-MS). The ME was prepared using surfactants under agitation with an Ultra-Turrax mixer, characterized physicochemically, and evaluated for stability. The larvicidal activity against *A. aegypti* was determined following WHO guidelines, and the data was processed using R software. GC-MS analysis identified menthol (57.14%) and menthone (17.53%) as the major compounds in the oil, which is consistent with previous literature. The ME containing 10% EO demonstrated 4 months stability, with a droplet size of 11.41 ± 0.56 nm, charge of -8.35 ± 3.24 and PDI of 0.17 ± 0.06 . In the larvicidal assay, the EO exhibited an LC_{50} of 172.27 ± 6.54 $\mu\text{g/mL}$. Additionally, the ME (10% EO) resulted in the death of 100% of mosquito larvae within 24 hours. The potential of the ME to inhibit egg hatching will be evaluated soon. These promising findings position MEs as an innovative, eco-friendly, and highly effective option for combating *A. aegypti*, significantly reducing environmental impact while enhancing public health efforts.

Keywords: Dengue, larvicidal, monoterpenes, diterpenes.





ANTI-PROTOZOAN RESPONSE OF PRODUCTS FROM *Duguetia stelechantha*

Auxiliadora Cristina Correa Barata Lopes^{1*}, Cáritas de Jesus Silva Mendonça², André Luís Menezes Carvalho³, Caroline Martins de Jesus⁴, Lucilene Amorim Silva⁴, **Cláudia Quintino da Rocha^{1,2}**

rocha.claudia@ufma.br

¹Programa de Pós-Graduação em Biodiversidade e Biotecnologia da Rede BIONORTE (PPG-BIONORTE), UFMA, Avenida dos Portugueses, 1966. São Luís, MA, Brazil. ²Programa de Pós-Graduação em Química, UFMA, Avenida dos Portugueses, 1966. São Luís, MA, Brazil. ³Programa de Pós-Graduação em Ciências Farmacêuticas, UFPI, Teresina, PI, Brazil. ⁴Programa de Pós-Graduação em Ciências da Saúde, UFMA, Avenida dos Portugueses, 1966. São Luís, MA, Brazil.

Duguetia stelechantha, known as ata brava, is a tree of the Annonaceae family. Different species of the Annonaceae family have been reported to be biologically active, and *Duguetia* species have been identified metabolites from different classes that perform promising biological activities, such as essential oils (EOs) with proven antiprotozoal activity. There are few chemical and biological records of *D. stelechantha* in the literature, so this study aimed to investigate the biotechnological potential of the species. The aim was to obtain EO from *D. stelechantha* leaves (EO-DU), develop a microemulsion (ME) (ME-DU) to incorporate the EO, and evaluate the antiprotozoal activity of these bioproducts. Chemical characterization by GC/MS of the hydrodistilled EO-DU identified β -pinene (46.17%), α -pinene (20.2%), and spathulenol (6.68%) as the major constituents. Headspace GC/MS analysis of ME-DU confirmed the incorporation of EO in the formulation. Physicochemical characterization of ME indicated that particle size, polydispersity index, and zeta potential are in accordance with the literature. The antiprotozoal activity evaluated the action of these natural products on *Leishmania* (L.) *amazonensis* promastigotes, which classified ME-DU (IC₅₀=4.47 μ g/mL) as an active sample, and EO-DU (IC₅₀=138.30 μ g/mL) and the ME blank (IC₅₀=185.60 μ g/mL) as moderately active. ME-DU had a lower IC₅₀ than EO-DU, providing an antileishmanial action approximately 30 times more effective than EO-DU. ME-DU also achieved an IC₅₀ close to that of the drug used as a positive control, pentamidine (IC₅₀ = 4.00 μ g/mL). The selectivity index (S.I) indicates whether a sample is more toxic to the parasite or the cell. After cytotoxicity testing in Raw 264.7, the S.I was calculated, indicating that EO-DU (CC₅₀=44.77 μ g/mL) is more toxic to cells than to the parasite. ME-DU (CC₅₀=8.87 μ g/mL) is more selective for parasite inhibition and less cytotoxic, as the IC₅₀ for *L. (L.) amazonensis* is lower than what is considered cytotoxic. The results demonstrate the potential of the species, and the incorporation of EO into ME increased the bioavailability of bioactives, optimizing biological activity, and reduced the toxicity of compounds. The authors thank the support from their institutions and the financial support of PPBioAmar/CNPq, FAPEMA and CAPES.

Keywords: *Annonaceae*, *Duguetia*, formulation, leishmania, microemulsion, essential oil





**SCREENING OF WOUND HEALING AGENTS - IN VITRO
EVALUATION OF 1,8-CINEOLE ON CELL VIABILITY,
PROLIFERATION AND MIGRATION**

***Clara Giuliana Magossi*^{1*}**, Robson Pontes¹, Josélia Cristina de Oliveira Moreira¹, Ana Lucia Tasca Gois Ruiz¹

* c290053@dac.unicamp.br

1- Faculdade de Ciências Farmacêuticas, LAFTE_x, Rua Cândido Portinari, 200, Cidade Universitária Zeferino Vaz, Campinas, São Paulo, 13083-871, Brasil.

Wound healing is a complex biological process involving inflammation, cell proliferation, and tissue remodeling. Keratinocytes and fibroblasts play essential roles in skin re-epithelialization and extracellular matrix remodeling, particularly through collagen production. Various natural products, including terpenoids, have been identified as promisor agents for promoting wound healing. Commonly found in several essential oils, the monoterpene 1,8-cineole is known for its anti-inflammatory and antimicrobial properties. This study investigated the effects of 1,8-cineole on the viability and proliferation of both tumor [melanoma (SK-MEL-28), and squamous cell carcinoma of pharynx (FaDu)] and non-tumor [immortalized human keratinocytes (HaCaT), and immortalized murine fibroblasts (3T3 and L-929)] cell lines. Additionally, the effect of 1,8-cineole on cell migration was evaluated in L-929 cells using the scratch assay. All cell lines were cultured in RPMI 1640 medium supplemented with 5% fetal bovine serum (FBS) and maintained at 37 °C in a humidified atmosphere containing 5% CO₂. After 48 h of exposure in 96-well plates, 1,8-cineole exhibited neither cytostatic (GI₅₀ > 300 µg/mL) nor cytotoxic (IC₅₀ > 300 µg/mL) effects in any of the cell lines tested. For the migration assay, L929 cells were cultured in 24-well plates, and wound closure was monitored at 0, 18, 36, and 48 h after treatment. A significant difference was observed between positive control (RPMI 1640 plus 5% FBS) and negative control (RPMI 1640 plus 0% FBS) at 36 and 48 h. However, the treatment with 1,8-cineole (1.5 to 300 µg/mL) diluted in RPMI 1640 plus 0% FBS had no effect on L-929 cell migration, regardless of exposure time or concentration. After 48-h, all experimental group showed relative cell viability close to 100%. These finding suggest that 1,8-cineole does not affect cell proliferation and migration. Future studies will assess the effect of 1,8-cineole on *in vitro* collagen production to further applications as wound healing agent.

Acknowledgments: CAPES, CNPq, FAEPEX/Unicamp.

Keywords: *Eucalyptol, Skin, preclinical evaluation, cell migration, wound healing*





EFFECT OF THE AQUEOUS STEM EXTRACT OF *Costus spicatus* ON THE MODULATION OF BREAST CANCER MODELS

Gracimério José Guarneire^{1*}, Ana Araujo Sathler², Giovanna Duarte Silva¹, Rebeca Rocha Rodrigues¹, Samuel Gouveia Silva Neres Cardoso¹, Roberta Mello Cachuba¹, Nerilson Marques Lima³; Talles Caires Chaves¹, Sandra Bertelli Ribeiro Castro¹, Caio César Souza Alves¹, Alessandra Paula Carli¹

gracimerio.guarneire@ufvjm.edu.br

1- Federal University of the Jequitinhonha and Mucuri Valleys, 39803-371 Teófilo Otoni - Minas Gerais, Brazil. 2- Federal University of the Juiz de Fora, 35010-180 Governador Valadares - Minas Gerais, Brazil. 3- Federal University of Alfenas, Institute of Chemistry, 37130-001, Alfenas, Minas Gerais, Brazil

Natural products have gained prominence due to bioactive compounds with antitumor potential. *Costus spicatus*, a plant known for its traditional medicinal uses (Lorençone et al., 2021), has shown potential anticancer properties. Despite this promising bioactivity, its effects on breast cancer cells remain poorly explored. Therefore, this study aimed to evaluate the effect of the aqueous stem extract of *C. spicatus* (AQCa) on the modulation of the antitumor response *in vitro* and *in vivo* in a mammary adenocarcinoma model (SisGen - A126B1D). Initially, cell viability was assessed using the MTT assay after 48 h in macrophage cell lines RAW 264.7 and J774A.1, and in tumor cell lines MCF-7, MDA-MB-231, and 4T1, at concentrations of 333, 100, 33.3, and 10 µg/mL. In the *in vivo* model, 50 µL of a cell suspension containing 4T1 cells was inoculated into the mammary gland of female BALB/c mice (CEUA/Mucuri – 02-2023). From the 10th day after inoculation, mice were treated daily by gavage with AQCa (75, 150, or 300 mg/kg) for 18 days, either alone or in combination with doxorubicin (5 mg/kg). *In vitro*, the results showed that AQCa reduced tumor cell viability at higher concentrations, particularly in the triple-negative MDA-MB-231 cell line, which exhibited only 51.8% of viable cells. *In vivo*, the AQCa 300 mg/kg group displayed inhibition of tumor growth, with a significant reduction in tumor volume (271.925 mm³) compared to the untreated group (521.333 mm³), and even lower than that observed for doxorubicin (329.7 mm³). These findings indicate that AQCa contains bioactive compounds capable of significantly inhibiting tumor growth, with low toxicity to normal cells, highlighting its potential as an adjuvant agent in breast cancer treatment. Further studies are required to elucidate its molecular mechanisms of action and assess its clinical applicability.

Keywords: *Costus spicatus*, antitumor effect, breast cancer, murine model.

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BIOPROSPECTING PIPER SPECIES FOR ANTIMICROBIAL ACTIVITIES

Bruna Cianciulli Barbosa dos Santos^{1*}, Estela Ynés Valencia Morante²,
Júlia Naelly Machado Silva³, Lydia Fumiko Yamaguchi³,
Cristian Fabian Paz Robles⁴, Massuo Jorge Kato³

brunacbsantos@ifsp.edu.br

1- IFSP, Campus Suzano, Av. Mogi das Cruzes, 1501, Suzano, SP, Brazil. 2- ICB-USP, Departamento de Microbiologia, Av. Prof. Lineu Prestes, 1374, São Paulo, SP., Brazil. 3- IQ-USP, Departamento de Química Fundamental, Av. Prof. Lineu Prestes, 748, São Paulo, SP, Brazil.
4- Universidad de La Frontera, Av. Francisco Salazar, 01145, Temuco, Chile.

A set of crude extracts, fractions and pure compounds from *Piper* species was submitted to antimicrobial assays, aiming at detection of bioactive compounds. Among them, methanolic extracts from roots, leaves, branches and stems of *P. flavoviride* were selected for further chromatographic fractionation, yielding as major compounds 2,2-dimethyl-6-carbomethoxychroman-4-one and methyl taboganate, besides their benzoic acid derivatives, nervogenic acid, 2,2-dimethyl-8-(3-methyl-2-butenyl)-2*H*-chromene-6-carboxylic acid, pinocembrin, tembamide and tembamide acetate. The fraction rich in chromanone presented inhibitory activity against *Staphylococcus aureus* (inhibition zone = 15 mm), *Pseudomonas aeruginosa* (inhibition zone = 9 mm) and *Chromobacterium violaceum* (MIC = 125 µg/mL). The fraction rich in methyl taboganate presented inhibitory activity against *C. violaceum* (MIC = 125 µg/mL). Nervogenic acid (inhibition zone = 11 mm), chromene (inhibition zone = 12 mm) and tembamide acetate (inhibition zone = 13 mm) presented inhibitory activity against *S. aureus*.

Keywords: *Piper* sp., Piperaceae, bioprospecting, antimicrobial activity.





EXPLORING THE ANTILEISHMANIAL PROPERTIES OF *LANTANA CAATINGENSIS* MOLDENKE (VERBENACEAE): A PHYTOCHEMICAL APPROACH

Iolanda Souza do Carmo¹, **José de Sousa Lima Neto^{2*}**, Paulo de Sousa Lima Júnior³, Sidney Gonçalo de Lima¹, Jardes Figuerêdo do Rêgo⁴, Valéria Carlos de Sousa,⁵ Laiz Pinheiro Santos,⁵ Rita de Cássia Viana de Carvalho,⁵ Lucas Maciel Mauriz Marques,⁶ Norberto Peporine Lopes,⁶ Fernando Aécio de Amorim Carvalho⁷, Antônia Maria das Graças Lopes Citó¹

jose.sln@ufma.br

1 - Programa de Pós-Graduação em Química, UFPI, Av. Universitária, sn, lado ímpar, Teresina, PI.
2 - LEAF, Departamento de Biologia, UFMA, Av. Portugueses, 1966, São Luís, MA. 3 - Curso de Farmácia, UFPI, Av. Univsersitária, sn, lado ímpar, Teresina, PI. 4 - Coordenação do Curso de Engenharia Civil, AFYA, Teresina, PI. 5 - BioLeish, UFPI, Av. Universitária, sn, lado ímpar, Teresina, PI. 6 -NPPNS_LAB, Departamento de Ciências BioMoleculares, FCFRP, USP, Av. do Café, Ribeirão Preto, SP. 7 – Departamento de Biofísica e Fisiologia, UFPI, Av. Universitária, sn, lado ímpar, Teresina, PI.

Lantana caatingensis Moldenke (Verbenaceae) is an endemic plant from northeastern Brazil. However, its chemical composition is almost unknown. This study aimed to characterize the chemical compounds found in *L. caatingensis* and investigate the antileishmanial potential of its hydroalcoholic extract and polar fractions. Compounds present in the hydroalcoholic extract obtained from *L. caatingensis* leaves and its polar fractions (ethyl acetate and methanolic) were analyzed by Liquid chromatography with a photodiode-array detector coupled an electrospray ionization quadrupole Time-of-Flight mass spectrometry. An antileishmanial assay was performed in a 96-well plate against *Leishmania major* promastigotes using resazurin on a plate spectrophotometer and the results were expressed as percentage of growth inhibition. Nine compounds were determined in the investigated extract and fractions, classified as flavonoids and C-glycosides derivatives, as well as the phenylethanoid glycosides and the antileishmanial activity revealed that both the hydroalcoholic extract and the ethyl acetate fraction were active against of *L. major* promastigotes with inhibitory concentration of 71.78 and 26.86 $\mu\text{g mL}^{-1}$, respectively, while the methanolic fraction was inactive (478.40 $\mu\text{g mL}^{-1}$). This is the first report on the chemical composition and antileishmanial activity of *L. caatingensis* extracts. These results contribute to further knowledge on species belonging to the *Lantana* genus. The authors thank the support from their institutions, Capes, CNPq and PPBioAmar.

Keywords: flavonoids, phenylethanoids, mass spectrometry, promastigotes, natural products





CYTOTOXICITY OF *LOBELIA BRASILIENSIS* (CAMPANULACEAE) LEAF AND FLOWER EXTRACTS IN MURINE L929 FIBROBLASTS

Amanda Aparecida Marques de Castro^{*}, Lilian Santana Coelho, Rosangela Martines Echeverria, Christopher William Fagg, Omar Enrique Estrada-Semprun, Yris Maria Fonseca-Bazzo, Yanna Karla de Medeiros Nóbrega, Pérola Oliveira Magalhães, Dâmaris Silveira

aamc.amanda@gmail.com

Laboratory of Natural Products, Faculty of Health Sciences, University of Brasília (UnB), Campus Darcy Ribeiro, Asa Norte, Brasília, DF, 70910-900, Brazil

Lobelia brasiliensis A.O.S.Vieira & G.J.Sheph. (Campanulaceae), an endemic and rare species of the Federal District, is considered a bioindicator of flooded areas (*veredas*), remains pharmacologically unexplored despite the documented bioactivity of congeners within its genus. Therefore, in this study, the toxicity of ethanolic extracts, obtained from leaf and flower of *L. brasiliensis*, on murine L929 cells was investigated. The cytotoxicity was assessed via MTT assay [1], with extracts tested at concentration ranging from 0.0625 mg/mL to 1 mg/mL. Cell density was adjusted to 20,000 cells/well, and the tests were conducted in triplicate. The experiment included controls for cells (negative control), MTT reagent, solvent, and the color of the extracts. Absorbance was measured at 570 nm. The leaf extract showed mild cytotoxic activity against L929 cells, with an estimated IC₅₀ value of 1.169 mg/mL. In contrast, the flower extract exhibited markedly potent cytotoxicity, reducing cell viability to 5.484% at 1 mg/mL, with an IC₅₀ value of 0.317 mg/mL. approximately 3.7-fold more potent than the leaf extract. The disparity suggests a distinct phytochemical profile between plant organs. These findings provide the first evidence of the cytotoxicity potential of *L. brasiliensis* and highlight its flowers as a particularly promising source of bioactive compounds. Further phytochemical investigation to isolate and identify the compounds responsible for the activity, alongside assays on a broader panel of cell lines, is warranted to assess its therapeutic potential.

Keywords: *Lobelia brasiliensis*, MTT, Cerrado, cytotoxicity

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CHEMICAL PROFILE AND *IN VITRO* EVALUATION OF *Tamarindus indica* L. (FABACEAE) ON *Helicobacter pylori* AND ITS IMPLICATIONS IN INFECTION

Ester da Silva Tonini^{1*}, Rodrigo de Almeida Romagna¹, Lorena Carnielli Queiroz¹, Rita de Cássia Ribeiro Gonçalves¹, Rodrigo Rezende Kitagawa¹

ester.tonini@edu.ufes.br

1- Department of Pharmaceutical Sciences, Health Sciences Center, Federal University of Espírito Santo, Espírito Santo, 29047-105, Brazil.

The current scenario indicates high rates of *Helicobacter pylori* resistance to established treatments, highlighting the need for new therapeutic alternatives, and a valuable tool is ethnopharmacological research. For *H. pylori*, a bacterium with high global prevalence (43.9%) and associated with the main cause of peptic ulcers and gastric cancer, this screening can be performed using plants that exhibit gastroprotective and antiulcer properties, a potential observed in traditional medicine in *Tamarindus indica* L. (Fabaceae). In this scenario, this study aimed to evaluate the chemical profile of *T. indica* seeds and fruit peels and their anti-*H. pylori* activity and evaluate *in vitro* the implications of the infection, such as oxidative stress, peptic ulcers and gastric cancer, through antioxidant, wound healing, and cytotoxic assays for gastric adenocarcinoma cells (AGS). The chemical profile was evaluated through preliminary phytochemistry tests and liquid chromatography combined with mass spectrometry (LC-MS). The anti-*H. pylori* property was evaluated through the broth microdilution technique with ATCC and clinical strains. The antioxidant potential was evaluated through assays with DPPH, ABTS and superoxide radicals. The cytotoxic activity was assessed using the MTT method in AGS tumor and non-tumor fibroblast cell lines (L-929) for selectivity analysis. Lastly, the healing effect was assessed using the *scratch* assay. In the preliminary phytochemistry, the methanolic extracts of the fruit peel (EBC) and seed (EBS) demonstrated the presence of phenolic compounds such as flavonoids and tannins, however, only EBS indicated the presence of saponins. LC-MS analysis suggested the presence of trans-cinnamic acid and epiandrosterone in EBS, associated with the observed antioxidant effects, with EC₅₀ values close to the standard, anti-*H. pylori* with a minimum inhibitory and bactericidal concentration of 512 µg/mL, and a selective cytotoxic effect against AGS. While EBC showed relevant dose-dependent wound healing activity, this action may be related to the annotated flavonoid pinocembrin. Therefore, the fruit peel and seed of *T. indica* L. have been shown to have a synergistic effect in the treatment of *H. pylori* and its implications for infection, although further studies are needed to understand the mechanisms of action of the isolated compounds.

Keywords: *Helicobacter pylori*; *Tamarindus indica*; Ethnopharmacology; Seeds; Fruits.





***PTERODON EMARGINATUS* VOGEL OLEORESIN CO-LOADED WITH DOXORUBICIN IN pH-SENSITIVE NANOCAPSULES AS POTENTIAL THERAPY FOR BREAST CANCER**

Janaina de Alcântara Lemos^{1*}, Giovanna Oliveira Melo¹, Sued Eustáquio Mendes Miranda⁴, Mauro Lúcio Gonçalves Oliveira⁵, Vanessa Carla Furtado Mosqueira², Lucas Antônio Miranda Ferreira¹, Anna Eliza Maciel de Faria Mota Oliveira³, André Luís Branco de Barros¹

jana_alemos@hotmail.com

1-Departamento de Produtos Farmacêuticos, FaFar, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, 31270-901, MG, Brazil. 2-LDGNano, Faculdade de Farmácia, UFOP, Campus Morro do Cruzeiro, S/N Morro do Cruzeiro, Ouro Preto, 35400-000, MG, Brazil. 3-Laboratório de Nanobiotecnologia Fitofarmacêutica, Universidade Federal do Amapá, Campus Universitário Marco Zero do Equador, Rodovia Josmar Chaves Pinto, Km 02, Macapá, 68902-280, AP, Brazil. 4-Centro de Desenvolvimento de Tecnologia Nuclear, CDTN, Av. Antônio Carlos, 6627, Belo Horizonte, 31270-901, MG, Brazil. 5-LQA-LARA, Instituto Mineiro de Agropecuária IMA-MG - BR 040 km 688 CEASA-MG, S/N, 32145-900, Belo Horizonte, MG, Brazil.

Nanocarriers have emerged as a promising strategy for the delivery of bioactive natural products with low hydrophilicity, enabling targeted tissue distribution with greater specificity. Therefore, this study aimed to develop multifunctional nanocapsules capable of co-delivering natural anti-inflammatory and antitumor agents along with chemotherapeutics, with the goal of enhancing efficacy, specificity, and safety. The phytochemical profile of *Pterodon emarginatus* Vogel oleoresin was determined using gas chromatography (GC) and liquid chromatography (HPLC) coupled with mass spectrometer. Conventional and PEGylated nanocapsules were prepared via nanoprecipitation method and stored at 4°C for stability assay. The mean diameter and polydispersity index were determined by dynamic light scattering and zeta potential was associated with electrophoretic mobility. The encapsulation content was evaluated by centrifugation-ultrafiltration, where nonencapsulated doxorubicin and total were analyzed by spectrophotometry. *In vitro* release profile was obtained by dialysis method, using Hepes buffer pH 7.4 and 5.0, as acceptor compartment, at 37°C under agitation. The amount of doxorubicin released from nanocapsules was measured by HPLC. Cell viability (4T1 tumor and fibroblasts cells) was assessed by the Sulforhodamine B assay. While antitumor efficacy and toxicity *in vivo* were evaluated in 4T1 tumor-bearing mice. Diterpenes and sesquiterpenes were identified in the oleoresin. Conventional and PEGylated nanocapsules oleoresin-loaded with or without doxorubicin were monodisperse (polydispersity index <0.1) with a size of less than 150 nm and negative zeta potentials (-30 mV). The nanocapsules remained stable over a 30-day period, maintaining their original physicochemical properties. Encapsulation efficiency was greater than 90%, with release modulated by pH medium. *In vitro* data showed high selectivity and improved cytotoxicity against tumor cells for PEGylated nanocapsules oleoresin-loaded combined with doxorubicin. Additionally, *in vivo* data showed not only increased efficacy but also reduced toxicity



to liver and heart tissue and less body weight loss. Therefore, the results presented in this paper show that *Pterodon emarginatus* Vogel oleoresin co-loaded with doxorubicin in PEGylated nanocapsules can be considered a promising system for the tumors treatment. The authors thank the support from their institutions and CAPES, CNPq and FAPEMIG for their financial support.

Keywords: *Pterodon emarginatus*, PEGylated nanocapsules, doxorubicin, antitumor activity, drug delivery, natural products



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BIOGUIDED STUDY OF *Jatropha gossypifolia* - *IN VITRO* ANTI- *Helicobacter pylori* AND CYTOTOXICITY AGAINST GASTRIC ADENOCARCINOMA CELLS

Aliny Rodrigues de Jesus da Conceição^{1*}, *Ester da Silva Tonini*¹, *Rodrigo de Almeida Romagna*¹, *Lorena Carnielli Queiroz*¹, *Rita de Cássia Ribeiro Gonçalves*¹, *Rodrigo Rezende Kitagawa*¹

rodrigo.romagna@edu.ufes.br

1- Department of Pharmaceutical Sciences, Health Sciences Center, Federal University of Espírito Santo, Espírito Santo, 29047-105, Brazil.

Helicobacter pylori is a gram-negative bacterium that colonizes the human stomach, and its infection is strongly linked to the development of gastric inflammatory disorders, from gastritis to cancer and is designated as a Class I carcinogen by the International Agency for Research on Cancer (IARC). The global prevalence is approximately 43%, and the increasing resistance to the treatment compromises the eradication of the pathogen. This requires the search for alternative treatments, and this work aimed to assess the efficacy of *Jatropha gossypifolia* L. (Euphorbiaceae), whose chemical profile had previously been studied in recent research conducted in our laboratory, against *H. pylori* and gastric adenocarcinoma cells (AGS). Liquid-liquid extractions were performed using the ethanolic crude extract to yield hexane, ethyl acetate, and aqueous fractions. The most active fraction was analyzed using liquid chromatography combined with mass spectrometry (LC-MS). The spectrum data was processed and obtained in MZmine by comparing the compounds with the Global Natural Products Social Molecular Networking (GNPS) database. The anti-*H. pylori* activity was evaluated using the broth microdilution method with ATCC 43504 and a clinical strain to find the minimum inhibitory concentration (MIC). The minimal bactericidal concentration (MBC) was determined as the concentration that did not exhibit bacterial growth on blood agar. The cytotoxicity was assessed for AGS and L-929 cells, which is non-cancerous, by the MTT assay to determine the cytotoxic index (CI₅₀) and the selectivity index (SI). The crude extract and its derived fractions shown activity against *H. pylori* and AGS cells, especially the hexane fraction, which exhibited a MIC and MBC of 16 and 32 µg/mL, respectively, against the ATCC strain, and a MIC and MBC of 64 µg/mL for the clinical strain. The hexane fraction demonstrated CI₅₀ of 13.33 ± 0.29 µg/mL and a SI of 2.4, the best findings of the samples tested. The antibacterial and cytotoxic action may be attributed to the presence of terpenoids like jatrophenone, jatrophone and sumaresinolic acid together with flavonoids such as vitexin and isovitexin, as they were found in LC-MS. Further research should be conducted for the evaluation of safety and efficacy of this fraction *in vivo*.

Keywords: *Jatropha gossypifolia*, Euphorbiaceae, *Helicobacter pylori*, gastric cancer, terpenoids





Metabolomic and Morphological Analysis of Micromonospora Strains Isolated from Marine Sediments

Luiz Fernando Covizzi Castilho^{1*}, Renan S. Oliveira², Bruna V. Souza², Paula C. Jimenez², Suzan Pantaroto de Vasconcellos³, Vitor Gonçalves Vital³, Patrícia Sartorelli¹

lfccastilho@unifesp.com

1-LaBiORG, Departamento de Química, UNIFESP, R. Prof. Artur Riedel, 275 - Eldorado, Diadema – SP, 09972-270, Brazil.

2-BioproSP, Departamento de Ciências Biológicas, UNIFESP, Instituto do Mar, R. Carvalho de Mendonça, 144, Santos – SP, 11070-100, Brazil.

3-LabMSMA (Grupo BioMicro), Departamento de Farmácia, UNIFESP, R. São Nicolau, 210 - 1o Andar - Centro, Diadema - SP, 09913-030, Brazil.

Marine ecosystems are recognized as promising sources of microorganisms capable of producing bioactive secondary metabolites. In this context, two strains of *Micromonospora* sp. (BRB 607 and BRB 640), isolated from marine sediments, were cultivated in A1 broth (10g starch, 2g peptone, 4g yeast extract, 35.71g sea salt) at 28 °C, 120 rpm, followed by liquid–liquid extraction with ethyl acetate. The crude extracts were analyzed by liquid chromatography–mass spectrometry (LC-MS/MS), hydrogen nuclear magnetic resonance spectroscopy (¹H NMR), and scanning electron microscopy (SEM). SEM images revealed significant morphological changes between 6 and 22 days of cultivation, including filament formation and structures compatible with exopolysaccharides, suggesting biofilm development as an adaptive strategy to osmotic conditions. LC-MS/MS analysis, integrated with the GNPS platform, enabled the construction of molecular networks and the annotation of six compounds, with lumichrome (C₁₂H₁₀N₄O₂) identified as the major metabolite, previously reported for its antimicrobial activity. The ¹H NMR spectra of the extracts exhibited characteristic signals in the 6.5–8.0 ppm region, indicative of aromatic hydrogens, as well as signals between 3.0–4.0 ppm, associated with hydrogens bound to oxygenated carbons, and multiple signals within 0.8–2.0 ppm, typical of aliphatic chains. These findings reinforce the structural diversity of metabolites present in the crude extracts and corroborate the annotations obtained via GNPS. In addition, genomic DNA was extracted following a protocol adapted from Sachinandan et al. (2010), yielding A260/A280 ratios of 1.53 (BRB 607) and 2.14 (BRB 640), confirming adequate purity for downstream analyses. Altogether, the results obtained thus far highlight the metabolic diversity of marine *Micromonospora* strains and their potential as sources of bioactive compounds. Ongoing efforts involve metabolite isolation, structural characterization, and biological activity assays.

Keywords: *Micromonospora*, marine sediment, antimicrobial activity





VIRTUAL SCREENING OF RENISUS MEDICINAL PLANTS WITH GASTRIC ANTITUMORAL POTENTIAL

Pedro Henrique Tregnago*¹, Vitor Zorzal Majeski¹, Rita de Cassia Ribeiro Gonçalves¹,
Rodrigo Theofilo Valadares³, Warley de Souza Borges², Rodrigo Rezende Kitagawa¹

pedro.henrique.tregnago@gmail.com

1- Department of Pharmaceutical Sciences, Federal University of Espírito Santo, Vitória 29047-105, Espírito Santo, Brazil. 2- Department of Chemistry, Federal University of Espírito Santo -UFES, Avenida Fernando Ferrari 514, 29075-910 Vitória, ES, Brazil. 3- VIES Herbarium, Federal University of Espírito Santo -UFES, Avenida Fernando Ferrari 514, 29075-910 Vitória, ES, Brazil.

Gastric cancer is both the fifth most common type of cancer and the fifth cancer with the highest mortality rate in the world, with *Helicobacter pylori* infection being its main risk factor. When the cancer is discovered in more advanced stages, its prognosis often has a negative outcome, which highlights the demand for new treatment options. The use of medicinal plants and their phytochemicals represent important allies in the search for new compounds with potential for pharmacological use. Thus, the objective of this work was to select medicinal plant species from the RENISUS list with gastric antitumor potential through in silico studies and, subsequently, in vitro studies. Through virtual screening, medicinal plants were selected through a systematic review of the literature, searching for species with known gastroprotective and anti-*H. pylori* activity, but without studies for gastric cancer. Then, a database of its secondary metabolites was created and its biological activity was evaluated through a prediction model using the PASSOnline program. The plant with the most compounds with antitumor potential was selected and evaluated in silico, through molecular docking, and in vitro, through a cytotoxicity assay. Based on the literature survey and PASS analysis, the selected medicinal plant was *Casearia sylvestris* L. (Salicaceae), popularly known as guaçatonga. Its molecular docking analysis was performed using the transcription factor HIF-2 α as the target, where several compounds from *C. sylvestris* demonstrated potential interactions with the active site. The best docking scores were observed for the metabolites 15 ξ -Methoxy-cleroda-3,12-dien-18-carboxy-15,16-olide, α -zingiberene, and catechin, however, sesquiterpenes overall showed the most promising performance. In its cytotoxicity assay on AGS cells, its IC₅₀ was 138.20 $\pm$ 8.10 μ g/mL. The results of the trials carried out with *C. sylvestris* were promising, but further studies are still needed, evaluating fractions of its extract, especially the apolar fractions, and isolated compounds, to confirm the gastric antitumor activity predicted here.

Keywords: Gastric cancer; *Casearia sylvestris*; medicinal plants; RENISUS; virtual screening.





Exploring Brazilian Cyanobacteria for the Identification of New Bioactive Natural Products

Márcio Barczyszyn Weiss^{1*}, Jaewon Yoon¹, João P. B. Domingues¹, Samuel C. Amaral¹, Vítor F. Freire², Fernanda Rios Jacinavicius¹, Helori Vanni Forastieri³, Leticia Veras Costa Lotufo³, Ricardo M. Borges⁴, Roberto G. S. Berlinck², Camila Manoel Crnkovic¹

marciobweiss@gmail.com

1-Lab.azul, Departamento de Tecnologia Bioquímico-farmacêutica, FCF, USP, Av. Prof. Lineu Prestes, 580, São Paulo, SP, 05508-000, Brazil. 2- Organic Chemistry of Biological Systems, IQSC, USP, Av. Trab. São Carlense, 400, São Carlos, SP, 13566-590, Brazil. 3-LAFARMAR, ICB I, USP, Av. Prof. Lineu Prestes, 1524, 05508-000, São Paulo, SP, Brazil. 4-laabioipn, IPPN, UFRJ, Av. Carlos Chagas Filho, 373, 21941-902, Rio de Janeiro, RJ, Brazil.

Cyanobacteria are among the earliest life forms on Earth. These photoautotrophic prokaryotes inhabit diverse ecosystems, including rivers, forests, permafrost, and deserts, employing several strategies that include the production of a wide variety of natural products. Developing efficient strategies to optimize the screening of potentially novel and bioactive compounds is essential for discovering molecules of biotechnological interest. In this study, we present a pipeline to identify promising bioactive features from fractions of freshwater cyanobacterial strains isolated from Brazilian environments (Atlantic Rain Forest, Pantanal, and Cerrado). Samples were evaluated for their bioactivities and were analyzed using high-resolution mass spectrometry. Metabolomics was performed via GNPS molecular networking, while DAFdiscovery was used to highlight features potentially correlated with biological activity. SIRIUS supported annotation and chemical classification of metabolites. Dereplication revealed several potentially novel peptides and polyketides associated with bioactivity against mammalian melanoma (MCF-7) and colorectal cancer (HCT-116) cell lines. This study demonstrates the utility of metabolomics tools for the rapid prioritization of bioactive features, streamlining subsequent isolation and structural elucidation efforts. Our findings highlight the effectiveness of integrating computational tools with bioassays to accelerate the discovery of bioactive natural products.

Keywords: *Cyanobacteria, metabolomics, dereplication, molecular networking, mass spectrometry*





Larvicidal Activity of *Piper arboreum* and Its Synergy Effect with *Melaleuca alternifolia* Essential Oil Against *Spodoptera frugiperda*

Essential oil-based pesticides have been investigated as alternatives to traditional synthetic pesticides, primarily due to their advantages, including low environmental impact and the maintenance of soil health. In Brazil, various natural product-based materials are being studied to control *Spodoptera frugiperda*, a moth that consumes, in larval form, leaves from *Zea* spp., a plant of significant economic importance. On the other hand, the essential oil (EO) of native plants has shown bioactivities that are interesting for agricultural uses, including those of *Piper* spp. species, with approximately 400 species cataloged in Brazil. In this work, the seasonal chemical variability of EOs from *Piper arboreum*, the EO of *Melaleuca alternifolia* leaves, and the synergistic effects among these EOs were evaluated against the larvae of *S. frugiperda*. The EOs were extracted by hydrodistillation for 4 hours, and the larvae were exposed to the EO with the aid of a manual sprayer. Negative and positive controls were performed using pure propanone and Pirate® 0,1%, with mortalities of 0 and 100%, respectively. All tests were conducted in 10 replicates with five larvae, and the EO concentration was maintained at 2% from the synergy evaluation. The EOs from *P. arboreum*, analyzed in triplicate by GC-MS, and were then subjected to Principal Component Analysis (PCA). The *P. arboreum* EOs composition are rich in sesquiterpenoids (Autumn – 74.8%; Winter – 80.7%; Summer – 81.7% and Spring – 87.3%), mainly bicyclogermacrene ($17.0 \pm 1.70\%$), germacrene D ($9.40 \pm 2.07\%$) and *E*-caryophyllene ($9.28 \pm 1.03\%$), the *M. alternifolia* EO is rich in monoterpenoids (93.3%) with predominance of terpinen-4-ol (42.3%). The larvicidal activity of EO from *P. arboreum* (Autumn: 22%; Winter: 28%; Summer: 42% and Spring: 16%) and *M. alternifolia* (24%) were lower than EO mixture (Autumn: 86%; Winter: 92%; Summer: 88% and Spring: 70%), indicating synergy between the EOs. The PCA successfully separated the seasonal samples with PC1 (Variance Explained - VE: 60.28%) and PC2 (VE: 27.66%). The minor compounds were responsible for the separation, corroborating the hypothesis that indicates the synergy between classes of compounds, and not specific compounds.

Keywords: Agriculture, Biopesticides, *Piper* spp., Fall armyworm, Seasonality, Synergy





NEOLIGNANS FROM *Piper rivinoides* - KUNTH

Mariane Carolina Pesenti¹, Fabiele Kloster Campos Weiber¹, Pedro Henrique Danguì Bellardo¹, Aurea Portes Ferriani¹, Marta Cristina T. Duarte², Beatriz Helena L. N. Sales Maia^{1*}

marianepesenti@ufpr.br

1-LAPNEQ, Departamento de Química, UFPR, Av. Cel. Francisco H. dos Santos, 100, Curitiba, 81531-980, PR, Brazil.

2- CPQBA – Unicamp, Av. Alexandre Cazellato, 999, Paulínia, SP, 13140-000, Brazil.

The *Piper rivinoides* Kunth plant belongs to the *Piperaceae* family, is widely distributed throughout Brazil and consists mainly of neolignans, which show promise in various biological activities (Moreira et al, 2016). The crude extracts of the branches and roots obtained using hexane, ethyl acetate and methanol were evaluated against six microorganisms: *Candida albicans*, *Staphylococcus aureus*, *Staphylococcus epidermidis*, *Salmonella choleraesuis*, *Escherichia coli* and *Pseudomonas aeruginosa*. The slow evaporation of the hexane solvent from the root (PRRH) and branch (PRGH) extracts resulted in crystal formation that was analyzed by single crystal X-ray diffraction (XRD) and nuclear magnetic resonance (NMR - 1D and 2D, ¹H and ¹³C). The crude ethyl acetate branch extract (PRGA) was purified by vacuum column chromatography and the fractions were grouped based on their similarity. The slow evaporation of the solvent from one fraction resulted in a crystal that was also evaluated by XRD and NMR. XRD analysis identified the neolignan from the PRRH and PRGH extracts as grandisine (C₂₄H₃₂O₇) with *trans-cis-trans* stereochemistry, isolated for the first time in this plant by our research group (Azevedo, 2022). The second compound isolated from the PRGA extract fraction is a neolignan (C₂₄H₃₂O₈) not previously reported in the literature. The best results obtained in the antimicrobial analysis were for *E. coli* and *S. epidermidis* treated with the PRRH and PRGA extracts (MIC 0.25 mg mL⁻¹ and MBC >1.0 mg mL⁻¹), while the other extracts did not show significant activity. These results indicated the potential biological activity of *P. rivinoides* Kunth and may be associated with the presence of neolignans. Acknowledgments: PPGQ – UFPR, CNPq, and CAPES.

Keywords: Grandisine, secondary metabolites, antimicrobial activity, two-dimensional NMR, single crystal XRD.

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**SAKURANETIN AS A PROMISING PROTOTYPE IN DRUG DEVELOPMENT -
PHARMACOKINETICS AND *in vivo* ANTI-Schistosoma mansoni ACTIVITY**

Dalete Christine S. Souza^{1,4*}, Pedro Enrico H. Tesser¹, Ruqaya Jasim⁴, Rayssa A. Cajás²,
Thainá R. Teixeira², Josué de Moraes^{2,3}, Dion R. Brocks⁴, João Henrique G. Lago¹

christine.silva@ufabc.edu.br

¹Center for Natural and Human Sciences, Federal University of ABC, Santo André, Brazil; ²Research Center for Neglected Diseases, Guarulhos University, Guarulhos, Brazil; ³Research Center for Neglected Diseases, Universidade Brasil, São Paulo, Brazil; ⁴Katz Group Centre For Research, University of Alberta, Edmonton, Alberta, Canada.

Sakuranetin (SAK), a flavanone found in several plant families, exhibits various biological activities, including antimutagenic, anticancer, antiviral, anti-inflammatory, antidiabetic, and antiparasitic.¹ As part of our ongoing research on discovering new antischistosomal prototypes based on natural products², SAK underwent *in silico* and *in vitro* pharmacokinetic experiments and was then tested for *Schistosoma mansoni* using an *in vivo* model. To conduct this study, the aerial parts of *Baccharis lateralis* (Asteraceae) were defatted with hexane and then extracted with MeOH. The MeOH extract was partitioned into hexane (0.5 g) and CH₂Cl₂ (10.7 g). Part of the CH₂Cl₂ phase (10.0 g) was chromatographed over SiO₂ (eluent hexane:EtOAc in different proportions) to produce 12 groups (A–L). Group B (977 mg) was then chromatographed over Sephadex LH-20 using the following eluents: hexane:CH₂Cl₂ (1:4), CH₂Cl₂:acetone (3:2 and 1:4), and pure acetone. This process yielded 12 additional groups (B1–B12). As evidenced by NMR and MS analysis, group B8 (618 mg) contained pure SAK. *In silico* pharmacological analyses were performed using the SwissADME tool, which indicated no violations of drug-likeness or PAINS and high absorption by the GI tract. Thus, it was considered similar to orally administered drugs. Next, we validated an analytical method for the extraction and detection of SAK in rat plasma, following the recommendations of ANVISA and the FDA, for concentrations up to 50 ng/mL. We also performed a Plasma Protein Binding experiment, finding that only 8.3% of the drug was unbound. Liver microsomal vesicles were used to calculate the metabolic rate: 40% of the drug was metabolized within 120 minutes. Considering that the *in silico* and *in vitro* pharmacokinetic parameters indicated favorable drug-like properties, the *in vivo* anti-*S. mansoni* activity was assessed in mice infected subcutaneously and treated with a single oral dose of 400 mg/kg of SAK or PZQ (the standard drug), compared to untreated mice as the control group. After euthanizing the mice, the parasites were sexed and counted, and quantitative oograms and the Kato-Katz technique were used to assess the worm burden reduction (WBR) and egg burden reduction (EBR), respectively. As results, SAK achieved total WBR and EBR of 84 ± 6% and 96 ± 5%, respectively, compared to the standard drug, which achieved reductions of 88 ± 2% and 87 ± 2%. Based on these results, SAK is a promising candidate for the development of new oral schistosomiasis drugs.

References: ¹Stompor et al., 2020. *Nutrients* 12(2), 513; ²Souza et al., 2024. *Phytomedicine* 135, 156045.

Keywords: Sakuranetin, Pharmacokinetics, *Schistosoma mansoni*, drug development.

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ANTIOXIDANT POTENTIAL AND TOXICOLOGICAL EVALUATION OF *Clitoria guianensis* FROM THE BRAZILIAN CERRADO

Nathália A. A. Nunes^{1*}, Feliciano Da Silva Neto¹, Juliana Panato Didonet¹, Aline B. M. Del Conte², Elisandra Scapin¹, Juliana C. Holzbach¹

nathalia.aires@uft.edu.br

1-Curso de Engenharia Ambiental, Câmpus de Palmas, UFT, Avenida NS-15, Quadra 109 - Alcno 14, Norte, s/n - bloco D - Plano Diretor Norte, Palmas - TO, Brazil. 2 - Programa de Pós-Graduação em Biodiversidade e Biotecnologia da Rede BIONORTE, Brazil.

Clitoria guianensis, a species native to the Brazilian Cerrado and traditionally used in folk medicine, has been reported to contain bioactive compounds with pharmacological potential. However, the bioactive potential and toxicological characterization of its different plant parts remains scarce. This study aimed to investigate the antioxidant activity, and toxicity of *C. guianensis* stems and leaves. Stem extracts were obtained by sequential maceration with solvents of increasing polarity (hexane, ethyl acetate, and ethanol), while leaf extracts were prepared using ultrasound-assisted extraction under different ethanol concentrations and extraction times. The extracts were evaluated for total phenolic and flavonoid content, antioxidant potential (DPPH, ABTS, FRAP assays), and toxicity using *Artemia salina* and *Allium cepa* bioassays. Leaf extracts presented moderate yields of phenolics (35.17 ± 1.1 mg EAG g⁻¹) and flavonoids (34.38 ± 3.8 mg EQ g⁻¹), but no significant antioxidant activity under the tested conditions. Stem extracts exhibited low to moderate toxicity: the hexane extract showed $LC_{50} = 1445.0$ mg·L⁻¹ and the ethanol extract $LC_{50} = 245.5$ mg·L⁻¹ against *A. salina*, while *A. cepa* assays revealed no cytotoxic effects. Overall, *C. guianensis* demonstrated promising phytochemical potential and weak toxicity in specific extracts. These findings contribute to the chemical and toxicological knowledge of this Cerrado species and reinforce its relevance for pharmacological and biotechnological applications.

Keywords: Ultrasound-assisted extraction; antioxidant activity; toxicity





**METABOLOMIC PROFILE AND IN VITRO ANTI-INFLAMMATORY AND
CYTOTOXIC ACTIVITIES OF LICARIA ARMENIACA EXTRACTS**

*Lanalice R. Ferreira^{1*}, Laine C. Pinto², José Diogo E. Reis³, Paulo Wender P. Gomes³, Joyce
Kelly R. da Silva¹,*

joykellys@ufpa.br

- 1- Programa de Pós-Graduação em Química, Universidade Federal do Pará, Belém, Brazil*
- 2- Laboratório de Neuropatologia Experimental, Hospital Universitário João de Barros
Barreto, Universidade Federal do Pará, Belém, Brazil.*
- 3- Laboratório de Cromatografia Líquida, Universidade Federal do Pará, Belém, Brazil.*

Licaria armeniaca (Lauraceae) is a tree up to 7 m, widely distributed in the Amazonian rainforest, Brazil. A specimen was collected in Belém, PA, and its tissues were extracted by an ultrasound-assisted method using Ethanol/ water as solvent. Each tissue was extracted according to optimal conditions as follows: leaves (Ethanol 64.9%, t: 26.1 min, 6.23% m/v), thin branches (Ethanol 73.8%, t: 31.3 min, 11.0% m/v) and thick branches (Ethanol 50.0%, t: 35.0 min, 11.0% m/v). The extracts were analyzed by LC-MS/MS and the data were converted from RAW standard data format (Waters corp., Milford, USA) to mzML format using MSConvert 3.0.2. Feature extraction of the resulting file was processed using MZmine 4. The output files were for the CANOPUS chemical classes prediction and statistical analysis. The leaf extracts showed a predominance of alkaloids (46.34%), amino acids and peptides (19.51%), and shikimate and phenylpropanoid derivatives (12.20%). For thin branches and thick branches, the major classes were alkaloids (35.97%), amino acids and peptides (20.86%), and carbohydrates (12.23%), and alkaloids (32.14%), amino acids and peptides (25.00%), and fatty acids (14.26%), respectively. The cytotoxic activity of the extracts was evaluated by the MTT method against three cancer cell lines: gastric ascites (AGP01), glioblastoma (AHOL), lung cancer (A549), and non-malignant murine macrophage cells (RAW 264.7). The cell availability was measured after 24h, and the samples with an IC₅₀ value < 25 µg/mL were considered active. The leaf extract was selective to glioblastoma cell lines (IC₅₀, 11.52 µg/mL) while the thin and thick branches extracts were active against gastric ascites (IC₅₀, 15.71 and 13.59 µg/mL, respectively). However, the thick branches extract was the only activity against lung cancer (IC₅₀, 16.95 µg/mL). Regarding the cytotoxicity against normal cells (RAW 264.7), the thick branches extract displayed low toxicity. The in vitro anti-inflammatory activity was assessment using an LPS model stimulating macrophage cells with Lipopolysaccharide (LPS) to induce an inflammatory state, then testing the effect of extracts in reduction of inflammatory markers such as nitric oxide (NO) and anion superoxide. The reduction of nitrite concentration compared to LPS group was significant to leaf and thick branches extracts in all concentrations tested (6.25-25 µg/mL), meanwhile to thin branches extract was efficient only at 12.5 e 6.25 µg/mL. Regarding to superoxide anion formation, the extracts of thin and thick branches reduced in all concentrations tested. However, the leaf extract was effective only at 12.5 µg/mL.

Keywords: *alkaloids, amino acids and peptides, shikimate derivatives, MTT assay, LPS model.*





POTENTIAL OF PYRANOCARBAZOLE ALKALOIDS IN THE CONTROL OF CITRUS CANKER

Chrystiane Helena Campos de Matos^{1*}, Carlos André Ferreira Moraes¹, Danielle Fernandes da Silva¹, Jéssica Cristina Amaral², João Batista Fernandes¹, Maria Fátima das Graças Fernandes da Silva¹

chrystiane campos@gmail.com

1 – Laboratório de Produtos Naturais, Universidade Federal de São Carlos, Departamento de Química – DQ, Rodovia Washington Luis km 235, São Carlos, SP, 13565-905, Brazil. 2 – Laboratório de Fisiologia e Bioquímica Fitopatológica, Escola Superior de Agricultura Luiz de Queiroz (ESALQ – USP), Departamento de Fitopatologia e Nematologia., Av. Pádua Dias 11, Piracicaba, SP, 13418-900, Brazil.

Citrus canker, caused by the bacterium *Xanthomonas citri*, is a phytopathological disease of high economic relevance, compromising both productivity and fruit quality in citrus crops. The search for natural antimicrobial agents is an important strategy for developing sustainable alternatives to synthetic pesticides, aiming to reduce environmental impacts and bacterial resistance. In this study, five pyranocarbazole alkaloids were isolated from the leaves of *Murraya koenigii* using the ethyl acetate extract. The extract was subjected to adsorption liquid chromatography with silica gel 230–400 mesh as the stationary phase and a solvent mixture with increasing polarity as the mobile phase. The fractions obtained were further processed by solid-phase extraction using a C18 (octadecyl – 10 g) silica-based cartridge (C18 SPE) and subsequently analyzed for chemical profiling by high-performance liquid chromatography (HPLC) using an analytical C18 column with ultrapure Milli-Q® water (line A) and HPLC-grade acetonitrile (Sigma-Aldrich®) (line B) as mobile phases in reverse-phase mode. The samples were monitored at a wavelength of λ 250 nm. Structural characterization of the alkaloids was confirmed by nuclear magnetic resonance (NMR) spectroscopy. For antibacterial activity assessment, the compounds were solubilized in DMSO and tested in triplicate against *X. citri* using the broth microdilution method in 96-well plates, with standardized bacterial inoculum. Appropriate controls were included: DMSO, copper, inoculum alone, and compounds dissolved in DMSO alone, ensuring result reliability and absence of contamination. All compounds exhibited a minimum inhibitory concentration (MIC) of 1000 μ g/mL, demonstrating consistent antibacterial activity. The results indicate that pyranocarbazole alkaloids have potential as natural antibacterial agents against *X. citri*, providing a promising basis for the development of formulations applicable to citrus plants, with prospects for activity optimization and in planta studies in future investigations.

Keywords: citrus, antibacterial activity, *Xanthomonas citri*, bioactive compounds, integrated pest management (IPM), Rutaceae.





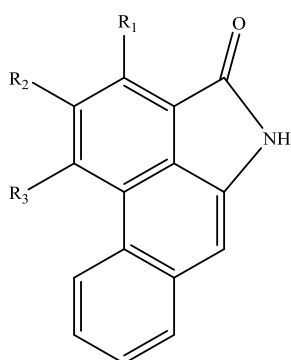
ARISTOLACTAMS FROM *Piper truncatum* VELL. WITH ANTI-*Trypanosoma cruzi* ACTIVITY

Sávio R. Soares^{1*}, Marina de M. Gonçalves¹, Vanessa Albuquerque²,
André G. Tempone², João Henrique G. Lago¹

savio.rodrigues@ufabc.edu.br

¹Center for Natural and Human Sciences, Federal University of the ABC, Santo Andre, SP Brazil.

²Laboratory of Pathophysiology, Butantan Institute, São Paulo, SP, Brazil.



1 R₁ = H; R₂ = R₃ = OCH₃

2 R₁ = H; R₂ = OCH₃; R₃ = OH

3 R₁ = OCH₃; R₂ + R₃ = OCH₂O

In continuation of our studies on the isolation of antiprotozoal metabolites from *Piper* species¹, the present study aims to detect anti-*Trypanosoma cruzi* metabolites from *P. truncatum*. Initially, the branches were defatted with hexane, then extracted with MeOH. Evaluation of the anti-*T. cruzi* potential revealed potent activity to MeOH extract, with 100% of trypomastigote forms killed at 300 µg/mL. After partitioning with hexane, CH₂Cl₂, and EtOAc, we observed that the bioactivity was concentrated in the CH₂Cl₂ phase. Thus, 1 g of this material was chromatographed over silica gel, yielding 26 fractions (A–Z). Groups M, Q, and V exhibited potent activity against *T. cruzi* and were purified by HPLC, which afforded three aristolactams (**1–3**). The ¹H NMR spectra of compounds **1** and **2** showed aromatic hydrogen signals between δ 9.1–7.1 and singlets corresponding to methoxyl groups between δ 4.1–4.0. The spectra also showed signals attributed to the amide N–H hydrogen at δ 10.8 (s). The respective ¹³C NMR spectra showed signals of the amide carbonyl group at δ 168, methoxyl carbons at δ 60–57 and sp² carbons of a phenanthrenic system at δ 154–105. These signals allowed for the identification of aristolactam BII (**1**) and piperolactam A (**2**).² The ¹H NMR spectrum of compound **3** showed characteristics of the phenanthrene moiety observed in **1** and **2**, as well as a singlet at δ 6.47 attributed to methylenedioxy hydrogens and another singlet at δ 3.87 corresponding to an additional methoxy group.³ These results indicated the structure of **3**, a previously unreported aristolactam, as shown in Figure 1. Finally, the molecular formulas of compounds **1–3** were confirmed by ESI-HRMS analysis. Among the isolated aristolactams, compound **1** exhibited significant activity against amastigotes, with an EC₅₀ of 8.6 µM and reduced toxicity (CC₅₀ >200 µM), a comparable to the results for the positive control, benznidazole, which has an EC₅₀ of 5.5 µM and a CC₅₀ >200 µM.

Keywords: Chagas disease, aristolactams. **References:** ¹Gonçalves M.M. et al., *Chem. Biodivers.* **2024**, 21, e202400547.

²Qu, W. et al., *Nat. Med.* **2011** 9, 425–8., ³Holzbach, J.C. et al., *Molecules* **2010**, 15, 9462–72. **Acknowledgements:** CAPES/FAPESP/CNPq





IN SILICO EVALUATION OF FLAVONOIDS FOR INHIBITION OF THE ENZYMES GLUCOSE 6-PHOSPHATE DEHYDROGENASE, SHIKIMATE KINASE AND ASPARTATE SEMIALDEHYDE DEHYDROGENASE ENZYMES OF *Helicobacter pylori*

Leonardo Dias da Silva¹, Dalila Nickel Loose¹, Amanda Cavalcante Gonzaga Nunes¹, Lorena Carnielli Queiroz¹, Rodrigo Rezende Kitagawa¹, **Rita de Cassia Ribeiro Gonçalves¹**

rita.goncalves@ufes.br

¹Graduate Program of Pharmaceutical Sciences, Health Sciences Center, Federal University of Espírito Santo, Avenida Marechal Campos 1468, Maruípe, 29047-105, Vitória, Espírito Santo, Brazil.

Helicobacter pylori is a microaerophilic, Gram-negative bacterium that colonizes the human gastric mucosa and constitutes the main risk factor for gastric adenocarcinoma. Increasing bacterial resistance and adverse effects of conventional treatment encourage the search for therapeutic alternatives, including natural compounds with antimicrobial potential. This study aimed to perform an *in silico* evaluation of flavonoids described in the literature as having anti-*H. pylori* activity and evaluate their ability to inhibit three target enzymes of bacterial metabolism: glucose-6-phosphate dehydrogenase (HpG6PD), shikimate kinase (SK), and aspartate semialdehyde dehydrogenase (ASADH). The flavonoids were selected from a literature review using the PubMed and SciELO database. Their physicochemical and pharmacokinetic properties were predicted by SwissADME server. Subsequently, molecular docking assays were performed on SwissDock/AutoDock Vina, with pose analysis in Discovery Studio. Forty flavonoids with anti-*H. pylori* activity were identified, of which 23 presented adequate pharmacokinetic properties: partition coefficient ranging from 3.76 to 0.51, high gastrointestinal absorption, non-permeability in the blood-brain barrier and compliance with Lipinski's rule. Docking indicated relevant interactions with the three enzymes. For SK, morin (-7,122 kcal/mol), diosmetin (-6,377 kcal/mol) and taxifolin (-6,533 kcal/mol) presented the best interaction. For ASADH and HpG6PD, licoisoflavone B presented the highest layers (-8,150 and -8,695 kcal/mol, respectively), followed by luteone (-7,467 and -8,255 kcal/mol) and isowigtheone (-7,256 and -8,039 kcal/mol). These results highlighted a potential against *H. pylori* infection and its complications. Flavonoids such as licoisoflavone B, luteone, isowigtheone, and morin have a promising profile against the essential enzymes of *H. pylori*. These results reinforce the need for *in vitro* experimental validation to confirm their therapeutic applicability.

Keywords: *Helicobacter pylori*. Stomach cancer. Flavonoids.

Acknowledgments: UFES and FAPES





CITOTOXIC ACTIVITY SCREENING OF MARINE ORGANISMS ON HCT-116, MCF7 AND A549 CELL LINES

Rodrigo Rezende Kitagawa^{1,2}, Jéssica Raquel Borges Monteiro^{1*}, Rita de Cássia Ribeiro Gonçalves², Marie L. Matos-Hernández³, Eduardo J. Caro-Díaz³

rodrigo.kitagawa@ufes.br

1-Programa de Pós-graduação em Química, UFES, Av. Fernando Ferrari 514, Vitória, ES, Brazil. 2-Programa de Pós-graduação em Ciências Farmacêuticas, UFES, Av. Marechal Campos 1468, Vitória, ES, Brazil. 3- Marine Natural Products Lab, Molecular Research Center, UPR, San Juan, Puerto Rico.

Cancer is one of the main causes of mortality worldwide, with significant socioeconomic impact. Despite the advances obtained with conventional therapies, many types of neoplasms still demonstrate resistance, which reinforce the continuous need for new therapeutic approaches. In this scenario, marine organisms have stood out as relevant sources of promising bioactive secondary metabolites for the development of innovative antitumor agents. In this study, the cytotoxic activities of three cyanobacteria (*Phormidium laetevirens*, *Blennothrix lynghyaceae* and *Anabaena* sp), one sponge (*Dysidea avara*) and four macroalgae (*Ulva* sp., *Dichotomaria marginata*, *Laurencia dendroidea* and *Laurencia elata*) - that were collected in Gramutê Beach, Aracruz, Espírito Santo, Brazil and Bahía de Jobos, Salinas, Puerto Rico and identified by metagenome shotgun and metabarcoding - were analyzed against the three tumor cell lines with the highest incidence worldwide: lung carcinoma (A549), breast cancer (MCF7) and colorectal cancer (HCT116). This analysis was performed by MTT cell viability tests to measure the IC₅₀ (μl/mL) with two distinct cytotoxic standards: cisplatin (synthetic) (HCT116: IC₅₀=7.85; MCF7: IC₅₀=13.22; A549: IC₅₀=4.00) and quercetin (natural) (HCT116: IC₅₀=37.02; MCF7: IC₅₀=69.17; A549: IC₅₀=25.64) at 6 different concentrations for all samples. *Phormidium laetevirens*, *Blennothrix lynghyaceae*, *Ulva* sp. and *Dichotomaria marginata* demonstrated cell viability close to 100% at all concentrations tested. *Anabaena* sp. demonstrated cell viability close to 90% on MCF7 and A549 cell lines, however it demonstrated IC₅₀=49.14 on HCT116 cell line. *Dysidea avara* (HCT116: IC₅₀=40.39; MCF7: IC₅₀=41.88; A549: IC₅₀=34.18), *Laurencia dendroidea* (HCT116: IC₅₀=29.21; MCF7: IC₅₀=73.17; A549: IC₅₀=41.06) and *Laurencia elata* (HCT116: IC₅₀=30.30; MCF7: IC₅₀=60.97; A549: IC₅₀=33.24) demonstrated low cell viability in all tumor cell lines tested at a concentration of 100μl/mL, with *D. avara* being the sample with the highest cytotoxic potential when compared to the standards tested. Sponges and red algae have solid evidence of cytotoxic metabolic profile in literature, being a strategic and promising source, whose explored potential contributes to the development of new anticancer therapies.

Keywords: Cancer, marine organisms, secondary metabolites, cytotoxicity, anticancer therapies.





**IN VITRO ANTILEISHMANIAL ACTIVITY OF DICENTRINE FROM BRANCHES
OF *Ocotea langsdorffii* (LAURACEAE)**

Eduardo Oliveira S. da Silva^{1*}, Camila S. de Freitas², Daniela C. Tristão¹,
Guilherme M. Antar³, Elaine S. Coimbra⁴, João Henrique G. Lago¹, Eduardo A. F. Coelho²
eduardo.stelmo@ufabc.edu.br

¹Center of Natural Sciences and Humanities, Federal University of ABC, Santo Andre, SP.

²Faculty of Medicine, Federal University of Minas Gerais, Belo Horizonte, MG.

³Department of Biological Sciences, Federal University of Espirito Santo, São Matheus, ES

⁴Institute of Biological Sciences, Federal University of Juiz de Fora, Juiz de Fora, MG.

Leishmaniasis is a neglected tropical disease caused by protozoan parasites of the genus *Leishmania*. Current chemotherapeutic options, such as pentavalent antimonials, pentamidine, amphotericin B, and miltefosine, have several limitations including high toxicity. Continuing our studies on the discovery of new antileishmanial compounds from Brazilian plant biodiversity, this study evaluated the antileishmanial activity of alkaloid dicentrine from *Ocotea langsdorffii*, a chemically unknown lauraceous species. To this end, the branches of *O. langsdorffii* (250 g) were defatted with hexane and subject to chemically active extraction to afford an alkaloidal phase (113 mg). A portion of this material (100 mg) underwent CC over silica gel, yielding a fraction (55 mg), which was then purified by CC over silica gel, producing pure dicentrine (8.2 mg). Dicentrine exhibited antileishmanial activity against the promastigote forms of *L. infantum*, *L. amazonensis*, and *L. braziliensis*, with EC₅₀ values of 1.64, 0.95, and 0.86 µg/mL, respectively. This potency is similar to that of the positive control, AmpB. Cytotoxicity was evaluated against murine macrophages and afforded CC₅₀ values of 162.5 and 0.79 µg/mL for dicentrine and AmpB, respectively. The selectivity index (SI) of dicentrine against the tested parasites was determined to be 99.1, 171.7, and 188.3, respectively; the SIs for AmpB were 6.1, 3.2, and 4.0, respectively. When tested against intracellular amastigotes of *L. braziliensis*, dicentrine caused a concentration-dependent reduction in infection. At concentrations of 1, 2, and 4 µg/mL, dicentrine led to reductions in the degree of infection of 11.3%, 23.9%, and 26.3%, respectively. Additionally, the percentage of recovered amastigotes decreased by 74.2%, 81.1%, and 84.0%, respectively, after treatment. The mechanism of action revealed that dicentrine induces mitochondrial disruption and ROS accumulation in parasite promastigotes. Dicentrine also showed potential to reduce the percentages of infected macrophages and amastigotes against the three *Leishmania* species. These findings improve our understanding of the antileishmanial effects of dicentrine and support its potential as a promising candidate for the development of future drugs against leishmaniasis.

Keywords: *Ocotea langsdorffii*, alkaloids, dicentrine, leishmaniasis, *L. infantum*, *L. braziliensis*, *L. amazonensis*.





PROSPECTION OF PROTEASE INHIBITORS FROM VALE DO MUCURI PLANTS WITH IN VITRO ANTITUMOR ACTIVITY IN BREAST CANCER

Samira Charbaje Colen Ludgero¹, Gracimério José Guarneire¹, Sandra Bertelli Ribeiro Castro¹, Caio César Souza Alves¹, Alessandra Paula Carli¹, Laís Kelly Moraes de Souza Valverde², Maria Eugênia Hott Corrêa²

samira.ludgero@ufvjm.edu.br

¹Programa de Pós-Graduação em Ciências Biológicas, Universidade Federal dos Vales do Jequitinhonha e Mucuri (UFVJM), Teófilo Otoni, MG, Brazil. ²Faculdade de Medicina do Mucuri – FAMMUC- (UFVJM), Teófilo Otoni, MG, Brazil

Breast cancer is one of the leading causes of mortality among women in Brazil, reinforcing the need for new, more effective and selective therapeutic approaches. Plant compounds stand out as promising sources of bioactive molecules, including protease inhibitors, capable of modulating tumor processes related to invasion and metastasis. This study evaluated the cytotoxic potential of hydroethanolic extracts of Espinheira Santa (*Maytenus ilicifolia*) and Aveloz (*Euphorbia tirucalli*) in breast cancer cell lines. The plants were used as representative material in the study, with analysis focused on their main metabolites. Cytotoxicity was evaluated using MTT assays in cells (MCF-7, MDA-MB-231, and 4T1). The results indicated that the *M. ilicifolia* extract did not promote a reduction in MCF-7 (~18%) and 4T1 (~12%), with no relevant impact on MDA-MB-231. The *E. tirucalli* extract showed a cytotoxic effect on MDA-MB-231 (~14%) and 4T1 (~14%), although it was not consistently detrimental to MCF-7 predictions. The statistical tests used were Welch's t-test and Mann-Whitney U-test. The findings suggest that *M. ilicifolia* may be associated with hormone receptor-dependent mechanisms (as in MCF-7), while *E. tirucalli* did not demonstrate efficacy against the more detrimental strains (MDA-MB-231 and 4T1). These preliminary findings reinforce the importance of new results from studies involving fractionation and identification of active compounds, for validation. the therapeutic potential of these species.

Keywords: breast cancer; *Maytenus ilicifolia*; *Euphorbia tirucalli*; protease inhibitors; antitumor.





**DEREPLICATION OF ESSENTIAL OILS FROM *Nectandra paranaensis*
(LAURACEAE) WITH ANTI-*Trypanosoma cruzi* ACTIVITY**

Daniela da C. Tristão¹, Marina de M. Gonçalves¹, Giovanna T. Santos¹, Sarah L. Reis¹,
Vanessa Albuquerque², Roberto B. Almeida³, André G. Tempone², João Henrique G. Lago¹

marina.monroe@ufabc.edu.br

¹Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André, SP, Brazil;

²Laboratório de Fisiopatologia, Instituto Butantan, São Paulo, SP, Brazil.

³Instituto de Biociências, Universidade de São Paulo, SP, Brazil.

Neglected tropical diseases affect approximately one billion people worldwide. One such disease is Chagas disease, which is caused by *Trypanosoma cruzi* and has only two available treatments: benznidazole and nifurtimox. In this context, natural products are essential for identifying new bioactive compounds. This study reports the anti-*T. cruzi* evaluation and chemical dereplication of essential oils (EOs) from *Nectandra paranaensis* (Lauraceae), a previously uninvestigated species. Initially, leaves and twigs were extracted separately using a Clevenger-type apparatus to obtain their EOs. Dereplication using gas chromatography-mass spectrometry (GC-MS) analysis revealed 37 compounds in the leaves (90.5% of the total composition) and 34 compounds in the twigs (90.0% of the total). The composition of both is aligned with the genus description, with the majority of the compounds being oxygenated sesquiterpenes (46.5% in the leaves and 65.5% in the twigs), followed by hydrocarbon sesquiterpenes (42.2% in the leaves and 24.5% in the twigs). Guaiol was the main component detected in the leaf (11.1%) and in the twig (26.7%) oils. Other abundant compounds in the leaves were α -eudesmol (10.4%), δ -cadinene (9.4%), *E*-caryophyllene (5.7%), and spathulenol (4.3%), while the twigs were mainly composed of β -eudesmol (12.1%), *E*-caryophyllene (5.7%), bulnesol (5.0%), and spathulenol (4.3%). Additionally, hexane extracts were prepared from the leaves and twigs of *N. paranaensis* and showed a similar profile by NMR and TLC analysis. Therefore, the hexane extract from the twigs underwent chromatographic fractionation, yielding pure spathulenol (**1**), guaiol (**2**), β -eudesmol (**3**), and ylangenol (**4**). The EC₅₀ values of compounds **2**, **3**, and **4** against trypomastigotes of *T. cruzi* were determined to be 7.6, 21.5, and 11.6 μ M, respectively. These compounds exhibited reduced toxicity against NCTC cells (CC₅₀ > 200 μ M). Compared to the control benznidazole (EC₅₀ = 18.7 μ M and CC₅₀ > 200 μ M), compounds **2** and **4** exhibited potent activity. Similarly, 100% of parasite death occurred at 200 μ g/mL of both EOs, with no toxicity against NCTC cells (CC₅₀ > 200 μ g/mL), which suggests that the effect is due, at least in part, to the predominance of guaiol (**2**) in both oils.

Keywords: Chagas disease, volatile oils, sesquiterpenes, guaiol





EXPLORING THE ANTIOXIDANT AND PHENOLIC PROFILE OF *CISSUS GONGYLODES*: PERSPECTIVES FOR BIOACTIVE COMPOUNDS

Ana Maria da Silva Souza^{1*}, Gabriela Cristina Ferreira Mota¹, Lúcia Pinheiro Santos Pimenta¹.

*anamsilvasza@gmail.com

1-CerQBio, Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Cissus gongylodes (Baker) Planch is a liana belonging to the Vitaceae family, popularly known as "cipó-de-uvas", "uvas-do-mato", and "cura tudo". Its tea is traditionally used in treating renal diseases, such as kidney stones and pyelonephritis, in addition to being employed for its analgesic properties¹. Intending to identify new biological activities of *Cissus gongylodes* with therapeutic potential, this study evaluated the antioxidant activity of its stems and leaves, followed by quantification of phenolic compounds in each aerial part. Leaves and stems were extracted separately by decoction. 10 g of powdered material in 200 mL of water, yielding the aqueous extracts (CGGA and CGFA). The residual material of each infusion was then subjected to 80% hydroalcoholic extraction, yielding the ethanolic extracts (CGGE and CGFE). The antioxidant activity of the extracts was assessed by the DPPH• radical scavenging method (2,2-diphenyl-1-(2,4,6-trinitrophenyl)hydrazin-1-yl), with the highest activity determined for the leaf extracts. The ethanolic extract (CGFE) showed the most significant inhibitory potential ($IC_{50} = 2.79 \pm 0.92$ mg/mL), followed by the aqueous extract (CGFA, $IC_{50} = 3.42 \pm 1.19$ mg/mL). The stem extracts exhibited lower antioxidant activity, with the aqueous extract (CGGA) showing the weakest inhibitory potential, requiring higher concentrations to achieve radical inhibition ($IC_{50} = 9.52 \pm 0.82$ mg/mL). Extracts were further subjected to phenolic quantification using the Folin-Ciocalteu method. The ethanolic leaf extract (CGFE) presented the highest phenolic content, expressed as gallic acid equivalents (78.53 ± 0.81 mg GAE/g of sample), and the aqueous stem extract (CGGA) showed the lowest phenolic concentration (16.21 ± 0.70 mg GAE/g of sample). These results are consistent with its antioxidant activity, since phenolic compounds are widely reported in the literature as potent antioxidants². Based on these findings, further studies will focus on the metabolic profiling of the extracts by NMR and LC-MS to advance the understanding of this species.

Keywords: *Cissus gongylodes*, antioxidant activity, phenolic quantification.

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DETERMINATION OF ANTIFUNGAL ACTIVITY, MECHANISMS OF ACTION AND ANTIBIOFILM CAPACITY OF CRUDE HYDROALCOHOLIC EXTRACT AND FRACTIONS OF *MYRCIA NEOOBSCURA* LEAVES AGAINST *CANDIDA KRUSEI*.

Leticia Bachmann^{1*}, Eduarda R. Botelho², Patrícia H. Arrabal², Pâmela E. Munzlinger³, Larissa M. Krepsky⁴, Lucas F. Mariotto⁵, Michele D. Alberton¹, Tatiani K. R. Botelho¹.

¹Postgraduate Programme in Biodiversity, Universidade Regional de Blumenau – FURB; ²Centre of Health Sciences, Universidade Regional de Blumenau – FURB; ³Postgraduate Programme in Applied Chemistry, Universidade do Estado de Santa Catarina – UDESC; ⁴Postgraduate Programme in Pharmaceutical Sciences, Universidade do Vale do Itajaí – UNIVALI, Itajaí, SC, Brazil; ⁵Department of Natural Sciences, Universidade Regional de Blumenau – FURB. *letbachmann@furb.br

Infections caused by yeasts of the genus *Candida* are responsible for high morbidity and mortality rates. *Candida krusei* has intrinsic resistance to fluconazole and can quickly acquire resistance to other antifungals. Biofilm formation is one of the main virulence factors of the genus, decreasing susceptibility to antifungals and being associated with increased mortality. With the scarcity of therapeutic options and the increase in resistance to antifungal drugs, new treatment options are needed. Natural products are an important source of resources for obtaining bioactives and developing drugs for various diseases. *Myrcia neoobscura* is an endemic plant of the Atlantic Rainforest, belonging to the genus *Myrcia*, several of whose species have demonstrated important antifungal activities. The objective was to evaluate the antifungal activity of the crude hydroalcoholic extract and ethyl acetate, aqueous, insoluble, hexane and dichloromethane fractions of *M. neoobscura* leaves against *C. krusei*, determine the mechanisms of action, evaluate the biofilm formation capacity of *C. krusei* and the antibiofilm action of *M. neoobscura*. Determination of antifungal activity was carried out with a clinical strain of *C. krusei* using the broth microdilution methodology and tested against the extract and fractions of *M. neoobscura* leaves. With these results obtained the mechanisms of action, the biofilm-forming capacity and the antibiofilm activity of *M. neoobscura* were determined. All *M. neoobscura* samples tested showed strong antifungal activity against *C. krusei*, especially the aqueous fraction with MIC of 7.81 µg/mL. Analysing the mechanisms of action, it is suggested that *M. neoobscura* may act simultaneously on the fungal membrane and cell wall. Regarding the biofilm formation, *C. krusei* showed moderate biofilm formation. The extract and all fractions of *M. neoobscura* at MIC and MICx2 concentrations showed antibiofilm capacity against *C. krusei* mature biofilm, with a significant difference ($p < 0.01$) in relation to the negative control and no significant difference between different concentrations. *M. neoobscura* showed activities with strong potential for antifungal and antibiofilm use against *C. krusei*. Also, two possible different modes of actions were found. These results can be explained by the abundant presence of phenolic compounds, such as flavonoids and flavonols, in *M. neoobscura* leaves.

Keywords: *Candida*, biofilm, *Myrcia neoobscura*, bioprospecting, antifungal





IN SILICO STUDY OF SILYMARIN COMPOUNDS AGAINST *Helicobacter pylori* VIRULENCE FACTORS

Vitor Zorzal Majeski^{1*}, Pedro Henrique Tregnago¹, Dalila Nickel Loose¹, Amanda Cavalcante Gonzaga Nunes¹, Lorena Carnielli Queiroz¹, Rodrigo Rezende Kitagawa¹, Rita de Cassia Ribeiro Gonçalves¹

vitorzmajeski@hotmail.com

1- Graduate Program of Pharmaceutical Sciences, Federal University of Espirito Santo, Av. Mal. Campos, 1468, Maruípe, Vitoria 29047-105, Espirito Santo, Brazil.

Helicobacter pylori is a bacteria capable of colonizing the human stomach, which makes it the greatest risk factor for stomach cancer development. The drugs used in its treatment, like clarithromycin, have already shown resistance, showing the need for the development of new drugs against this infection. Silymarin, which is a complex of flavonolignans extracted from the plant *Silybum marianum* (L.) Gaertn., is traditionally and safely used to treat liver diseases and has already shown anti-*H. pylori* activity in previous *in vitro* assays. This study aimed to evaluate the potential of the main silymarin compounds (silybinin A and B, isosilybinin A and B, silychristin, isosilychristin, taxifolin and silydianin) of inhibiting virulence factors of *H. pylori* and their drug-likeness properties through *in silico* techniques. The platforms SwissADME and ADMETlab 3.0 servers were used to analyse the physicochemical, pharmacokinetics and druglikeness profile. The results demonstrated that the compounds exhibit values for LogP ranging from 0,85 to 1,85, LogS ranging from -4,45 to -3,33. All compounds were approved in the Lipinski rule. The molecular docking was executed with GOLD software with the protein targets BabA (PDB: 4ZH7), CagA (PDB: 4IRV) and VacA (PDB: 2QV3), and it was detected that most of the compounds are able to establish interactions the essential aminoacids CYS189, GLY191 and SER244 of BabA (with the best fitness score 57,7528 for isosilybinin A), with the essential aminoacids VAL107, PHE219 and TRP212 of CagA (with the best fitness score 63,0801 for silychristin), and with the aminoacids VAL266 and ASN289 of VacA (with the best fitness score 54,5783 for isosilybinin B). Therefore, it is possible to conclude that the silymarin compounds possess good drug-likeness profile and are capable to establish positive molecular interactions with the tested proteins, and therefore, are suitable enter experimental essays with the possibility of representing a new frontier against *H. pylori* and the consequential reduction of the risk of stomach cancer development in the future. The authors thank the support from UFES and FAPES.

Keywords: *Helicobacter pylori*; virulence factors; natural compounds, silymarin; in-silico techniques.





INHIBITORY POTENTIAL OF ETHANOLIC EXTRACT AND THE FLOWER FRACTIONS OF *Couroupita guianensis* AGAINST TARGET ENZYMES OF *Leishmania donovani*

Edgar J. Laice, Beatriz M. Silva, Bruno C. B. Marques, Douglas G. dos Santos, Luzineide W. Tinoco

[*edyllaice01@gmail.com](mailto:edyllaice01@gmail.com), lwtinoco@ippn.ufrj.br

Laboratório de Análise e Desenvolvimento de Inibidores Enzimáticos – Instituto de Pesquisa de Produtos Naturais – Universidade Federal do Rio de Janeiro - 21491 599, Brazil.

Plant-derived secondary metabolites play an important role in drug discovery due to their structural diversity and affinity for biological targets. Leishmaniasis, caused by parasites of the genus *Leishmania*, is a neglected tropical disease with therapeutic options increasingly limited by drug resistance, highlighting the urgency of identifying novel molecular targets. Among them, the nucleoside hydrolase (*LdNH*) and ornithine decarboxylase (*LdODC*) enzymes of *L. donovani* stand out as promising candidates, since *LdNH* is absent in mammals and *LdODC* shows significant structural differences from the human ODC, while both perform essential functions in parasite metabolism. This study aimed to identify inhibitors of *LdNH* and *LdODC* from flower extracts of *Couroupita guianensis*. Native to the Amazon region, this species is traditionally used for the treatment of inflammation, pain, and skin infections. From 340 g of dried flowers, ultrasound-assisted extraction with 70% ethanol was conducted, yielding 3.8%. The extract was fractionated in a Biotage C18 reversed-phase column (25 g, Isolera One system), generating 45 fractions that were grouped according to chemical similarity. The fractions were analysed by ¹H NMR (500 MHz) and tested for inhibition of *LdNH* and *LdODC*. Fractions showing inhibition greater than 50% were considered active. For *LdNH*, active fractions included F5B, F8B, and F9B. For *LdODC*, the active fractions were F2B, F3B, F4B, F5B, F6B, 13B, and F14B. The F5B fraction was notable for showing significant inhibition in both assays. Its ¹H NMR spectrum exhibited signals at 7.0–7.5 ppm (aromatic/heteroaromatic hydrogens), 3.2–3.8 ppm (hydrogens bound to electronegative atoms), and 0.8–1.2 ppm (methyl and methylene groups). These characteristics suggest the presence of flavonoids, substituted phenols, glycosides, or alkaloids. In conclusion, *C. guianensis* flower fractions demonstrated inhibitory potential against enzymes essential for *L. donovani*. The F5B fraction, active against both *LdNH* and *LdODC*, will undergo LC-MS and 2D NMR analyses for structural elucidation of its active metabolites.

Keywords: nucleoside hydrolase, ornithine decarboxylase, secondary metabolites.





**ANTIMICROBIAL AND ANTIBIOTIC SYNERGISTIC EVALUATION OF
PORPHYRIDIDIUM PURPUREUM CHLOROFORMIC EXTRACT**

Rodolfo Moreira Baptista^{1*}, Natália Popiurek dos Santos²; Bruno Galler Kubelka³, Marcelo Gonçalves Montes D'oca⁴, Daniela Fernandes Ramos²

rodolfombaptista@outlook.com

1- Departamento de Farmácia e Nutrição, Centro de Ciências Exatas, Naturais e da Saúde, UFES, Alto Universitário, S/N - Guararema, Alegre, ES, Brazil. 2-NUDEFA, Faculdade de Medicina, FURG, R. Gen. Osório, S/N - Centro, Rio Grande, RS, Brazil. 3-AlgaSul Biotecnologia de Microalgas, Av. Itália, s/n - km 08, Carreiros, Rio Grande, Brazil. 4- Laboratório Kolbe de Síntese Orgânica, Departamento de Química, UFPR, Av. Cel. Francisco H. dos Santos, 100 - Jardim das Américas, Curitiba, PR, Brasil

Until 2050, is estimated that bacterial resistance will cause 39 million deaths worldwide. Therefore, natural compounds have been investigated as alternatives that work synergistically with antibiotics. *Porphyridium purpureum* is a microalgae known as a potential source of bioactive metabolites, such as fatty acids, with antimicrobial properties. These compounds destabilize the bacterial membrane, favoring the action of antibiotics. Therefore, this study aims to characterize the lipid profile of the chloroform extract of *P. purpureum* and evaluate its antimicrobial activity against gut pathogens. The biomass was obtained in a 15 L photobioreactor with F/2 medium and light irradiance at 450 nm. After 9 days, the biomass was lyophilized and subjected to extraction with chloroform (1:6 g/mL) by percolation. The extract was rotary evaporated and resuspended in 50% DMSO (40 mg/mL). Chemical analysis was performed using Gas Chromatography-Mass Spectrometry (GC-MS), and the samples were identified by the NIST 2020 library. The antimicrobial activity was performed by broth microdilution method to determine the Minimum Inhibitory Concentration (MIC) against *Escherichia coli* (ATCC 25922) and *Salmonella enterica* Typhimurium (ATCC 14028). The activity evaluation was made with the extract isolated (800–6.25 µg/mL) and combined with ciprofloxacin (32–0.25 µg/mL). Therefore, the Fractional Inhibitory Concentration Index (FICI) was determined, where FICI ≤ 0.5 suggests a synergistic effect. GC-MS analyses allowed the identification of the following major compounds: palmitic acid (42.05%), arachidonic acid (22.73%), linoleic acid (17.91%), eicosapentaenoic acid (8.64%), oleic acid (4.35%), linolenic acid (2.30%) and stearic acid (2.02%). Did not show antimicrobial activity in the concentrations tested, but, when the extract, at 6.25 µg/mL, were combined with ciprofloxacin, it was observed bacterial growth inhibition. Thereby, the MIC against *S. typhimurium* was reduced from 4 to 1 µg/mL (FICI = 0.25) and *E. coli* from 4 to 2 µg/mL (FICI = 0.50). These results suggest synergism between *P. purpureum* chloroformic extract and ciprofloxacin, which can be a strong tool against infections caused by bacterial, especially against gut pathogens.

Keywords: fatty acids, antibacterial activity, microalgae, natural products, marine.



Pombalia atropurpurea as a source of cyclotides with larvicidal activity

Ana Letícia P. Santos (Post-Doc)¹, Meri Emili F. Pinto (Post-Doc)¹, Suzana A. S. Queiroz (PhD)¹, Juliana P. Souza (Professor)², Lorena Carneiro Albernaz (Post-Doc)³, Laila Salmen Espindola (Professor)³ and Vanderlan Bolzani (Professor)¹.

alp.santos@unesp.br

¹Institute of Chemistry, São Paulo State University-UNESP-IQ, Araraquara, SP, Brazil, ²Department of Biological Sciences, Federal University of Santa Catarina-UFSC, Santa Catarina, SC, Brazil, ³ Faculty of Health Sciences/Medicine, University of Brasília-UnB, Brasília, DF, Brazil.

Cyclotides are disulfide-rich mini proteins found in some plant families: Violaceae, Rubiaceae, Fabaceae, Solanaceae and Poaceae.¹ They have a distinct circular backbone with 28-37 amino acid residues, a head-to-tail cyclization, and a knotted arrangement of three conserved disulfide bonds named CCK (Cyclic Cystine Knot). Currently, around 720 cyclotides have been discovered, according to Cybase: a database of cyclic protein sequences and structures.² These stable structures are resistant to proteolytic degradation¹ and are involved in plant defense. A wide range of biological activities and/or therapeutic applications have been reported for these peptides, including insecticidal, nematocidal, molluscicidal, antimicrobial, anti-HIV, and antitumor activities.³ Aiming to contribute even more in the area of cyclotides, our research group is dedicated to studying this class of natural products present in plants. Cyclotides from stems of *Pombalia atropurpurea*, Violaceae family, were extracted, defatted, and lyophilized, resulting in the crude extract, which was submitted to SPE-C18 cartridges and eluted with a mixture of 20%, 40%, 60%, 80%, and 100% buffer B (100% CH₃CN, 0.1% CF₃COOH) in A (H₂O, 0.1% CF₃COOH). The 40%, 60%, and 80% fractions, considered rich in cyclotides, were tested with *Aedes aegypti* larvae, resulting in 87%, 53%, and 100% larval mortality within 72 h, respectively. From the 40% fraction, four peptides were isolated, and three of them showed excellent larvicidal potential in 72 h. From the 60% fraction, three cyclotides were isolated, but only one exhibited larvicidal activity in 48 h. Five cyclotides were extracted from the stems, and three of them are new in the literature.

Keywords: Circular miniproteins, cyclotides, cyclic peptides, *Pombalia atropurpurea*, Violaceae.

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***IN SILICO AND IN VIVO ANTIOXIDANT ACTIVITY OF CAFESTOL AND ITS
p-METHOXYBENZOATE DERIVATIVE***

**Yasmin Oliveira de Santana^{1*}, Maria Alice Esteves¹, Daniela Dias² Elis Eleuthério²,
Claudia Rezende¹**

yasmin41oliveira@gmail.com; claudia.rezendeufri@gmail.com

1 Departamento de Química orgânica UFRJ, Rio de Janeiro, RJ, Brazil. 2- Departamento de Bioquímica, Instituto de Química, UFRJ, Rio de Janeiro, RJ, Brazil.

Cafestol is an *ent*-kaurane diterpene alcohol found in coffee beans (*Coffea arabica* L. and *C. canephora* P., Rubiaceae) that exhibits antioxidant activity through modulation of the Nrf2/Keap1 pathway, which protects against oxidative stress, a process implicated in diseases such as cancer, atherosclerosis, and Alzheimer.^[1] This study aimed to evaluate the antioxidant activity of cafestol and a novel 4-methoxybenzoate derivative (**1**) using *in silico* and *in vivo* approaches, with *Saccharomyces cerevisiae* as a model organism. Molecular docking was conducted in AutoDock 1.5.7 using Keap1 (PDB ID: 1U6D), cafestol (PubChem CID: 108052) and **1**, designed in Spartan. Derivative **1** was synthesized by esterification of cafestol with 4-methoxybenzoic acid, DMAP, and EDC·HCl (24 h, 40 °C), characterized by 1D and 2D ¹H and ¹³C NMR, as also its melting point. For viability assays, *S. cerevisiae* strain BY4741 was treated with cafestol or compound **1** (20 μM), incubated at 28 °C for 1 h with shaking at 180 rpm, and subsequently exposed to 1 mM H₂O₂. Colonies were counted after 5 days. Data were analyzed by one-way ANOVA followed by Tukey's test. Docking analyses revealed binding energies of −14.04 kcal/mol for the compound **1** and −11.02 kcal/mol for cafestol, suggesting a stronger interaction between **1** with Keap1, which can be correlated with its higher antioxidant potential. In cell viability assays, neither cafestol nor **1** showed cytotoxicity, with survival rates above 90% in non-stressed cells. Under oxidative stress conditions, cell viability was 48% for cafestol and 61% for compound **1**.

In conclusion, the structural modification of cafestol as 4-methoxybenzoate derivative (**1**) gave a good reaction yield 60% which led to an increase in antioxidant activity, as demonstrated by both computational and biological assays.

Keywords: *Coffee, Saccharomyces cerevisiae, Oxidative stress, Antioxidant activity, Molecular docking*





OPTIMIZATION OF MORUS NIGRA L. LEAF EXTRACT FOR TYROSINASE INHIBITION: INFLUENCE OF ETHANOL CONCENTRATION, TIME, AND EXTRACTION METHOD

Maria Beatriz Macedo Gonçalves^{1*}, Samuel Leite Cardoso¹, Patrícia Marques Rodrigues¹, Damaris Silveira¹, Yris M. Fonseca Bazzo¹, Pérola Oliveira Magalhães¹

maria.beatriz01@gmail.com

1- Laboratory of Natural Products, Health Science School, University of Brasilia, Brazil

Morus nigra L., also popularly known as black mulberry, exhibits various therapeutic effects that have been demonstrated in studies, such as anti-inflammatory and antihyperlipidemic actions, and most notably, its potential depigmenting effect through the inhibition of L-tyrosinase, an enzyme that catalyzes melanin synthesis. Due to their significant potential, including therapeutic applications, industries are increasingly using plant extracts to obtain components capable of assisting various sectors, from the food industry to pharmaceuticals. Therefore, optimizing the extraction process is necessary to reduce resource consumption, such as time and money. Given these contexts, the present study aimed to optimize the process of obtaining the hydroethanolic extract from *Morus nigra* L. leaves by varying ethanol concentration, extraction time, and method. These variables were tested through enzymatic assays for L-tyrosinase inhibition and compared with a positive standard, followed by high-performance liquid chromatography (HPLC) analysis to evaluate the compounds extracted in each sample. This study allowed us to infer that the isolated flavonoids, isoquercetin and chlorogenic acid, do not directly inhibit the enzyme. However, reducing the ethanol concentration in the extract may be a viable approach to optimize and replace the standard extract while also saving resources. Another important factor is the extraction time, as extracts obtained in 2 hours through active maceration showed high IC₅₀ values compared to the others.

Keywords: *Morus nigra* L.; extraction optimization; L-tyrosinase; inhibition; hydroethanolic extract;





ACTINOBACTERIA FROM *TETRAGONISCA ANGUSTULA* MICROBIOME: A PROMISING SOURCE OF ANTIMICROBIAL COMPOUNDS.

Gabriel de Deus Correia^{1*}, Rafael Gonçalves Padilha ¹, Rodolfo Bizarria Júnior ¹, Fábio Santos do Nascimento ², Mônica Tallarico Pupo ¹.

gabriel.deusc@usp.br

1-Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Avenida do Café s/n, Ribeirão Preto, SP, 14040-903 Brazil 2- Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto, Universidade de São Paulo, Avenida do Café s/n, Ribeirão Preto, SP, 14040-901 Brazil.

With the spotlight on growing antimicrobial resistance (AMR), research on natural products discovery from microorganisms represents a rich source of novel bioactive metabolites. In this context, social insects such as *Tetragonisca angustula* and their microbiomes emerge as a promising model for study, since stingless bees (tribe Meliponini, Hymenoptera) may establish symbiotic interactions with microorganisms that play important roles in the hive. In this study, actinobacteria isolated from *T. angustula* bees obtained from colonies maintained in the meliponary of the Department of Biology, Faculty of Philosophy, Sciences, and Letters on the Ribeirão Preto campus, University of São Paulo were tested in antagonism assays using the overlay soft agar method against several pathogens to evaluate their bioactive profiles. The isolates exhibited activity against *S. aureus* ATCC 3538, *C. albicans* ATCC 10231, *P. larvae* ATCC 9545 and *Beauveria bassiana*. Extracts from the most promising strains were obtained from both solid and liquid cultures and tested against the same pathogens in 10 mg/mL concentration. Several extracts revealed inhibitory potential and for each active strain, one extract was selected based on bioactivity and chemical profile obtained by HPLC-DAD-ELSD analysis. The selected extracts were fractionated through solid-phase extraction (SPE) using MeOH/H₂O, and both chemical profile and bioactivity of the fractions were evaluated. Fractions with promising activity are currently undergoing further bioassays and HPLC-MS/MS analysis. The results demonstrate that the microbiome of *T. angustula*, particularly the isolated actinobacterial strains, represents a promising source of bioactive compounds with antimicrobial activity. The 16S rRNA genes from the active strains were amplified and sequenced for identification and phylogenetic analysis. Among the 24 strains isolated, 39% exhibited inhibition activity against human and entomopathogenic pathogens, with the genus *Streptomyces* being most frequently associated with bioactivity. These findings suggest that actinobacteria, specially from *Streptomyces* genus, may play a defensive role in the hive, producing specialized metabolites against entomopathogens in the beehive.

Keywords: Stingless bees, actinobacteria, microbiome, bioactive metabolites.





**ISOLATION AND CYTOTOXICITY ASSESSMENT OF FLAVONE C-GLYCOSIDES
EXTRACTED FROM CORN STIGMAS (*Zea mays* L.)**

Leonardo Gomes Costa^{1*}, Omar Enrique Estrada Semprún², Josana de Castro Peixoto¹,
Leonardo Luiz Borges¹, Fernando Gomes Barbosa¹, Marco Aurélio Batista¹, Anielly
Monteiro de Melo¹, Cristiane Maria Ascari Morgado³, André José de Campos³, Cátia Lira do
Amaral⁴, Joelma Abadia Marciano de Paula¹

leonardogomescostaifg@gmail.com

1-PD&I Bio, Laboratório de Pesquisa, Desenvolvimento e Inovação de Produtos da Biodiversidade,
Universidade Estadual de Goiás, UEG, BR 153, n 3105, Anápolis, GO, Brazil. 2-LaProNat,
Departamento de Farmácia, FAR, UnB, Campus Universitário Darcy Ribeiro. Asa Norte, Brasília –
DF, Brazil. 3-LabPOS, Laboratório de Pós-Colheita, Universidade Estadual de Goiás, UEG, BR-153,
n. 3105, Anápolis, GO, Brazil. 4-LAB Epitox, Laboratório de Epigenética e Toxicologia,
Universidade Estadual de Goiás, UEG, BR 153, n 3105, Anápolis, GO, Brazil.

The recovery of agro-industrial waste is essential for the circular economy, supporting sustainable development and waste reduction. Corn stigmas (*Zea mays* L.), often discarded, are used in traditional medicine for their diuretic properties, and studies show that they are a promising source of flavonoids. This study aimed at the isolation and structural elucidation of corn stigma C-glycosides flavones and the evaluation of cytotoxicity in human lymphocytes. Corn stigmas were collected from establishments that sell corn-based foods in Anápolis, GO, Brazil (seeds Agrocere 1051 - SISGEM: A913311). The plant material was dried, ground, and then processed to isolate C-glycoside flavones, as described in patent BR1020240269403. The structural identification of the compounds was performed by one-dimensional and two-dimensional NMR ¹H and ¹³C. The isolated compounds were tested for cytotoxicity in human lymphocyte by tripan blue exclusion assay (CAAE: 66860023.1.0000.8113), using primary cells isolated from healthy donors. The main flavones isolated and identified were maysin (2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-[4-hydroxy-6-methyl-5-oxo-3-(3,4,5-trihydroxy-6-methyloxan-2-yl)oxyoxan-2-yl]chromen-4-one) and apimaysin (2,6-Anhydro-1-deoxy-5-O-(6-deoxy-α-L-mannopyranosyl)-6-C-(5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-1-benzopyran-6-yl)-xylo-3-hexulose). After three hours of treatment, maysin and apimaysin showed cell viability above 90% across all tested concentrations (110-2100 µg/mL). These results suggest low cytotoxicity of the main flavones found in corn stigma. Additional studies are needed to verify safety for pharmacological or nutraceutical applications.

Keywords: Circular economy, maysin, apimaysin, cytotoxicity, *Zea mays*.





**MARINOLIDE A, A NEW GERMACRANOLIDE FROM *Mikania nummularia*,
DISPLAYS *in vivo* ANTISCHISTOSOMAL ACTIVITY**

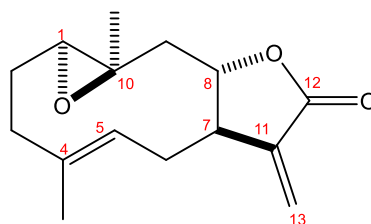
Marina de M. Gonçalves^{1*}, Leonardo M. Carneiro¹, Roberto Baptista P. Almeida²,
Thainá R. Teixeira³, Monique C. Amaro³, Josué de Moraes³, João Henrique G. Lago¹

marina.monroe@ufabc.edu.br

1-Center for Human and Natural Sciences, Federal University of ABC, Santo André, SP, Brazil. 2-Department of Botany, University of São Paulo, São Paulo, SP, Brazil. 3-Research Center for Neglected Diseases, University of Guarulhos, Guarulhos, SP, Brazil.

In the search for new drug prototypes against schistosomiasis, the hexane extract from the aerial parts of *Mikania nummularia* DC (Asteraceae) showed 100% mortality of *Schistosoma mansoni* at 200 µg/mL. Chromatographic fractionation afforded one pure compound whose structure was elucidated using NMR, ESI-HRMS and ECD analysis. The ¹H NMR spectrum revealed signals of exocyclic methylene hydrogens at δ 6.23 (d, *J* = 2.8 Hz, H-13a) and 5.63 (d, *J* = 2.8 Hz, H-13b), carbinol hydrogens at δ 4.40 (m, H-8) and 2.76 (dd, *J* = 10.6 and 2.6 Hz, H-1) and vinyl hydrogen at δ 5.32 (t, *J* = 7.7 Hz, H-5). The ¹³C NMR spectrum showed 15 signals including an α,β-unsaturated carbonyl system at δ 169.2 (C-12), 138.7 (C-11) and 122.7 (C-13), an endocyclic double bond at δ 137.1 (C-4) and 122.5 (C-5), as well as carbinol carbons at δ 79.3 (C-8), 61.6 (C-1) and 57.0 (C-10). The ESI-HRMS spectrum showed the [M + Na]⁺ ion at *m/z* 271.1318 (error = 2.9 ppm) and the [2M + Na]⁺ ion at *m/z* 519.2726 (error = 0.8 ppm), confirming the molecular formula as C₁₅H₂₀O₃, with six unsaturation. Based on these data and in the correlations observed in the HMBC spectrum, the structure of this compound was proposed as 1,10-epoxy-germacra-4,11(13)-dien-12,8-olide, named marinolide A. Finally, analysis of NOESY correlations and ECD data, the absolute configuration 1*S*,7*R*,8*S*,10*R* was proposed to this non-previously reported sesquiterpene lactone. For *in vivo* evaluation, *S. mansoni*-infected mice were treated with a single oral dose of 400 mg/kg of marinolide A on 49th day post-infection. On day 63th, the analysis revealed a 47% reduction in total worm burden compared to untreated controls, with no significant difference between male and female worms, and with reduced toxicity. These findings suggest that marinolide A, may serve as a promising scaffold for future structural optimization and development of new schistosomicidal agents.

Figure 1: Marinolide A, a new germacranolide isolated from *M. nummularia*



Keywords: *Schistosoma mansoni*, germacranolide, *Mikania nummularia*





ISOLATION AND CHARACTERIZATION OF BIOACTIVE PEPTIDES FROM THE MARINE ACTINOBACTERIA *Streptomyces* sp. BRA-214

Yann Florencio Lin^{1*}, Patricia Sartorelli², Paula Christine Jimenez¹

yann.lin@unifesp.br

1-BioprosSP, Instituto do Mar, UNIFESP, R. Carvalho de Mendonça, 144, Santos, SP, Brazil.

2-LaBiORG, Instituto de Ciências Ambientais, Química e Farmacêuticas, UNIFESP, R. Prof. Artur Riedel, 275, Eldorado, Diadema, SP, Brazil.

The marine ecosystem offers an extensive diversity of bioactive natural products. Algae, invertebrates and marine microorganisms are sources of specialized metabolites that act on multiple molecular targets. Preliminary studies from our group identified that the marine actinobacteria *Streptomyces* sp. BRA-214, recovered from sediments collected at the St. Peter and St. Paul Archipelago, produced peptides that interact with survivin, an apoptosis inhibitor protein and a relevant anticancer target. In this context, this study aimed at the isolation and structural characterization of peptides obtained from strain BRA-214. Initially, a screening comprising the cultivation of the bacteria in four distinct liquid culture mediums was carried out to identify improved conditions for production of the metabolites of interest. The extracts from each medium were obtained in ethyl acetate and evaluated by thin-layer chromatography (TLC) and cytotoxicity against HCT-116 cells. The extracts obtained in A1 (1% starch, 0.4% yeast extract and 0.2% peptone in reconstituted sea water) and ISP2 cultures were the most interesting concerning biological activity and chemical diversity, thus the strain was cultivated in large scale (5L) in the selected medium (A1). The extract was fractionated in Sephadex LH-20 column chromatography, yielding 45 fractions, which were analysed and pooled by similarity based on TLC. The fractions were interpreted in terms of metabolites intensity present in HPLC and some peaks based on previous results were selected for partial purification and initial characterization in ¹H NMR. Enriched fractions and purified compounds were interpreted in UHPLC-ESI-HRMS-MS and their respective mass spectra were compared with previous data and searched in Norine/GNPS databases. Four peptides were annotated and one of them, a major component from a peptide enriched fraction with *m/z* 704, was isolated and elucidated for its chemical structure, suggesting that it is an unprecedented compound. The identification and isolation of the peptides will allow further studies to advance beyond the affinity of these molecules with survivin, and reinforce the importance of addressing underexplored locations in search of new natural products with pharmacological relevance.

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Keywords: Marine natural products, peptide prospecting, chemical characterization, anticancer activity, biotechnology.





ANTITUMOR POTENCIAL OF PROPOLIS EXTRACT FROM *DUCKEOLA GHILIANII* AND *FRIESEOMELITTA LONGIPES*: AMAZONIAN STINGLESS BEES

Távila Tatiane Amorim Cavalcante^{1*}, Ana Lígia Leandrini de Oliveira², Jorge Luís Santos Silva¹, Carla Larissa de Souza Monteiro², Ítalo Hugo Maciel Pimentel¹, Patrícia Rayná Simas¹, Jerusa Araújo Quintão Arantes Faria¹

taviamorimcavalcante@gmail.com

1-Programa de Pós-graduação em Imunologia Básica e Aplicada -Instituto de Ciências Biológicas – ICB, Universidade Federal do Amazonas (UFAM), Av.Gen.Rodrigo Octávio Jordão Ramos, 3000 - Coroado I, Campus Universitário - Senador Arthur Virgílio Filho - Setor Sul, Bloco G, CEP: 69077-000, Manaus-AM. 2- Instituto de Ciências Farmacêuticas, UFAM.

Propolis from *Apis mellifera* has been widely studied for its cytotoxic, antitumor, pro-apoptotic, and potential anti-mutagenic activities, but the biological potential of propolis from *Duckeola ghilianii* and *Frieseomelitta longipes* remains scarcely explored. Thus, this study aimed to evaluate the antitumor activity of propolis extracts from *Duckeola ghilianii* (DGPE) and *Frieseomelitta longipes* (FLPE). In vitro assays were performed to evaluate the effects of these propolis extracts on A549 cell viability, colony formation and migration profile. Cells were treated with DGPE, FLPE and paclitaxel (PTX) at their maximum non-cytotoxic concentrations, both alone and in combination, for 48 hours and their cell viability was determined using the resazurin assay. Clonogenic assays were performed by plating 100 cells per well in a 12-well plate. Cells were treated with a sub-cytotoxicity dose of DGPE or FLPE (7,5 and 15µg/mL) and PTX (0.05mM), which was used as positive control. After 10 days of culture, cells were stained with 1% crystal violet solution. Cells migration was assessed by wound healing assay and a transwell chamber (8 µm), with epidermal growth factor EGF (30ng/mL) as a positive control. Our results showed a reduction in viability in the group treated with DGPE and PTX, demonstrating a synergism of PTX with DGPE but not with FLPE. Cells treated with DGPE significantly reduced colony formation compared to the control. In contrast, FLPE showed a significant increase in the number of colonies, suggesting a possible activation of epithelial-mesenchymal transition (EMT). In the wound healing experiment, both propolis extracts showed a reduction in cell migration compared to the control. However, in the transwell chamber assay, DGPE-treated cells showed a migration rate similar to the control, while FLPE revealed an increase in migrated cells, reinforcing the hypothesis of EMT induction at low and non-cytotoxic concentrations. The findings indicate that even at a sub-cytotoxic dosage, DGPE has promising antitumor potential, while FLPE can modulate mechanisms related to EMT. Thus, there is a clear need for further studies on the antineoplastic effects of this natural product, especially considering its modulation of the tumor microenvironment, projecting as a promising natural product of oncological interest.

Keywords: propolis; stingless bees; *Duckeola ghilianii*; *Frieseomelitta longipes*; cancer.



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EVALUATION OF THE NITRIC OXIDE PRODUCTION IN MACROPHAGES TREATED WITH *Anthaenania lanata* EXTRACTS

Franciane Pereira Brant^{1*}, Benedicto Soares Neto², Maria Clara Lima Senra de Oliveira²,
Fernando Staub Medaglia², João Luccas de Oliveira Martins², Olívia Rosa Fernandes²,
Sandra Bertelli Ribeiro Castro¹, Caio César de Souza Alves¹

franciane.brant@ufvjm.edu.br

1- Programa de Pós-graduação em Ciências da Saúde, Universidade Federal dos Vales do Jequitinhonha e Mucuri (UFVJM), Diamantina, Minas Gerais, Brasil, CEP 39100-000. 2- Faculdade de Medicina do Mucuri (FAMMUC), Universidade Federal dos Vales do Jequitinhonha e Mucuri (UFVJM), Teófilo Otoni, Minas Gerais, Brasil, CEP 39100-000.

Anthaenania lanata, capim-açu, is a grass from the Poaceae family with a wide distribution in Latin America, especially in Brazil. Traditional populations in the Mucuri Valley and the North of Minas Gerais report its use in treating respiratory illness. Excess nitric oxide (NO) can amplify inflammatory processes, aggravating immune disorders, and studies have shown that NO can influence the prevalence, pathogenesis, and progression of asthma. Objective: To evaluate the action of the aqueous and the ethanolic extracts of *A. lanata* on the NO production. Materials and Methods: The aerial parts of *A. lanata* were obtained at two different times, late summer and winter, recorded in SisGen (A6A292B), and aqueous and ethanolic extraction of their compounds was performed. J774A.1 macrophages (2×10^5 cells.mL⁻¹) were cultured in supplemented RPMI-1640 medium, stimulated or not with LPS (1 µg.mL⁻¹) and IFN-γ (0.9 ng.mL⁻¹) and treated with aqueous or ethanolic extracts at concentrations of 333, 100, 33 and 10 µg.mL⁻¹. The MTT test was carried out to assess viability in unstimulated cells. NO production was assessed by the Griess method in the supernatant of stimulated cells. Results: The aqueous extract had a lower effect on NO reduction and showed greater cytotoxicity when collected in late summer. The ethanolic extracts reduced the NO production (late winter 2.27 ± 0.91 , 3.68 ± 0.75 , 3.70 ± 0.72 , late summer 2.11 ± 0.35 , 2.27 ± 0.35 , 2.30 ± 0.37 vs. 5.66 ± 0.67 (stimulated not-treated cells)) at higher concentrations (333, 100, and 33 µg.mL⁻¹), with lower cytotoxicity, especially when collected in late summer. Conclusion: The ethanolic extract of *A. lanata* from late summer effectively reduced NO production without altering viability. Further studies should be carried out to evaluate its potential use for treating inflammatory disorders such as asthma.

Keywords: *Anthaenania lanata*, ethanolic extract, inflammation.

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CYTOTOXIC THIAZOLE-PRODUCING *Myxococcus* sp. BRX-014 ISOLATED FROM A BRAZILIAN MANGROVE

Renan da Silva de Oliveira^{1*}, Luís Guilherme Pereira Feitosa², Elthon Gois Ferreira³, Anna Caroline Campos Aguiar⁴, Leticia Veras Costa-Lotuf³, Paula Christine Jimenez¹

*rs.oliveira@unifesp.br

1- Instituto do Mar, Departamento de Ciências do Mar, Universidade Federal de São Paulo, Santos, SP – Brazil, 11.070-100. 2- Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, Ribeirão Preto, SP – Brazil, 14.040-903. 3- Instituto de Ciências Biomédicas, Departamento de Farmacologia, Universidade de São Paulo, São Paulo, SP – Brazil, 05.509-900. 4- Departamento de Microbiologia, Imunologia e Parasitologia, Universidade Federal de São Paulo, São Paulo, SP - Brazil, 04.023-900.

Myxobacteria are recognized as prolific producers of structurally diverse and biologically active metabolites. Although predominantly studied from terrestrial soils, their occurrence in coastal ecosystems such as mangroves remains largely underexplored. This gap is particularly evident in Brazil, where studies on myxobacterial diversity and biotechnological potential are still scarce. In this context, the present study investigates the potential of strain BRX-014, isolated from the Portinho Mangrove in São Paulo, Brazil. Phylogenetic analysis based on 16S rDNA sequencing identified the strain as a member of the genus *Myxococcus*, forming a distinct clade that suggests a potentially novel lineage. Its organic extracts demonstrated potent and selective cytotoxicity against human fibrosarcoma (HT-1080) and colorectal carcinoma (HCT-116) cell lines. Bioassay-guided fractionation afforded a dichloromethane fraction with pronounced bioactivity, displaying potent cytotoxicity (IC₅₀ = 0.58 µg/mL) and strong antiparasitic activity against *Plasmodium falciparum* 3D7 (IC₅₀ = 0.9 µg/mL). Metabolomic analysis of the BRX-014 extract (HRMS/GNPS) revealed a large cluster of ions annotated as myxothiazol correlates, suggesting the presence of novel thiazole-related metabolites. Fractions enriched in these ions were purified by HPLC and will be subjected to further structural elucidation. The detection of ions consistent with myxothiazol derivatives provides a plausible mechanistic rationale for the observed bioactivities, given that myxothiazols are potent inhibitors of the mitochondrial cytochrome bc₁ complex. This study highlights the unexplored potential of myxobacteria for the discovery of novel bioactive molecules, while also underscoring the importance of Brazilian mangroves as reservoirs of distinctive microbial diversity.

Keywords: Myxobacteria; Myxothiazol; Marine natural products; Anticancer; Antimalaria





PHYTOCHEMICAL PROFILE AND ANTIOXIDANT ACTIVITY OF *Solanum cernuum* VELL

Jéssica Pereira Silva^{1*}, José Alisson da Silva Lima¹, Maria Luiza de Almeida Aquino
Soares¹, Victor Campana Leite¹ Nicolas de Castro Campos Pinto¹

jessicapereira.silva@estudante.ufjf.br

1- Laboratory of Natural Products and Bioactive Compounds, Institute of Biological Sciences,
Department of Biochemistry, Federal University of Juiz de Fora – UFJF, Rua José Lourenço Kelmer,
s/n - São Pedro, Juiz de Fora - MG, 36036-900, Brazil.

The chemical and biological properties of *Solanum cernuum* Vell., popularly known as panacea, remain poorly documented. However, it has long been associated with anti-inflammatory and gastroprotective folk medicine, suggesting it may represent an underexplored reservoir of potential bioactive compounds. Further investigation on its antioxidant activity, as well as identifying its bioactive compounds, may broaden its potential therapeutic applications, as the oxidative stress is linked to the development of various chronic diseases. Accordingly, the present study aimed to evaluate the antioxidant potential of the ethanolic extract (EE) of *S. cernuum* leaves and obtain its phytochemical profile. *S. cernuum* leaves were collected at the UFJF Pharmacy School Garden (SisGen ADBB5C6), and a voucher was deposited in the CESJF herbarium (no. 80114). The EE was obtained by static maceration for 72 hours and stored at 4 °C. Antioxidant activity was assessed by hydroxyl radical (•OH) inhibition assay and by the ORAC method (Gligorovski et al., 2015; Pilaquinga et al., 2021) with modifications. Gallic acid and Trolox[®] were used as reference substances, respectively. Phytochemical characterization was performed by LC-MS using a C18 column (2.1 × 100 mm, 1.7 µm) at 40 °C, with a water/methanol gradient mobile phase at a flow rate of 0.4 mL/min; ionization occurred in negative mode (100–1000 m/z) with leucine-enkephalin as lock mass, and the spectra were compared with databases (MassBank, MoNA) and literature reports. The EE (12.5 µg/mL) showed significant antioxidant activity in the ORAC assay, and the analysis of fluorescence decay revealed no statistical differences among the time-points evaluated up to 60 min compared to Trolox[®] (12.5 µg/mL). The hydroxyl radical (•OH) inhibition assay showed that EE exhibited higher activity than gallic acid at the maximum concentration used (166.6 µg/mL). Even at the lowest tested concentration, EE showed over 70% of •OH inhibition (IC₅₀ < 6.25 µg/mL). Phytochemical analysis revealed the presence of cytidine-5'-diphosphate, caffeic acid-3-O-glucuronide, isocernumidin, cernumidin, hyperin, quercitrin, isorhamnetin-3-O-galactoside, isorhamnetin-3-O-glucoside, quercetin-7-O-rhamnoside, afzelin, and isorhamnetin-3-O-rhamnoside. These results contribute for better understanding of *S. cernuum* biological potential and expand the knowledge of its phytochemical constituents.

Keywords: *Solanum cernuum*, Antioxidant activity, Phytochemical profile, Mass spectrometry



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ONE STRAIN–MANY COMPOUNDS: STUDIES WITH *Streptomyces* sp. (BRA-010), A STRAIN RECOVERED FROM THE TUNICATE *Eudistoma vannamei*

Elthon Gois Ferreira^{1*}, Nicolas Ledres¹, Luís Guilherme Pereira Feitosa², Paula C. Jimenez³, Norberto Peoporine Lopes², Letícia Veras Costa-Lotufo¹

elthonferreira@usp.br

1-Laboratório de Farmacologia Marinha - Lafarmar, Departamento de Farmacologia, ICB-I, USP, Av. Prof. Lineu Prestes, 1524 - Butantã - São Paulo - SP. 2- Faculdade de Ciências Farmacêuticas de Ribeirão Preto (FCFRP), USP, Av. Prof. Dr. Zeferino Vaz - Vila Monte Alegre, Ribeirão Preto – SP, Brazil. 3. Instituto do Mar, UNIFESP, Santos-SP.

Marine bacteria and fungi possess genomes rich in biosynthetic gene clusters (BGCs) that are often unexpressed under standard laboratory conditions. The OSMAC (One Strain–Many Compounds) strategy offers an effective means to activate these silent pathways through variations in cultivation parameters. Complementarily, metabolomics provides systematic profiling of metabolic outputs and facilitates the annotation of bioactive compounds. Together, these approaches play an important role in the chemical mining of marine natural products. The present work aimed to perform chemical mining of compounds with anticancer potential from the BRA-010 strain under modified cultivation conditions. The marine strain BRA-010 deposited in the microorganism bank (MicroMarin) was reactivated in liquid culture medium A1 (starch, peptone and yeast extract) for 7 days under agitation at 200 rpm. The strain was cultivated in duplicate for 7 days under agitation at 200 rpm in different cultures with the elicitors: dimethylsulfoxide (DMSO), ampicillin, procaine hydrochloride, sodium butyrate, nickel sulfate and ethanol. Each culture broth was extracted during 1 h with equal volume of ethyl acetate, to obtain a crude extract of each culture. Cytotoxicity of the extracts and isolated compound was evaluated through the MTT assay after 72h exposure against colorectal carcinoma (HCT-116) and breast adenocarcinoma (MCF-7 and MDA MB 231) and melanomas (SK-MEL-28 and SK-MEL-147) cancer cell lines, and IC₅₀ values were obtained. The organic extracts obtained from the BRA-010 strain in the presence of different elicitors demonstrated cytotoxic activity against only the HCT-116 cell line, except when ethanol was used as an elicitor. The analysis of the extracts with different elicitors by HPLC-MS/MS did not show significant variations between the chemical profiles of cultures, highlighting the presence of tirandamycin A as the majoritary compound in most samples. These results suggested that *Streptomyces* sp. (BRA-010) was not sensitive to the presence of the elicitors to active the production of different metabolites.

Keywords: Marine Natural Products, Marine microorganism, OSMAC, Chemical Elicitors, Cytotoxic activity





EVALUATION OF THE CYTOTOXIC ACTIVITY OF TAGITININ C IN BREAST CANCER CELLS

Fernanda Brito Leite^{1*}, Wanderleya Toledo dos Santos¹, Albert Katchorian Netto², Daniela Chagas de Paula², Ana Cláudia Chagas de Paula Ladvocat¹.

fernandabrito.leite@estudante.ufjf.br

1-Department of Pharmaceutical Sciences, Federal University of Juiz de Fora, 36036-900, Juiz de Fora, Minas Gerais, Brazil. 2-Chemistry Institute, Federal University of Alfenas, 37130-001, Alfenas, Minas Gerais, Brazil.

Breast cancer is the second most common cancer in women and the second leading cause of cancer-related death among them. It has been the focus of scientific studies worldwide with the clear objective of reducing its incidence and improving its treatment. Given the severity of the disease and the significant adverse effects associated with current therapies, it is urgent and essential to invest in research aimed at developing new treatments. Based on this scenario, the aim of the present study was to investigate the cytotoxic activity of the sesquiterpene lactone Tagitinin C (TC), a compound isolated from *Tithonia diversifolia*, in a breast cancer cells *in vitro*. TC has been described as having antimicrobial, antifibrotic, and cytotoxic properties against some human cancer cell lines. In this study, its cytotoxic activity was widely evaluated for the first time against breast cancer cells (MCF-7) and human fibroblasts (CCD-1059Sk). Cytotoxicity was assessed using the MTT reagent (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide), and the IC₅₀ (the concentration required to inhibit 50% of cell viability) was calculated. From the results obtained, it was also possible to determine the selectivity index for cancer cells, the antiproliferative effect of TC, the inhibition of colony-forming capacity, and the reduction of the invasive potential of tumor cells treated with TC. Additionally, the type of cell death and the expression of apoptotic markers were evaluated using the RT-PCR technique. Thus, the results demonstrate the cytotoxic potential of TC, contributing to the discovery and development of new treatments that may be more effective, selective, and with fewer adverse effects for patients. The authors thank their institutions for their support and the financial support provided by FAPEMIG, CAPES, and CNPq.

Keywords: Breast cancer; *Tithonia diversifolia*; Tagitinin C, MCF-7, cytotoxicity, apoptosis.





PHYTOCHEMICAL INVESTIGATION AND CYTOTOXIC ASSESSMENT OF *Jacaranda caroba*

Alexandre Milanez Brandão^{1*}, Eliane Cristina Costa¹, Fernanda Rodrigues de Souza¹,
Michele Conceição Miranda¹, Lavínia Mota Cristianismo Silva¹, Rafael Cesar Gonçalves
Pereira², Lara Vieira de Almeida Peçanha², Lucienir Pains Duarte², Heveline Silva²,
Grasiely Faria de Sousa², Roqueline Rodrigues Silva¹

alexandre.milanez@ufvjm.edu.br

1-Departamento de Química, FACET, UFVJM, Alto da Jacuba, 5000, Diamantina, MG, Brasil.

2-Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brasil.

The genus *Jacaranda* comprises approximately 49 species distributed across Central America, South America, and the Caribbean. Among them, *Jacaranda caroba*, commonly known as “caroba-do-campo,” is traditionally used as a diuretic and for the treatment of syphilis. Its leaves, macerated in sugarcane spirit, are applied topically as a wound-healing agent or ingested for the treatment of ulcers. In this study, a phytochemical prospecting guided by cytotoxicity bioassays was conducted against the tumor cell lines MDA-MB-231 (metastatic breast adenocarcinoma) and A431 (epidermoid carcinoma), as well as the non-tumorigenic mammary epithelial cell line MCF-10, employed for selectivity analysis, using chloroform and methanolic leaf extracts. Chromatographic fractionation of the extracts yielded 11 fractions from the chloroform extract (1–11) and 6 from the methanolic extract (12–17), which were evaluated for cell viability using the MTT assay after 72 h of exposure. Among the samples of the chloroform extract, fraction 6 stood out, which after purification, resulted in the white solid 6.1. These samples presented the lowest inhibitory concentrations. Subfraction 6.1 exhibited IC₅₀ values of 2.60 ± 0.003 µg/mL for MDA-MB-231 and 2.45 ± 0.001 µg/mL for A431. Despite the pronounced inhibitory potential, both showed low selectivity (SI $\approx$ 1.1). Chemical characterization of subfraction 6.1 by infrared spectroscopy and nuclear magnetic resonance revealed the presence of a mixture of uvaol, erythrodiol, and ursolic acid lactone. Fractions 7 and 8 of the chloroform extract, as well as ursolic acid isolated from both extracts, exhibited IC₅₀ values around 11 µg/mL with SI $\approx$ 1.0. Fraction 14 of the methanolic extract emerged as the most active against the MDA-MB-231 cell line, displaying an IC₅₀ of 24.17 ± 0.001 µg/mL and SI = 2.8, and its characterization revealed the predominant presence of 3-O-acetylursolic acid. Additionally, three pentacyclic triterpenes were isolated, including corosolic acid and a mixture of 3 β -hydroxy-urs-21-en-28,20 β -lactone with 3,28 β -dihydroxy-urs-21-ene, the latter being reported for the first time in the genus. The cytotoxic activity observed was mainly associated with pentacyclic triterpenes, with a possible synergistic effect among compounds. These findings highlight the potential of *J. caroba* as a source of pharmacologically relevant molecules and reinforce the need for further studies aimed at improving selectivity and elucidating mechanisms of action.

Keywords: *Jacaranda caroba*, cytotoxic assessment, MDA-MB-231, A431





METABOLOMIC PROFILE AND ANTIMICROBIAL POTENTIAL OF THE ENDOPHYTE *COLLETOTRICHUM KARSTI*, FROM *DUGUETIA LANCEOLATA*: A MULTI-OMICS APPROACH INTEGRATING *IN SILICO* SCREENING

Jackson Monteiro^{1*}, Gabriel Martins da Silva¹, Ana Clara Lima Nunes Silva¹, Marisi G. Soares², Lhaís Araújo Caldas³, Renata C. Pascon¹, Marcelo A. Vallim¹, Patricia Sartorelli¹

*jackson.monteiro@unifesp.br

1-Instituto de Ciências Ambientais, Químicas e Farmacêuticas, Universidade Federal de São Paulo, 09972-270, Diadema-SP, Brazil. 2-Instituto de Química, Universidade Federal de Alfenas, 37130-000, Alfenas-MG, Brazil. 3-Netherlands Institute of Ecology, Wageningen, Holanda,

The escalating crisis of antimicrobial resistance (AMR) necessitates innovative strategies to accelerate the discovery of novel antibiotic scaffolds from underexplored sources such as endophytic fungi. To address this, we implemented a modern dereplication workflow integrating multi-omics data with predictive *in silico* tools to rapidly prioritize bioactive candidates from *Colletotrichum karsti*, an endophyte isolated from *Duguetia lanceolata*. The fungus was cultivated under four distinct conditions (solid-state fermentation on rice and wheat bran; liquid culture in Potato Dextrose and Czapek broths), and its metabolic profiles were acquired using LC-MS/MS. The resulting data was processed into molecular networks on the GNPS2 platform, where key metabolites were annotated by integrating spectral library matches and molecular family information. This chemical data was then correlated with the fungus's biosynthetic potential, mapped through genome mining with FungiSmash, which revealed a rich repertoire of 65 Biosynthetic Gene Clusters (BGCs). This multi-omics evaluation allowed the high-confidence annotation of several expressed metabolites, including a putative Betaenone analog, a Botrydial derivative, and the diketopiperazine Maculosin, directly linked to their corresponding BGCs. Crucially, an *in silico* pipeline was employed prior to any *in vitro* assays, predicting potent antibacterial activity against clinically relevant genera such as *Staphylococcus* sp., *Pseudomonas* sp., and *Klebsiella* sp., including resistant phenotypes. A subsequent selectivity screen (KinScreen) distinguished candidates with ideal safety profiles, such as the Betaenone analog, from others predicted to be potent but non-selective inhibitors of human kinases. Therefore, *in vitro* antimicrobial assays are currently in progress to confirm the predicted bioactivity of the crude extracts from all culture conditions. These experiments, targeting a panel of the selected bacterial genera including clinically relevant resistant strains like MRSA, will serve to bridge the gap between computational prediction and experimental validation in the search for novel antibiotics.

Keywords: *Colletotrichum karsti*; Endophytic Fungus; Multi-omics; *In silico* Screening; Antibacterial Activity.





***CHEMICAL COMPOSITION AND ANTIMICROBIAL ACTIVITY OF
ESSENTIAL OIL FROM *Eugenia dysenterica* DC. AGAINST BACTERIA
CAUSING BOVINE MASTITIS***

Fernando Gomes Barbosa^{1,2*}, Gabriel Fernandes Silva², Anielly Monteiro de Melo²,
Leonardo Gomes Costa², Monatha Nayara Guimarães Teófilo², Josana de Castro Peixoto²,
Leonardo Luiz Borges², Eliete Souza Santana², Joelma Abadia Marciano de Paula²

fernandogbio@hotmail.com

*1-Secretaria Estadual de Educação de Goiás, 5^a Av., Goiânia - GO, 74643-030, Brazil. 2-
Universidade Estadual de Goiás - Laboratório de Pesquisa, Desenvolvimento e Inovação de Produtos
da Biodiversidade, Fazenda Barreiro do Meio, Anápolis - GO, 75132-903, Brazil.*

Bovine mastitis poses a health and economic challenge in dairy farming, affecting food security and the income of rural producers. The objective of this work was to investigate the antimicrobial activity of the essential oil from leaves of *Eugenia dysenterica* DC. (Myrtaceae), known as “cagaiteira”, a plant native to the Brazilian Cerrado, against bacteria isolated from clinical and subclinical cases of bovine mastitis. For the extraction of essential oil, leaf samples were collected in Rianápolis-GO (Sisgen A1D543E), dried, ground, and subjected to hydrodistillation for 3 hours in a Clevenger apparatus. Gas chromatography coupled with mass spectrometry was used to analyze the compounds of essential oil. The antimicrobial activity was evaluated using the broth microdilution test, following the protocol recommended by the Clinical and Laboratory Standards Institute. The microorganisms were isolated from cattle milk with clinical and subclinical mastitis: *Staphylococcus* spp.; *Streptococcus* spp.; *Escherichia coli*; *Pseudomonas aeruginosa*, and two standard strains from the American Type Culture Collection (*Pseudomonas aeruginosa* - ATCC 27855; *Escherichia coli* - ATCC 25312). The yield of essential oil was 0.4% (w/w). The main constituents of the oil included the sesquiterpene hydrocarbons β -selinene (23.04%) and α -selinene (19.19%), along with the monoterpene hydrocarbons myrcene (18.24%) and β -pinene (10.24%). Using concentrations between 0.5 mg/ml and 388 mg/ml, the minimum inhibitory concentration (MIC) and the minimum bactericidal concentration (MBC) were determined for *Pseudomonas aeruginosa* (MIC: 127 mg/ml; MBC: 388 mg/ml). The results highlight the potential of “cagaiteira” leaves for developing products that can help control bovine mastitis, especially amid increasing bacterial resistance.

Keywords: *Eugenia dysenterica*, “cagaita”, essential oil, bovine mastitis, bioinputs.





EVALUATION OF THE ANTIUNGAL AND ANTIDIABETIC ACTIVITIES OF *Miconia rubiginosa* AND THE ANNOTATION OF COMPOUNDS BY HPLC-ESI-MS/MS.

Tiara da Costa Silva^{1,7*}, Diego G. Prado¹, Mário M. Martins², Vinícius P. Bittar³, Ana L. S. Borges³, Mariana B. Santiago⁴, Rosana Romero⁵, Carlos H. G. Martins⁴, Luís C. S. Cunha⁶, Raquel M. F. de Sousa¹, Foued S. Spindola³, Alberto de Oliveira¹.

tiara.silva@uftm.edu.br; alberto@ufu.br

1-NuPpEn, Instituto de Química, UFU, Av. João Naves de Ávila, 2121, Uberlândia, MG, Brazil. 2-NANOS, Instituto de Biotecnologia, UFU, R. Rua Acre, 1004, Uberlândia, MG, Brazil. 3-LABIBI, Instituto de Biotecnologia, UFU, R. Acre, 1004, Uberlândia, MG, Brazil. 4-LEA, Instituto de Ciências Biomédicas, UFU, R. Pará, 1720, Uberlândia, MG, Brazil. 5-Herbário, Instituto de Biologia, UFU, R. Ceará 1084, Uberlândia, MG, Brazil. 6- NuBiProN, IFTM, R. João Batista Ribeiro, 4000, Uberaba, MG, Brazil. 7-ICENE, UFTM, Av. Randolpho Borges Júnior 1400, Uberaba, MG, Brazil.

M. rubiginosa (Melastomataceae), popularly known as caporoquina, is a plant used in folk medicine to treat throat infections. Although few biological studies have been reported on this species, its antimicrobial activity is notable. Several bioactive compounds have been isolated from *M. rubiginosa*, including phenolic compounds and triterpenes. This study aimed to investigate the antifungal and antidiabetic activities of *M. rubiginosa* and to annotate its compounds using HPLC-ESI-MS/MS. Hexane (HE, 0.34 g) and ethanolic (EE, 3.60 g) extracts were obtained from 22.19 g of *M. rubiginosa* leaves by maceration. The antifungal activity was evaluated against *Candida* strains using the broth microdilution method, with the results expressed as MIC. The EH was inactive against the tested strains (MIC > 3000 µg mL⁻¹). Conversely, EE showed potent activity against *C. albicans*, *C. glabrata*, and *C. tropicalis* (MICs = 2.93, 1.46, and 11.72 µg mL⁻¹, respectively). The inhibitory activity of the α -amylase enzyme was also assessed. The EH showed no inhibition, while EE exhibited strong α -amylase inhibition (92.91%) with an IC₅₀ of 0.74 µg mL⁻¹. In the glycation inhibition assays (fructose-BSA over 7 days and MGO-BSA over 28 days), both HE and EE demonstrated significant inhibition of fructose-BSA on day 7 (59.95% and 86.46%, respectively). MGO-BSA inhibition was more pronounced on day 3 (24.52% for HE and 62.06% for EE). Based on these results, the EE was analyzed using HPLC-ESI-MS/MS, leading to the annotation of 30 specialized metabolites. These included: phenolic compounds (such as *p*-coumaric acid hexoside and gallic acid derivatives), hydrolysable tannins (pedunculagin), proanthocyanidins (epi)catechin dimers and pentamers, and various flavonoids (aglycones such as kaempferol and heterosides such as rutin). In conclusion, *M. rubiginosa* has proven to be a rich source of bioactive compounds with significant biological potential. Further studies are needed to fully understand the relationship between its chemical composition and its observed activities.

Keywords: *Miconia rubiginosa*, HPLC-ESI-MS/MS, anti-*Candida*, antidiabetics, phenolic compounds.





PHYTOCHEMICAL PROFILING AND BIOLOGICAL POTENTIAL OF PIPER MARGINATUM AND ITS ENDOPHYTIC FUNGI: INSIGHTS FOR COSMETIC APPLICATIONS

Isabella B. P. Martins^{1*}, Patrícia P. Augusto¹, Carolina R. da Silva¹, Patrícia S. Lopes¹,
Vânia R. Leite e Silva¹, Adriana P. M. G. Macedo³, Lorena R. F. de Souza³, Thiago A. M.
Veiga¹

isabella.bibiano@unifesp.br

1- Instituto de Ciências Ambientais, Químicas e Farmacêuticas, Universidade Federal de São Paulo, Diadema, Brasil

2- Instituto de Química, Universidade Federal de Catalão, Brasil

Biodiversity represents a valuable reservoir of bioactive compounds with therapeutic and cosmetic applications. *Piper marginatum*, a pantropical species traditionally used in folk medicine, is known for its diverse phytochemical profile, yet its potential remains underexplored, particularly regarding its associated endophytic fungi.^{1,2} This study aimed to investigate the chemical profile and biological activities of *P. marginatum* extracts, as well as to report, for the first time, the isolation of its endophytic fungi, opening new opportunities for bioprospecting and the discovery of bioactive natural products aligned with the growing demand for sustainable and safe cosmetic ingredients. Supported by LiveAloe company and FINEP (0558/21), and carried out in collaboration with UFG, UFCat, and the universities of Berlin and Wuppertal (Germany), this study investigates the chemical profile and biological activities of *P. marginatum* extracts, aiming to evaluate their potential for application in cosmetic formulations. An in-house database of compounds reported for the plant was constructed and applied in dereplication strategies, submitting UHPLC-HRMS data to Bruker Target Analysis software and GNPS molecular networking. Chemical profiling revealed the presence of flavonoids, terpenes, alkaloids, and phenylpropanoids. In the antioxidant assay, the glycerinated extract showed the most promising performance, at 25 μ M it significantly reduced reactive oxygen species levels, with fluorescence values comparable to resveratrol, confirming its strong antioxidant potential. Moreover, anti-inflammatory evaluation in THP-1 macrophages indicated that the ethanolic extract was able to reduce pro-inflammatory cytokine secretion at concentrations up to 10 μ g/mL without compromising cell viability, suggesting selective immunomodulatory activity. Altogether, these findings highlight *P. marginatum* as a promising source of bioactive metabolites, with significant antioxidant and anti-inflammatory potential for cosmetic development. Moreover, the first isolation of 20 fungal endophytes from this species establishes an unprecedented platform for future studies, expanding chemodiversity and reinforcing the valorization of Brazilian biodiversity, as extracts obtained from these microorganisms are also being evaluated in antioxidant assays. This research was supported by CNPQ, FINEP (0558/21), FAPESP (2024/03978-6) and CAPES.

Keywords: *Piper marginatum*, molecular dereplication, antioxidant, endophytic fungi

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ANTI-*Leishmania infantum* ACTIVITY OF ACETOGENINS FROM *Porcelia macrocarpa* (ANNONACEAE)

Dorca Ferreira^{1*}, Ivanildo A. Brito¹, Thais A. Costa-Silva², André G. Tempone²,
João Henrique G. Lago¹

dorca.ferreira@ufabc.edu.br

¹Center for Natural and Human Sciences, Federal University of ABC, Santo André, SP, Brazil.

²Laboratory of Pathophysiology, Butantan Institute, São Paulo, SP, Brazil.

Visceral leishmaniasis is a neglected disease with a significant public health impact, with approximately 30,000 new cases reported annually¹. In this context, discovering new drugs to treat this disease is crucial. As part of our ongoing research on *Porcelia macrocarpa*,² five chemically related acetogenins (**1–5**, Figure 1) were isolated from the seeds of this specie. ¹H NMR spectra of **1–5** showed characteristic signals of the γ -lactone ring at δ 2.56–2.57 (dt, J = 9.9 and 4.8 Hz, H-2), 4.30–4.38 (dd, J = 4.8 and 3.1 Hz, H-3), 4.44–4.45 (dq, J = 6.5 and 3.1 Hz, H-4) and 1.43 (d, J = 6.5 Hz, H-5).² To compounds **1–4**, a triplet at δ 2.13 was also observed, assigned to the propargylic hydrogens H-10' and H-13'. Additionally, in the ¹H NMR spectra of **2–4**, were observed signals at δ 5.80–5.81 (ddt, J = 16.9, 10.2 and 6.6 Hz) and 4.95–4.96 (m), indicating the presence of a terminal double bond in the side chain. These signals were absent from the ¹H NMR spectra of compounds **1** and **5**, which showed one broad singlet at δ 1.27 and one triplet at δ 0.85 (J = 6.8 Hz), which is characteristic of a terminal methyl group.² Analysis of ¹³C NMR spectra of **1–5** confirmed the presence of γ -lactone ring due to the signals at δ 177 (C-1), 47 (C-2), 71 (C-3), 78 (C-4) and 13 (C-5). In the ¹³C NMR spectra of **1–4**, were observed signals at δ 81 (C-11') and 80 (C-12'), characteristic of sp carbons, while spectra of **2–4**, signals at δ 139 and 114, characteristic of terminal double bonds were detect. On the other hand, except to the signals of γ -lactone ring, no signals of sp and sp² carbons were observed in the ¹³C NMR spectrum of **5**, indicating a saturated side chain. Analysis by ESI-HRMS showed [M+H]⁺ ions at m/z 393.3382 (C₂₅H₄₅O₃, **1**), 391.3227 (C₂₅H₄₃O₃, **2**), 363.2900 (C₂₃H₃₉O₃, **3**), 419.3522 (C₂₇H₄₇O₃, **4**) and 397.3681 (C₂₅H₄₉O₃, **5**). Additionally, fragmentation patterns at m/z 143, 255 and 307, observed in the MS/MS spectra, indicated that the triple bond in compounds **2–4** are located at C-11'. Initially, no toxicity against NCTC cells was observed for compounds **1–5** (CC₅₀ > 200 μ M). Their antileishmanial effect was then evaluated *in vitro* against the amastigote form of *L. infantum*. Among compounds with a C₂₀ side chain, **2** displayed activity (EC₅₀ = 23.5 μ M), while **1** and **5** were inactive (EC₅₀ > 150 μ M). These results suggest that the terminal double bond in the side chain plays an important role in activity. Based on this profile, the effects of **2–4** on *L. infantum* suggested that elongating the side chain (C₂₂ - compound **4**) decreased activity (EC₅₀ > 150 μ M), while reducing it (C₁₈ - compound **3**) enhanced the potency (EC₅₀ = 11.3 μ M). Interestingly, compound **3** showed similar effect of that determined to the positive control, miltefosine (EC₅₀ = 17.8 μ M). Therefore, these data suggest that the antileishmanial activity of acetylenic acetogenins depends on a combination of double and triple bonds in the side chain and an appropriate side-chain length.

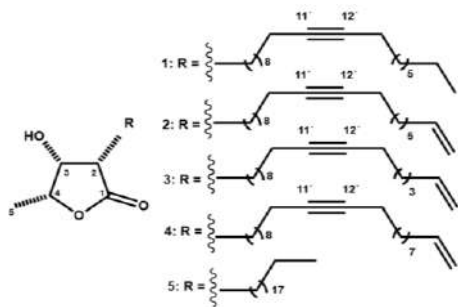


Figure 1. Molecular structures of the acetogenins **1–5** isolated from *P. macrocarpa*

Keywords: *Porcelia macrocarpa*, acetogenins, antileishmanial activity.

References: ¹WHO, *Leishmaniasis* **2023**; ²Brito et al., *Phytochemistry* **2025**, 231, 114360.

Acknowledgments: CAPES, CNPq, and FAPESP.





MARINE BACTERIAL EXTRACTS FROM RESTINGA ECOSYSTEMS AS POTENTIAL ANTI-BIOFILM AGENTS AGAINST *Pseudomonas aeruginosa* VIA CO-CULTURE STRATEGIES

Leidy Johana García Maza^{1,2*}, Rafaela Conceição de Souza¹, Alexandre José Macedo^{1,2}

garcia.maza@ufrgs.br

1- Centro de Biotecnologia, Universidade Federal do Rio Grande do Sul (UFRGS), Av. Bento Gonçalves, 9500, Campus do Vale, Prédios 43421/43431, Porto Alegre - RS, CEP 91501-970. 2- Faculdade de Farmácia, Universidade Federal do Rio Grande do Sul (UFRGS), Av. Ipiranga, 2752 - Azenha, Porto Alegre - RS, 90610-000.

Infectious diseases remain a major global health burden, accounting for nearly 20% of worldwide deaths (Martens et al., 2017). The declining efficacy of antibiotics against bacterial pathogens is mainly driven by intrinsic, acquired, and adaptive tolerance, with biofilm formation being one of the most critical adaptive defenses. Biofilms are linked to approximately 80% of chronic infections (Rather et al., 2021), notably chronic wound infections often caused and aggravated by the Gram-negative pathogen *Pseudomonas aeruginosa*. Addressing these challenges requires exploring novel sources of antimicrobial agents. Since oceans cover around 70% of Earth's surface, marine ecosystems represent an underexplored reservoir of bioactive molecules. Their long evolutionary history has generated vast biodiversity and unique adaptive strategies, enabling the production of chemically diverse metabolites. Among them, marine-derived bacteria are particularly promising as producers of secondary metabolites with potential anti-biofilm applications. In this study, 65 supernatants were obtained from mono-cultures of environmental marine bacteria isolated from the Restinga ecosystems on the South coast of Rio Grande do Sul, and 65 additional supernatants were produced through co-culture with the human pathogen *Pseudomonas aeruginosa* PA01. This work aimed to evaluate, using mixed-culture strategies, the scope and limitations of secondary metabolite production in inhibiting bacterial growth and biofilm formation by *Pseudomonas aeruginosa* ATCC 27853. Based on biological activity results, six supernatants were selected for secondary metabolites extraction: four from mono-culture (5M, 31M, 39M, 42M) and two from co-culture (12C, 15C). Then, anti-bacterial and anti-biofilm assays were also performed. Notably, regardless of cultivation strategy 12C showed bacterial growth inhibition by over 50%, while others selected extracts exhibited anti-biofilm activity more than 85%. 16S rRNA sequencing was performed to identify the promising marine-derived bacteria. The authors thank the support from their institutions, and the financial support of CAPES, CNPq, FAPERGS and the REDE MaRe (Rede de Pesquisa dos Ecossistemas Mangue e Restinga).

Keywords: Secondary metabolites, Marine-derived bacteria, Biofilm formation, Bacterial growth, Biological activity.





**PHYTOCHEMICAL PROSPECTING OF PSYCHOACTIVE INDOLE ALKALOIDS
FROM *Mimosa tenuiflora***

Natália Thatianne Duarte dos Santos^{1*}, Simone Alves Serafim Rocha¹, Suellen Vitória Santos de Oliveira¹, Yanna Julie da Silva Freitas², Jane Eire Silva Alencar de Menezes², Hécio Silva dos Santos², Roberto Lima de Albuquerque², Leandro Bezerra de Lima¹

* dnatalia959@gmail.com

1- Laboratório de Cromatografia (LC), Universidade do Estado do Rio Grande do Norte, UERN, Av. Professor Antônio Campos, S/N, Costa e Silva, Mossoró, Rio Grande do Norte, RN, 59625620, Brazil.

2- Laboratório de Bioensaios Químico-Farmacológico e Ambiental (LABQFAM), Universidade do Estado do Ceará (UECE), Av. Dr. Silas Munguba, 1700 - Campus do Itaperi, 60.714.903, Fortaleza, CE

Mimosa tenuiflora (Fabaceae), popularly known as Jurema-preta, is an endemic species of the Caatinga biome and widely distributed throughout Northeastern Brazil. With high ethnobotanical relevance, it has been traditionally employed in medicinal and ritual contexts and is recognized as a natural source of N,N-dimethyltryptamine (DMT), an indole alkaloid with marked psychoactive properties. Considering the increasing interest in psychedelic compounds for the treatment of resistant mental disorders, this study aimed to isolate and characterize DMT from the root bark of *M. tenuiflora*, evaluate its pharmacological effects, and perform *in silico* analyses of analogous tryptamines. The isolation was carried out by alkaline extraction, followed by structural characterization using ¹H and ¹³C NMR, TG/DTG, DSC, and thin-layer chromatography. *In vivo* assays with zebrafish (*Danio rerio*) demonstrated potential anxiolytic activity without evidence of acute toxicity. Computational analyses performed with SwissADME software indicated that DMT and related molecules exhibit pharmacokinetic parameters consistent with Lipinski's and Veber's rules, in addition to favorable oral bioavailability. Altogether, the findings reinforce the pharmacological relevance of *M. tenuiflora* as a source of bioactive metabolites and highlight DMT as a promising candidate for the development of novel therapeutic approaches targeting mental disorders, particularly treatment-resistant depression.

Keywords: *Mimosa tenuiflora*. N,N-dimethyltryptamine. Zebrafish. Psychedelics





**PHYTOCHEMICAL PROFILING AND NS2B-NS3 DENGUE VIRUS PROTEASE
INHIBITION BY *Banisteriopsis* SPECIES**

Jorge Luiz Souza Simão^{1*}, Isabella Marques do Nascimento¹, Ana Carolina Souza Parreira¹,
Jéssica Cristina Amaral², Collin Zimmer³, Tanja Schirmeister³, Lorena Ramos Freitas de
Sousa⁴, Vanessa Gisele Pasqualotto Severino¹

jorgesimao@discente.ufg.br

1- Chemistry Institute, UFG, Av. Esperança, Campus II, Goiânia - GO, Brazil; 2- Chemistry
Department, UFSCar, Rod. Washington Luis, Km 235, São Carlos – SP, Brazil; 3- Institute of
Pharmacy and Biochemistry, JGU, Staudinger Weg 5, 55128, Mainz, Germany; 4- Chemistry
Institute, UFCAT, Av. Dr. Lamartine Pinto de Avelar, Catalão – GO, Brazil;

The *Banisteriopsis* genus is notable for producing bioactive secondary metabolites with relevant therapeutic potential, such as glycosylated flavonoids, tannins, and β -carboline alkaloids. These metabolites make *Banisteriopsis* species promising candidates for investigation against Tropical Neglected Diseases, such as dengue virus (DENV), the most widespread arboviral disease globally, according to the WHO.^[1] DENV is transmitted by *Aedes aegypti* mosquitoes and can cause severe symptoms, including high fever and myalgia.^[1] In this view, this study aims to investigate the chemical profile of seven *Banisteriopsis* species (BAn – *B. anisandra*; BAr – *B. argyrophylla*; BC – *B. caapi*; BL – *B. laevifolia*; BM – *B. megaphylla*; BS – *B. stellaris*; and *B. vernoniifolia*) and evaluate their inhibitory activity against the NS2B-NS3 DENV protease, an essential molecular target for virus replication.^[2] Leaves of *Banisteriopsis* (SisGen A151706) were collected in Goiás, identified, and individually macerated with ethanol to obtain ethanolic leaf extracts (EEL). Chlorophyll was then removed from all *Banisteriopsis* EEL, and the extracts were evaluated against the NS2B-NS3 DENV enzyme using a fluorometric assay, according to the protocol described by Maus *et al.* 2023^[2]. Substrate hydrolysis was measured by the fluorescence of the reaction product 7-amino-4-methylcoumarin (AMC) at an excitation of $\lambda = 380$ nm and an emission of $\lambda = 460$ nm. Secondary metabolites were identified using LC-MS/MS analysis, followed by compound annotation through the FBMN at the GNPS platform (available on the link for [negative](#) and [positive](#) modes). Ethanolic leaf extracts (EEL) of *Banisteriopsis* without chlorophyll exhibited NS2B-NS3 protease inhibition above 94% (BAn – 97.4%; BAr – 96.9%; BL – 99.2%; BM – 95.3%; BV – 94.6%; BS – 97.9%), demonstrating a slight variation in inhibitory activity ($p < 0.05$). The species BL demonstrated the highest inhibition, reaching 99.2% against NS2B-NS3 DENV protease. GNPS analysis annotated several inhibitor metabolites of NS2B-NS3 protease, such as gallic acid, catechin, epigallocatechin, epigallocatechin gallate, luteolin, quercetin-3-*O*-hexoside-hexoside, quercetin-3-*O*-glucopyranoside, and kaempferol-3-*O*-hexoside-hexoside^[3]. In addition, GNPS analysis revealed the presence of β -carboline alkaloids, including tryptamine, 5-methoxytryptamine, tetrahydronorharmane, harmol, harmane, harmaline, and harmine, which are reported here for the first time in the BAr, BAn, BL, BM, BV, and BS species. Therefore, these ongoing investigations have enhanced the understanding of the biological potential and phytochemical profile of the *Banisteriopsis* genus.

Keywords: *Banisteriopsis*, arboviruses, Feature-Based Molecular Networking, dengue virus

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BIOSURFACTANT PROSPECTION IN MARINE Bacillus sp. STRAINS USING A COMPUTATIONALLY ASSISTED REVERSED DROP-COLLAPSE ASSAY

Felipe de Aguiar Porteiro^{1*}, Karolyne Bertholdo Ferreira¹, Paula C. Jimenez¹

felipe.porteiro@unifesp.br

1-Instituto do Mar, Universidade Federal de São Paulo, Santos-SP, Brazil.

Surfactants are compounds that reduce surface tension between two different phases. Also known as tensoactives, the increasing demand such substances is driven by their broad applications across chemical, pharmaceutical, food, and environmental industries. Among these compounds, microbial biosurfactants stand out due to key advantages such as high biodegradability, low toxicity, biocompatibility, and stability under varying pH, temperature, and salinity. The *Bacillus* genus is widely recognized as a biosurfactant producer; however, its marine species remain underexplored despite their significant biotechnological potential. The drop-collapse assay amply applied in screening protocols for the presence of surfactants in liquid samples; however, data analysis can be challenging due to the lack of methodization. Herein, this study evaluated six marine *Bacillus* strains from the MicroMarin culture collection — a repository of bacteria isolated from sediments and marine invertebrates collected along the Brazilian coast and islands — along with a reference strain (*B. subtilis*) for production of surfactant compounds. The strains were cultivated for 7 days in different solid media and assessed for biosurfactant production using an inverted version of the drop-collapse assay with various oils. A key methodological innovation of this work was the development of a Python script to standardize and automate droplet diameter measurements. This approach minimized subjectivity, improved reproducibility, and enabled systematic data recording and comparative analysis across different culture conditions, providing an efficient and original tool for similar studies. Among the tested strains, two – BRB191, recovered from sediments of Itaguapé Beach, Bertioga – SP, and BRB592, isolated from sediments collected at Saco da Ribeira Beach, Ubatuba – SP), phylogenetically related to *B. mexicanus*, demonstrated promising results for biosurfactant production, however, the media used for bacterial growth did not impact tensoactive activity of bacterial cultures. Additionally, selected strains were subjected to media with varying salinity and pH to investigate potential effects on surfactant production. In such conditions, significant increase in surfactant activity was observed when strains were grown in higher salinity levels. Also, extracts from hit-strains were chemically analyzed to confirm the occurrence of surfactants. These findings underscore the biotechnological potential of marine *Bacillus* strains within the MicroMarin collection in the production of industrially valuable bioproducts. Furthermore, these results highlight the relevance of integrating computational tools for assay standardization and data analysis.

Keywords: *Tensoactive, Firmicutes, Blue Biotechnology, Marine natural products, Python script.*





MEROTERPENOIDS FROM ROOTS OF *Piper* aff. *divaricatum* AND *Piper mosenii*

The Piperaceae family include a vast diversity of species globally, with Brazil harboring a significant number of genera and species. Within this context, the genus *Piper* exhibits the greatest species diversity. Among its representatives, *Piper* aff. *divaricatum* - a recently identified species - and *P. mosenii* have been the subject of a few chemical studies. This study reports the phytochemical investigation of hexane crude extracts from the roots of both species and its evaluation of antimicrobial activity. The extract from *P. aff divaricatum* was subjected to various chromatographic techniques, and subsequent structural elucidation was performed using spectroscopic methods (¹H and ¹³C NMR, including 1D and 2D experiments) which afforded compounds **1-3**. The hexane extract from *P. mosenii* led to the formation of crystals (compound **4**) that were analyzed by single-crystal X-ray diffraction (XRD). Four meroterpenes were described that included two chromenes, named (*E*)-2-(4',8'-dimethylnona-3',7'-dien-1-yl)-2-methyl-2H-chromene-6-carboxylic acid methyl ester (**1**), (*E*)-2-(4',8'-dimethylnona-3',7'-dien-1-yl)-8-hydroxy-2-methyl-2H-chromene-6-carboxylic acid methyl ester (**2**), and two benzoic acid derivatives named (*E*)-4-(3',7'-dimethylocta-2',6'-dien-1-yl)-3-hydroxybenzoic acid methyl ester (**3**) and 3-(1'-oxo-3'-methyl-2'-butenyl)-4-hydroxybenzoic acid methyl ester (**4**). Compound **1** is described for the first time in the literature. Furthermore, the antibacterial activity of the hexane extracts from *P. aff divaricatum* and *P. mosenii* demonstrated selective inhibition against *Staphylococcus epidermidis* (MIC 0.062 and 0.125 mg mL⁻¹, respectively), and *Escherichia coli* (MIC 0.031 and 0.25 mg mL⁻¹, respectively). Only *P. aff divaricatum* showed activity against *Staphylococcus aureus* (MIC 0.015 mg mL⁻¹). The chromatographic fractions from *P. aff divaricatum* that furnished compounds **1-3** exhibited broader antimicrobial activity, effectively inhibiting *S. aureus* (MIC 0.0078 mg mL⁻¹), *S. epidermidis* (MIC 0.125 mg mL⁻¹), *E. coli* (MIC 0.50 mg mL⁻¹) and *C. albicans* (MIC 0.078 mg mL⁻¹). The classes of isolated compounds are known for their pharmacological potential.

Acknowledgements:

Keywords: Piperaceae; Chromenes; Antimicrobial activity





EVALUATION OF THE SYNERGISTIC EFFECT OF *Bauhinia monandra* KURZ EXTRACT AND LASER ACUPUNCTURE IN THE MODULATION OF INFLAMMATORY MODELS

A. A. D. S. Castro^{1*}, R.C.C. Júnior¹, J.S. Nunes¹, E. A. Laurindo², L. C. Soares², T. M. Fernandes², N.M. Lima¹; S. B. R. Castro², C. Souza Alves², A. P. Carli¹.

*allyne.dias@ufvjm.edu.br

1 - Universidade Federal dos Vales do Jequitinhonha e Mucuri, Instituto de Ciência, Engenharia e Tecnologia, Teófilo Otoni, MG, Brasil, 39803-371. 2 - Universidade Federal dos Vales do Jequitinhonha e Mucuri, Faculdade de Medicina do Mucuri, Teófilo Otoni, MG, Brasil, 39803-371.

Bauhinia monandra Kurz, popularly known as "cow's foot," belongs to the Fabaceae family and is easily recognized by its bilobed leaves that resemble the shape of a cow's foot. It is a medicinal plant widely used in traditional medicine in Brazil and other tropical regions, especially for treating diabetes, inflammatory processes, and kidney disorders. Several studies have shown that the species is a source of bioactive compounds, such as flavonoids, glycosides, tannins, and protease inhibitors, associated with antioxidant, hypoglycemic, and anti-inflammatory properties. This study aimed to evaluate the anti-inflammatory potential of the ethanolic extract of *B. monandra* Kurz (EEBm) using *in vitro* and *in vivo* models. The leaves were obtained and recorded in SisGen (AFFF12E), and the ethanolic extraction of their compounds was performed. In an *in vitro* model, cell viability and nitric oxide (NO) production were evaluated in murine macrophages (J774A.1 and RAW 264.7) treated with EEBm. The cells were cultured under controlled conditions and exposed to different concentrations of the extract (333, 100, 33.3, and 10 µg/mL) in the presence or absence of inflammatory stimulus (LPS + IFN-γ) for 48 h. Cell viability was analyzed using the MTT assay, and NO production was measured using the Griess method. In the *in vivo* experiment, the paw edema model was performed in female BALB/c mice, aged 6 to 8 weeks, approved by CEUA-Mucuri (01-2025R). Induction was performed by inoculating 20 µL of carrageenan (2.5%) diluted in phosphate-buffered saline (PBS) into one of the hind paws. Animals were treated with EEBm at concentrations of 100 and 200 mg/kg and LaserAcupuncture (LA) in unilateral acupuncture points on the lower limbs. The findings suggest that EEBm has a safe profile regarding cell viability and exerts anti-inflammatory effects at both the cellular and systemic levels. The reduction in NO production *in vitro* and the inhibition of paw edema *in vivo* indicate that the bioactive compounds present in EEBm modulate central mechanisms of inflammation. Furthermore, the combination with LA demonstrated the potential to amplify therapeutic effects, constituting an innovative and promising strategy for the management of inflammatory processes.

Keywords: *Bauhinia monandra* Kurz. LaserAcupuncture; anti-inflammatory; arthritis.

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ANTIOPHIDIC POTENTIAL OF *Mimosa gracilis* var. *capillipes* AND *Mimosa modesta* var. *ursinoides*: METABOLOMIC AND IN SILICO APPROACHES AGAINST *Bothrops* AND *Crotalus* VENOMS

Alan Dumont Clemente^{*1, 2}, Heitor Akio Kimura^{3, 4}, João Paulo Sabino Pereira¹, Sokadjo Letchede Désire Kouassi¹, Anita Mitico Tanaka-Azevedo^{3, 4}, Marta Regina Magalhães⁵, Vanessa Gisele Pasqualotto Severino¹

alan.clemente@ifg.edu.br

¹Institute of Chemistry, Federal University of Goiás, Goiás, Brazil; ²Federal Institute of Education, Science and Technology of Goiás, Goiás, Brazil; ³Institute of Biosciences, Butantan Institute, São Paulo, Brazil; ⁴Institute for Technological Research – Butantan Institute, University of São Paulo, São Paulo, Brazil; ⁵Pontifical Catholic University of Goiás, Goiás, Brazil.

Snakebite envenomation, recognized by the WHO as a neglected tropical disease (NTD), affects approximately 5 million people worldwide annually, with nearly 1 million reported cases¹. In South America, the genera *Bothrops* and *Crotalus* are responsible for most envenomation cases. Among their toxins, phospholipase A₂ (PLA₂) plays a central role in inflammatory responses, while proteases contribute to local tissue damage and coagulation disorders. Although antivenom serum remains the primary treatment, it shows limited effectiveness against local damage, highlighting the need for complementary therapies. In this study, ethanolic extracts of *M. gracilis* var. *capillipes* and *M. modesta* var. *ursinoides* collected in Goiás, Brazil, authenticated with numbers 60.375 and 37.079, respectively, and extracted by maceration in ethanol, were investigated. The extracts were subjected to antioxidant activity evaluation (DPPH• method), in vitro antivenom assays-proteolytic, PLA₂, and coagulant inhibition LC-MS/MS, molecular networking via the GNPS platform, and molecular docking. Metabolomic analysis enabled the putative annotation of 77 compounds from various classes of secondary metabolites, including gallic acid, catechin, luteolin, kaempferol, and apigenin, all recognized for their antioxidant and anti-inflammatory properties. *In vitro* assays showed that *M. gracilis* leaf extracts and *M. modesta* root extracts exhibited high antioxidant activity, with EC₅₀ values of 1.25 and 3.25 µg/mL, respectively, and complete inhibition (100%) of proteolytic, PLA₂, and coagulant activities at concentrations of 1 mg/mL. The interaction between the extracts and venom proteins was confirmed by SDS-PAGE, with the disappearance of characteristic venom bands. Molecular docking indicated that, among the annotated compounds, six flavonoids exhibited higher predicted binding affinities to PLA₂ (PDB IDs: 1pa0, 3t0r, and 2qog) than rutin, a reference compound with demonstrated *in vivo* antivenom activity². To validate these findings, further in vitro and in vivo assays with the six selected flavonoids will be conducted to assess efficacy, toxicity, drug-likeness, and molecular dynamics. This study contributes to advancing the development of complementary therapies to conventional treatment for snakebite envenomation.

Keywords: Antivenom activity, Metabolomics, *Mimosa*, Phospholipase A₂ (PLA₂), Molecular docking, Snakebite envenomation.

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ANTIBACTERIAL ACTIVITY OF LAPACHOL DERIVATIVES AGAINST THE CITRUS CANKER PATHOGEN *XANTHOMONAS CITRI SUBSP. CITRI*

João Oiano-Neto^{1*}, Danielle Fernandes da Silva², João Batista Fernandes², Maria Fátima das Graças Fernandes da Silva².

joao.oiano@embrapa.br

1-Embrapa Pecuária Sudeste, Rod. Washington Luiz, km 234 s/nº, Fazenda Canchim, Caixa Postal 339, 13560-970, São Carlos SP, Brazil. 2- Laboratório de Química de Produtos Naturais, Departamento de Química, Universidade Federal de São Carlos, Rod. Washington Luís, km 235 SP-310, 13565-905, São Carlos SP, Brazil.

Citrus canker, mainly caused by *Xanthomonas citri subsp. citri*, is one of the most destructive citrus diseases, severely affecting yield, fruit quality, and international trade. In Brazil, especially in São Paulo State, the world's leading orange juice producer, millions of trees have been eradicated, resulting in significant economic losses. Current management relies on eradication programs and copper-based bactericides, which reduce incidence but promote bacterial resistance, soil accumulation, and environmental risks. Lapachol is a 1,4-naphthoquinone mainly isolated from *Tabebuia spp.* (Bignoniaceae), with a redox-active structure capable of generating reactive oxygen species, a mechanism underlying its broad antimicrobial spectrum. Its reported activities include antibacterial, antifungal, antiviral, antiparasitic, and insecticidal effects, in addition to antitumor properties. Importantly, both lapachol and its derivatives have demonstrated inhibitory action against phytopathogens, as well as herbicidal, reinforcing their applicability in agriculture. β -Lapachone, a structural isomer, further expands this potential by exhibiting selective antimicrobial and cytotoxic effects. Altogether, these features suggest that lapachol and its analogs represent promising candidates for the development of novel control strategies against *X. citri* and citrus canker, contributing to sustainable crop protection and reduced dependence on copper-based compounds. The aim was to evaluate the antibacterial activity of lapachol and its derivatives on *Xanthomonas citri subsp. citri*. Lapachol was isolated from wood of *Handroanthus sp.*, and its derivatives were synthesized according to procedures described in the literature, with modifications. All compounds were characterized by NMR spectroscopy. Minimum inhibitory concentrations (MICs) were determined following CLSI (Clinical and Laboratory Standards Institute) guidelines, using serial dilutions of compounds from 400 to 0.195 $\mu\text{g}\cdot\text{mL}^{-1}$. Copper sulfate was the positive control, and the inoculum was standardized to 10^6 CFU. All assays were performed in triplicate. The MIC values obtained in this study were: lapachol (412.7 μM), α -lapachone (103.2 μM), β -lapachone (6.4 μM), β -lapachone-3-sulfonic acid (4.8 μM), sodium salt of lapachol (189.2 μM), and copper sulfate (1566.3 μM). Notably, the MICs of α -lapachone, β -lapachone and β -lapachone-3-sulfonic acid were approximately 15, 245 and 326 fold lower, respectively, than that of copper sulfate; highlighting mainly the potential of β -derivatives as promising candidates for the control of *Xanthomonas citri*.

Keywords: *Xanthomonas citri subsp. citri*, citrus canker, citriculture, lapachol, β -lapachone.





MYXOBACTERIA FROM COASTAL ENVIRONMENTS FOR BIOPROSPECTING OF BIOACTIVE NATURAL PRODUCTS

Gabrielli Ribeiro Lopes da Silva¹; Yann F. Lin¹; Renan S. Oliveira¹; Elthon G. Ferreira²;
Letícia V. Costa-Lotufo²; Paula C. Jimenez^{1,*}

*pcjimenez@unifesp.br

¹BioproSP, Instituto do Mar, UNIFESP, R. Carvalho de Mendonça, 144, Santos, SP, Brazil;

²LaFarMar, Instituto de Ciências Biomédicas, Universidade de São Paulo, São Paulo-SP, Brazil

Myxobacteria are predatory bacteria known for their ability to produce bioactive secondary metabolites. Despite this potential, they remain understudied in Brazil, particularly in coastal and marine environments. Therefore, this study aimed to isolate, characterize, and assess the biotechnological potential of myxobacteria from the central coast of São Paulo State to expand the MyxoMarin microbiological collection, the first in the country dedicated to this bacterial phylum, ensuring long-term preservation and availability for further scientific research. Sixteen sediment samples were collected from beaches and mangroves, from which 21 bacterial isolates were recovered with typical myxobacterial characteristics (formation of fruiting bodies and swarms). After purification, strains were cultivated in VY/2 media with 2% XAD-16 resin and extracted with acetone:methanol 1:1 v/v to obtain the respective extracts, which, in turn, were evaluated for 1) cytotoxic activity against the human colorectal cancer cell line HCT-116, by means of the MTT assay; 2) trypsin and chymotrypsin protease inhibition activity; and 3) the chemical profile of the bioactive extracts by HPLC. Of the extracts obtained from isolates, 10 were considered cytotoxic ($IC_{50} < 50 \mu\text{g/mL}$), with BRX-053 ($1.57 \mu\text{g/mL}$), BRX-052 ($2.22 \mu\text{g/mL}$), and BRX-041 ($3.71 \mu\text{g/mL}$) revealing highest potency. In the trypsin and chymotrypsin inhibition assay, all extracts demonstrated some degree of activity, with BRX-041 (23%) and BRX-044 (20%) standing out for trypsin inhibition and BRX-041 (40%) and BRX-051 (43%) for chymotrypsin inhibition. HPLC analysis at 254 and 280 nm revealed similar chemical profiles among the most active extracts, suggesting the presence of related compounds. Future steps include taxonomical identification of the most promising strains and metabolomic analysis of bioactive extracts. These results highlight the potential of Brazilian coastal myxobacteria as an untapped source of new bioactive metabolites and, furthermore, consolidates the MyxoMarin as a strategic platform for bioprospecting marine natural products.

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Keywords: Microbiological collection; Marine natural products; Cytotoxicity; Protease inhibitors; Marine biotechnology.





CIRCADIAN VARIATION AND ANTILEISHMANIAL POTENTIAL OF THE VOLATILE COMPOUNDS OF *SCHINUS TEREBINTHIFOLIUS* RADDI

Idalina Candido^{1*}, Felipe Sales¹, André Gustavo Tempone², João Henrique Ghilardi Lago¹

i.candido@ufabc.edu.br

¹ -Center for Natural and Human Sciences, Federal University of ABC, Santo André, SP, Brazil.

² -Laboratory of Pathophysiology, Butantan Institute, São Paulo, SP, Brazil

Schinus terebinthifolius Raddi (Anacardiaceae), commonly known as the Brazilian pepper tree, has several well-documented therapeutic applications and properties, including anti-inflammatory, wound-healing, and antimicrobial activities. The essential oils from this plant displayed selective activity against cancer cells as well as allelopathic potential. As part of our ongoing research on antileishmanial agents derived from Brazilian flora, this study aimed to analyze the chemical composition of essential oils extracted from the leaves of *S. terebinthifolius* collected in Santo André, São Paulo, Brazil, at for different periods (6h, 12h, 18h, and 24 h) on December 15th, 2024, to assess a possible circadian variation, and to evaluate the potential of each oil and main compounds against promastigote forms of *Leishmania infantum*. During each period, the aerial parts were collected, and the essential oils were obtained individually by hydrodistillation using a Clevenger apparatus. The respective yields, calculated based on the fresh weight of the plant material, were 0,51% (6 h), 0,71% (12 h), 0,57% (18 h), and 0,55% (24 h). Chemically, the oils were found to consist mainly by non-oxygenated monoterpenes and sesquiterpenes. Quantitatively, minor variations were observed in each oil. The highest concentration of monoterpenes was observed at 6 h (58.0%), followed by a reduction in the subsequent time periods (49.9% at 12 h, 41.6% at 18 h, and 43.4% at 24 h). The proportion of the main monoterpenes, α - and β -pinene, changed from 28.4% and 12.9%, respectively, at 6 h, to 23.9% and 9.7% at 12 h, 19.7% and 9.7% at 18 h, and 22.0% and 8.6% at 24 h. Similarly, the amount of sesquiterpenes changed little over time, with higher amounts detected at 18 h (52.7%) and 24 h (49.1%). Among the main compounds identified were germacrene D and germacrene B, at 17.0% and 6.4% at 6 h, 16.6% and 9.8% at 12 h, 19.8% and 9.9% at 18 h, and 13.9% and 7.6% at 24 h, respectively. The effectiveness of each crude oil against promastigote forms of *Leishmania infantum* was determined *in vitro*, and all of the oils exhibited potency, resulting in 100% parasite death at a concentration of 200 mg/mL. To evaluate the effects of main compounds in bioactivity, a pool of the four oils was prepared and this material was subjected to column chromatography over SiO₂/AgNO₃, yielding α -pinene, β -pinene, α -copaene, germacrene D, and germacrene B in pure forms. These compounds were tested individually against *L. infantum* promastigotes and displayed EC₅₀ values of 15.5, 12.3, 18.1, 25.6, and 46.5 mg/mL, respectively, with reduced toxicity against NCTC cells (CC₅₀ > 200 mg/mL). These results indicate that the proportion of main compounds does not change over the course of a day and that these metabolites may be responsible for the antileishmanial effect of the crude oils (CNPq, FAPESP, CAPES).

Keywords: Volatile compounds; circadian variation; *Schinus terebinthifolius*; antileishmanial.





BIOACTIVE COMPOUNDS OF MANDEVILLA VELAME: CHEMICAL PROFILE AND ELASTASE INHIBITORY ACTIVITY

Luis Felipe Lima Guimarães^{1*}, Bianca Moreira Oliveira¹, Kyuri Ribeiro², Lorena Ramos Freitas de Sousa², Lucilia Kato¹

lucilia@ufg.br

1-Federal University of Goiás, Institute of Chemistry, 74690-900, Goiânia, GO, Brazil. 2-Federal University of Catalão, Institute of Chemistry, 75704-020, Catalão, GO, Brazil.

The species *Mandevilla velame*, belonging to the Apocynaceae family, is widely used by traditional communities of the Brazilian Cerrado for the treatment of renal disorders and blood purification [1]. Although no chemical or biological profile has been reported specifically for *M. velame*, studies within the genus *Mandevilla* Lindl. have described secondary metabolites with biological activities [2]. Thus, this study aimed to evaluate the chemical and biological profile of extracts and fractions from this species. Ethanolic extracts from leaves and stems were obtained through exhaustive maceration for nine days, with solvent renewed every three days, followed by chlorophyll removal. Fractions were obtained by liquid-liquid extraction with hexane and ethyl acetate. The chemical profiles of extracts and fractions were obtained by HPLC-ESI(+)-MS/MS. Data processed with MS-DIAL and SIRIUS were submitted to the GNPS platform and analyzed using the FBMN approach. Biological activity was evaluated against porcine pancreatic elastase (EC 254-453-6), using SucAla3-pNA as substrate and quercetin as positive control, and against mushroom tyrosinase (*Agaricus bisporus*, EC 1.14.18.1), using L-DOPA and kojic acid as control. Ethanolic extracts from leaves (79%) and stems (72.8%) showed strong inhibitory activity against elastase. Similar activity was observed for the acetate (80.2%) and hydromethanolic (75.3%) fractions of leaves, whereas the stem fraction were inactive. Annotation by MS/MS showed similarities among the fractions, highlighting the presence of flavonoids such as quercetin-*O*-hexoside (m/z 479.0810), condensed tannins such as aesculitannin B (m/z 865.1944), phenolic derivatives of phenylpropanoids such as chlorogenic acid (m/z 355.1008), and triterpenoids such as queretaroic acid (m/z 473.3602). Among them, flavonoids and tannins are particularly relevant due to their known antioxidant and enzyme-modulating properties. Although both extracts shared a similar chemical profile, the higher concentration and bioaccessibility of compounds in the leaves explain their superior elastase inhibitory activity. In contrast, *M. velame* extracts did not show significant activity against tyrosinase, with inhibition rates below 20%. Overall, this study reveals that the extracts, particularly the acetate and hydromethanolic fractions of the leaves, exhibited promising elastase inhibitory activity due to their flavonoid and tannin content. However, tyrosinase inhibition was unsatisfactory. These findings demonstrate that prospecting enzymatic inhibitors from plant extracts may represent a relevant tool for the development of biocosmetics. Acknowledgments: FINEP, CNPq, Livealoe, Bergische Universität Wuppertal.

Keywords: Mass spectrometry; Chemical profile; Elastase; HPLC-ESI(+)-MS/MS

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AYAHUASCA MITIGATES OXIDATIVE STRESS AND SENESCENCE IN 6-OHDA-INDUCED SH-SY5Y CELLS

Wanderleya Toledo dos Santos^{1*}, Albert Katchborian Neto², Fernanda Brito Leite Dornellas¹, Dawidson Assis Gomes³, Fernanda Maria Pinto Vilela¹, Marisi Gomes Soares², Danielle Ferreira Dias², Paula Carolina Pires Bueno⁴, Daniela Aparecida Chagas de Paula², Ana Cláudia Chagas de Paula Ladvocat¹

wanderleyatoledos@gmail.com

1-Faculty of Pharmacy, Department of Pharmaceutical Sciences, Federal University of Juiz de Fora, Rua José Lourenço Kelmer, Juiz de Fora, Minas Gerais, 36036-900, Brazil. 2-Chemistry Institute, Federal University of Alfenas, Alfenas, Minas Gerais, 37130-001, Brazil. 3- Department of Biochemistry and Immunology, Federal University of Minas Gerais, Av. Antônio Carlos, 6627, Belo Horizonte, Minas Gerais, Brazil. 4- Leibniz Institute of Vegetable and Ornamental Crops, IGZ, Theodor-Echermeyer-Weg 1, 14979 Großbeeren, Germany.

Parkinson's disease (PD) is a neurodegenerative disorder, characterized by the progressive loss of dopaminergic neurons and symptoms such as resting tremor and muscle rigidity, as well as non-motor symptoms, including mood and gastrointestinal alterations. Current therapies are only symptomatic and often associated with significant adverse effects, highlighting the urgent need for new therapeutic approaches. In this context, natural products have emerged as promising sources of biologically active molecules. Ayahuasca (Aya), a traditional ritualistic beverage, mainly composed of *Banisteriopsis caapi* and *Psychotria viridis*, showed promising neuroprotective results. Thus, this study aimed to investigate the neuroprotective mechanisms of action of Aya in cellular PD model, using human neuroblastoma cells (SH-SY5Y) subjected to 6-hydroxydopamine (6-OHDA)-induced toxicity. Initially, the cytotoxicity of Aya and reference drug (L-DOPA), was evaluated by the MTT assay after 48 h of treatment. Subsequently, the neuroprotective mechanism of action was evaluated. The oxidative stress was measured using the MitoSOX Green probe. The cellular senescence was also evaluated. The results demonstrated that Aya exerted a neuroprotective effect, associated with reduced mitochondrial oxidative stress and decreased cellular senescence induced by 6-OHDA at the concentration of 1.25 µg/mL. These findings suggest the therapeutic potential of Ayahuasca for PD, although further studies are required to elucidate possible additional details regarding its mechanisms of action. Acknowledgments: CAPES, FAPEMIG RED-00213-23, APQ02882-24, APQ00443-18, CNPq 408115/2023-8, 304916/2025-0, FAPESP 24/04606-5.

Keywords: Parkinson's disease, neuroprotection, natural products, Ayahuasca.





Myxobacteria Isolated from Ascidian Eudistoma vannamei and their biotechnological potential anticancer

Lívia Martins Costa^{1*}, Isolda de Sousa Monteiro¹, Elthon G. Ferreira², Letícia V. Costa-Lotuf², Paula Christine Jimenez¹

martins.costa@unifesp.br

¹Instituto do Mar, Universidade Federal de São Paulo, Santos-SP, Brazil; ²Instituto de Ciências Biomédicas, Universidade de São Paulo, São Paulo-SP, Brazil.

The marine ecosystem is a very rich source of microorganisms that produce bioactive metabolites with pharmacological potential. Among these microorganisms, myxobacteria stand out for their ability to generate secondary metabolites with antimicrobial and antitumor activities. In this context, the present study aimed to isolate, cultivate and evaluate the biotechnological potential of myxobacteria associated with the ascidian *Eudistoma vannamei*. were subjected to selective isolation techniques, resulting in seven distinct strains: five recovered by the *E. coli* bait method and two by cellulose supplementation. The isolated cultures were chopped until purified strains were obtained, and then cultured in liquid medium under agitation. After extraction with acetone and methanol, the extracts were dried, weighed and evaluated for yield and bioactivity. The cytotoxicity of the extracts was analyzed in HCT-116 cells (ATCC CCL-247), a human colorectal carcinoma cell line, by MTT assay. Two extracts presented IC₅₀ values below 20 µg/mL: BRX-092 (3.49 µg/mL) and BRX-093 (18.1 µg/mL). Two extracts exhibited IC₅₀ values between 20 and 100 µg/mL: BRX-088 (82.4 µg/mL) and BRX-095 (49.7 µg/mL). One extract presented an IC₅₀ value above 100 µg/mL: BRX-087 (139.7 µg/mL). The extract from strain BRX-089 inhibited more than 50% of cell proliferation even at the lowest concentration tested. Therefore, it was not possible to calculate an IC₅₀ value for this extract, indicating the need for testing at lower concentrations. In trypsin inhibition assays at 50 µg/mL, extracts BRX-100 (33.76%), BRX-093 (39.74%), and BRX-089 (39.31%) showed activity, suggesting multifunctional bioactivity. The results demonstrate the relevance of myxobacteria associated with ascidians as a source of innovative bioactive compounds with potential for pharmaceutical application.

Keywords: anticancer, bioprospecting, marine biotechnology, antimicrobial, marine natural products.





SEARCH FOR NEW ANTIMALARIALS FROM PLANTS USED IN TRADITIONAL MEDICINE FOR THE TREATMENT

Ana Júlia Marques de Abreu*, Victória Miranda Machado,
Ezequias Pessoa de Siqueira Filho, Isabela Penna Ceravolo

anaabreu@aluno.fiocruz.br

*Instituto René Rachou, Fundação Oswaldo Cruz, Avenida Augusto de Lima 1715, Belo
Horizonte, MG, 30.190-002, Brazil*

Human malaria remains one of the world's leading parasitic diseases, with a reported 263 million cases globally and approximately 140,000 cases in Brazil. One of the greatest challenges in the fight against malaria is the emergence and spread of resistance of the species *Plasmodium falciparum* to currently used antimalarial drugs. Given the great biodiversity of Brazilian biomes and the fact that several drugs, including the antimalarials quinine and artemisinin, were discovered from plants, we proposed to evaluate the antiplasmodial activity of plant extracts based on an ethnopharmacological approach. For this purpose, 21 plant species from 17 botanical families were selected from a search of scientific databases (Google Scholar and PubMed). These species had previously been described as used to treat malaria and/or fever but lacked detailed scientific or academic records. The crude extracts were obtained by macerating approximately 30 g of the dry plant in ethanol (leaves, roots, aerial parts, barks, flowers, and fruits) for seven days, followed by filtration and solvent evaporation. Each crude extract was then solubilized in DMSO. The evaluation of activity against blood-stage forms of *P. falciparum* was performed using the SYBR assay at seven dilutions starting from 50 µg/mL. The activity of each plant species was evaluated by determining the concentration that inhibits 50% of the parasite's growth (IC₅₀). Extracts that showed activity (< 20 µg/mL) had their cytotoxicity evaluated in mammalian kidney cells using the neutral red uptake assay, which determined the extract concentration that was cytotoxic to 50% of the cells (CC₅₀). The selectivity index (SI) was determined by the ratio of cytotoxicity to activity, where values less than 10 were considered toxic. Of all the medicinal plants tested, eight showed activity against the parasite in the *in vitro* assay, with IC₅₀ values ranging from 2.0 to 19.4 µg/mL and SI values ranging from 2 to 40. These results demonstrate the great potential of natural products for the discovery of new antimalarial drugs. With the isolation of the active compounds, it is expected that new drugs and therapeutic alternatives for the treatment of human malaria will emerge.

Acknowledgments: FAPEMIG, PIBIC/CNPq e Instituto René Rachou/FIOCRUZ-MG

Keywords: *malaria, ethnopharmacology, Plasmodium falciparum, natural products*



CHEMICAL COMPOSITION AND POTENTIAL ACTIVITY OF *Terminalia phaeocarpa* AND *Terminalia glabrescens* IN METABOLIC AND NEURODEGENERATIVE DISORDERS

Gabriel de Abreu P. Graca¹, José Hugo de Sousa Gomes¹, Gabriela Joice de Melo¹,
Rodrigo M. de Pádua¹, Fernão Castro Braga^{1*}

graca.gabap@gmail.com

1-Department of Pharmaceutical Products, Faculty of Pharmacy, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Diabetes mellitus type 2 (T2D) is a chronic metabolic disorder characterized by hyperglycemia and has recently been recognized as a risk factor for neurodegenerative diseases, particularly Alzheimer's disease (AD). Hyperglycemia contributes to neurodegeneration through oxidative stress, inflammatory response, and the formation of advanced glycation end products. Thus, glycemic control is critical to mitigate both the development and progression of AD among individuals with T2D. The *Terminalia* genus (Combretaceae) comprises over 250 species, many of which are traditionally used for their medicinal properties. Our research group previously reported the hypoglycemic activity of leaf extracts from *T. phaeocarpa* Eichler and *T. glabrescens* Mart.¹ In the present study, we investigated the hypoglycemic potential of ethanolic bark extracts of both species by evaluating their *in vitro* α -glucosidase inhibition activity. At 10 μ g/mL, inhibition reached $98.5 \pm 0.8\%$ for *T. phaeocarpa* and $98.07 \pm 1.5\%$ for *T. glabrescens*, with acarbose as positive control.¹ Additionally, we assessed the neuroprotective effects of leaf and bark extracts by measuring the reduction of glutamate-induced oxidative stress in SH-SY5Y neuroblastoma cells,² obtaining inhibition rates reaching up to $55.5 \pm 5.9\%$ at 30 μ g/mL. The chemical composition of the extracts was preliminarily analyzed by UHPLC-DAD-ESI-MS/MS. The ellagitannin 1- α -O-galloylpunicalagin was identified in bark extracts from both species; it had previously been isolated from *T. phaeocarpa* leaves by our group and associated with the hypoglycemic activity of that extract. A total of eight phenolic compounds have so far been identified in the bark extract of *T. phaeocarpa*, including tannins, flavonoids, and organic acids. Notably, the bark extract of *T. glabrescens* was found to be rich in proanthocyanidins. These metabolites may contribute to the antioxidant activity observed for the extracts. To the best of our knowledge, this is the first report on the biological activities and chemical composition of bark extracts from *T. phaeocarpa* and *T. glabrescens*.

Keywords: Diabetes, neurodegenerative diseases, *Terminalia* spp., UHPLC-DAD-ESI-MS/MS

¹ DE SOUSA GOMES, José Hugo *et al.* Polyphenol-rich extract and fractions of *Terminalia phaeocarpa* Eichler possess hypoglycemic effect, reduce the release of cytokines, and inhibit lipase, α -glucosidase, and α -amilase enzymes. Journal of ethnopharmacology, v. 271, p. 113847, 2021.

² ZHENG, Ting *et al.* Dexmedetomidine suppresses bupivacaine-induced parthanatos in human SH-SY5Y cells via the miR-7-5p/PARP1 axis-mediated ROS. Naunyn-Schmiedeberg's Archives of Pharmacology, v. 394, n. 4, p. 783-796, 2021.





ANTIMICROBIAL ACTIVITY AND CHEMICAL PROFILE OF ESSENTIAL OILS FROM *Duguetia lanceolata* LEAVES: A GNPS UNTARGET METABOLOMIC APPROACH

Simone S. Grecco^{1*}, Jackson Monteiro¹, Geovanna N. Antonelli¹, Erick P. Dantas¹, Marisi G. Soares², João H. G. Lago³, Renata C. Pascon¹, Marcelo A. Vallim¹, Patricia Sartorelli¹

*grecco.simone@unifesp.br

¹Instituto de Ciências Ambientais, Químicas e Farmacêuticas, UNIFESP, 09972-270, Diadema-SP, Brazil. ²Instituto de Química, UNIFAL, 37130-000, Alfenas-MG, Brazil. ³Centro de Ciências Naturais e Humanas, UFABC, 09210-180, Santo André - SP, Brazil.

The urgent need for novel antimicrobial agents has increased the interest in natural products, especially essential oils, as reservoirs of structurally diverse and bioactive molecules¹. In this study, we evaluated the antimicrobial properties of essential oils from *Duguetia lanceolata* leaves collected in different seasons, and correlated their chemical profiles with biological activity. Leaves were harvested in autumn (EO-A) and winter (EO-W), and the oils were analyzed by GC–MS supported by an untargeted GNPS metabolomic workflow. Antimicrobial activity was tested against Gram-positive and Gram-negative bacteria, as well as yeast strains, by disk diffusion and minimum inhibitory concentration (MIC) assays. EO-A demonstrated the most promising results, inhibiting the growth of *Acinetobacter baumannii*, *Candida krusei*, and *Candida parapsilosis* strains, often associated with multidrug resistance and nosocomial infections². MIC values ranged from 0.016 to 0.270 $\mu\text{g}\cdot\text{mL}^{-1}$, with EO-A consistently outperforming EO-W. Although both oils exhibited broad-spectrum activity, EO-W failed to inhibit several clinically relevant pathogens. These findings suggest that EO-A possesses not only a richer composition of monoterpenes, including limonene (28.5%) and (+)- β -pinene (15.0%), but also a more favorable antimicrobial profile compared to EO-W, which was enriched in sesquiterpenes such as β -bisabolene (16.4%) and β -gurjunene (6.4%)³. This work provides evidence that seasonal variation significantly modulates the antimicrobial efficacy of *D. lanceolata* essential oils. The superior activity of the autumn oil highlights the potential of this species as a natural source of antimicrobial agents and underscores the importance of seasonality in optimizing the collection of plant material for therapeutic applications. By combining metabolomics and bioassays, our results reinforce the value of Brazilian biodiversity in the search for new treatments targeting resistant pathogens.

Keywords: *Duguetia lanceolata*; Essential oils; Seasonal variation; GC–MS; Antimicrobial activity; GNPS untargeted metabolomics

References: ¹Yap, P.S.X., et al. 2014. *Open Microbiol J*, 8:6–14. ²Morrison, L., Zembower, T.R., 2020. *Gastrointest Endosc Clin N Am*, 4:619-635. ³Novais, M.H.G., et al., 2024. *Acta Trop* 253: 107168.

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**SCREENING OF ETHANOLIC EXTRACTS OF VARRONIA CURASSAVICA JACQ.
FOR COSMETIC APPLICATIONS: DEREPLICATION AND ENZYMATIC
INHIBITION ASSAYS**

João Vitor Souza de Oliveira^{1*}, Kyuri Ribeiro², Lorena Ramos Freitas de Sousa², Vanessa Gisele Pasqualotto Severino¹, Lucilia Kato¹

oliveira.joao@discente.ufg.br

1-Laboratório de Produtos Naturais e Síntese Orgânica, Instituto de Química, UFG, Av. Esperança, 74690-900, Goiânia, GO, Brazil. 2-Laboratório de Bioquímica e Química Orgânica – LaBiOrg, Universidade Federal de Catalão, Instituto de Química, 75704-020, Catalão, GO, Brazil.

Varronia curassavica Jacq. is a Brazilian native plant widely recognized for its anti-inflammatory activity, primarily attributed to α -humulene present in its essential oil. Although the essential oil has been extensively studied, the alcoholic extracts remain relatively underexplored [1]. To address this gap and better understand its potential applications, this study aims to chemically characterize the ethanolic extracts of Erva-baleeira and evaluate their activity in enzymatic inhibition assays with relevance to cosmetic applications. The extracts were obtained from leaves collected in Goiás using different extraction methods and analyzed by UHPLC-ESI(+)-HRMS/MS for chemical characterization. Raw data were processed using MZmine 4, employing dereplication tools such as GNPS and *in silico* platforms like SIRIUS. Enzyme inhibition was evaluated spectrophotometrically against porcine pancreatic elastase (EC 254-453-6) and mushroom tyrosinase (*Agaricus bisporus*, EC 1.14.18.1), with kojic acid and quercetin used as positive controls, respectively. The extracts exhibited strong elastase inhibition, reaching up to 96.41% at 100 μ g/mL. On the other hand, tyrosinase inhibition was limited, with a maximum of 5.94%. Dereplication indicated the presence of flavonoid molecules, including artemetin (m/z 389.1248), casticin (m/z 375.1082), and kaempferol-3-*O*-hexoside (m/z 449.1076). Since flavonoids are known to inhibit elastase [2], these compounds likely may contribute to the observed enzymatic activity. To further correlate structure with enzymatic activity, liquid-liquid partitioning of the most active extract was performed, and additional LC-MS analyses and enzymatic assays will be conducted for the fractions. While weak tyrosinase inhibition suggests minimal depigmenting potential, the strong elastase inhibition highlights the ethanolic extracts of *V. curassavica* as promising candidates for anti-aging strategies aimed at preserving dermal matrix integrity. The authors would like to acknowledge the support of the University of Wuppertal and Livealoe, as well as funding agencies such as FINEP, FAPEG, CNPQ, and CAPES.

Keywords: Erva-baleeira, elastase, dereplication, mass spectrometry.

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VIRTUAL SCREENING OF NATURAL PRODUCTS AS POTENTIAL INHIBITORS OF AMYLOID-BETA OLIGOMER-INDUCED NEUROTOXICITY

Mayara Carla dos Santos^{1,4*}, Priscila Baltazar Gonçalves², Yraima Lopes Cordeiro², Ana Carolina R. Sodero³, Julia Helena Rosauro Clarke⁴, Ivana Correa Ramos Leal^{1*}

mayaracarla.farm@gmail.com

¹Laboratório de Produtos Naturais e Ensaio Biológicos, Departamento de Produtos Naturais e Alimentos, Faculdade de Farmácia, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil.

²Laboratório de Biologia Molecular e Estrutural, Faculdade de Farmácia, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil. ³Laboratório de Modelagem Molecular e QSAR, Faculdade de Farmácia, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil. ⁴Laboratório de Investigação em Neuroprogramação, Instituto de Ciências Biomédicas, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil.

Alzheimer's disease (AD) is the leading cause of dementia worldwide, pathologically characterized by the aggregation of the amyloid-beta (A β) peptide. During the A β aggregation pathway, various aggregate species are formed, including oligomers, protofibrils, and fibrils. Among these, soluble A β oligomers (A β O) are considered the most neurotoxic species. Natural products (NPs) are recognized as a promising source of anti-amyloid compounds, including inhibitors of A β O-induced neurotoxicity¹. Brazilian biodiversity offers a rich source of structurally diverse natural compounds with significant potential for new drug discovery. In this study, we investigated the NuBBE database (NuBBEDB)² using a virtual screening approach, combining molecular docking and ADMET profile prediction to identify potential inhibitors of A β oligomer-induced toxicity. A total of 2,363 compounds were docked into the A β O structure (PDB ID: 6RHY) using AutoDock Vina³. The top 50 hits with the highest binding affinities were selected for each binding site: the hydrophilic edge pocket (P0 e P1) and the hydrophobic core pocket (P2). To predict their ADMET profiles, these compounds were analyzed using the Admet_Risk module in ADMET Predictor® 13. A risk score cutoff of Admet_Risk $\leq$ 6.5 was applied to prioritize the safest and most promising candidates for experimental validation and BBB_Filter. High-risk candidates were excluded, and the remaining hits were ranked based on lower ADMET risk scores and high BBB penetration probability. As a result, 14 compounds simultaneously met the Admet_Risk $\leq$ 6.5 criterion and were approved by the BBB_Filter. These compounds belong to the chemical classes of 12 tri- and di-type polycycle terpenoids and two indolic alkaloids. These results highlight promising candidates for further experimental validation. Their final binding affinities ranged from -9.407 to -7.293 kcal/mol at the hydrophilic edge binding pockets (P1 e P0) and from -7.747 to -5.504 kcal/mol at the hydrophobic core binding pocket (P2), highlighting their potential as candidates for inhibitors of A β O-induced toxicity. Herein, our goal is to identify the most promising candidates for further investigation through biophysical assays and imaging techniques.

Keywords: Alzheimer's Disease, Anti-amyloids, Amyloid-beta, Oligomers, Virtual Screening, Molecular Docking.



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FORMULATION OF A STABLE NANOEMULSION WITH THE ESSENTIAL OIL OF *PIPER BRACHYPETIOLATUM*

jvcdos.dbb25@uea.edu.br

João Vyctor C. de O. Santos¹, Marcelo de Sousa² Helena H. G Ramos², Brenda R. C. Leocadio², Juliana A. Ximenes², Antônia Q. de Souza¹, Rita de C. S. Nunomura²

1-Universidade do Estado do Amazonas Conheça a UEA Escola Superior de Ciências da Saúde Edifício Anexo, 4º andar Secretaria Estadual do PPG-BIONORTE/AM Av. Carvalho Leal, 1777, Bairro Cachoeirinha: CEP: 69065001 Manaus -AM. . Universidade Federal do Amazonas – UFAM, CEP 69080-900, Manaus - AM

Plant species of the Piperaceae family stand out for the commercial and pharmacological potential of their essential oils, recognized for antimicrobial, antioxidant, and insecticidal activities. However, the high volatility of these compounds limits their use. As an alternative, nanoemulsions have emerged to improve stability, bioavailability, and efficacy. This study aimed to develop and evaluate nanoemulsions containing the essential oil of *Piper brachypetiolatum*, given its potential biological activities, in order to enhance its bioactive properties and broaden its biotechnological and pharmaceutical applications¹. The leaves of *Piper brachypetiolatum* were subjected to hydrodistillation using a Clevenger apparatus, and the chemical profile of the essential oils was analyzed by GC-MS. The yield of *P. brachypetiolatum* essential oil was 0.85%, and GC-MS analysis revealed 12 compounds, mainly sesquiterpenes (50.0%) and oxygenated sesquiterpenes (25%). Nanoemulsions containing the essential oil of *Piper brachypetiolatum* were prepared according to established protocols². A total of 0.1 g of essential oil was diluted in 0.1 g of Tween 20 and 0.2 g of Tween 80, used as emulsifying agents. The mixture was subjected to mechanical stirring for 5 minutes, with 3-minute intervals between cycles. This process resulted in the formation of a stable nanosystem, in which the essential oil was efficiently incorporated into nanometric-sized particles. The formulations were subsequently characterized for particle size and zeta potential using a Zetasizer (Malvern, UK). The average particle diameter was 114.4 nm, within the typical range for nanoemulsions (20–200 nm), with a polydispersity index (PI) of 0.293, indicating a relatively homogeneous distribution. The zeta potential (–59.8 mV) suggested high colloidal stability, with low aggregation tendency and strong physicochemical stability of the system.

Keywords: Colloidal systems, polydispersity, emulsifiers, Piperaceae.

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PLANT-DERIVED INSECTICIDES: THE POTENTIAL OF CERRADO VEGETATION AGAINST LEAFCUTTER-ANTS

Eduarda Oliveira dos Santos^{1*}, Gabriele Fernanda da Silva¹, Anderson do Rego Pires¹

Lulliana Thalita Franco¹, Raul Vinícius Silva² Odair Correa Bueno², Maria Fátima das

Graças Fernandes da Silva¹, João Batista Fernandes¹

eduardaosantos853@gmail.com

1-Laboratório de Produtos Naturais, Departamento de Química, UFSCar, Rod. Washington Luís, s/n - Monjolinho, São Carlos - SP, Brazil. 2- CEIS-Centro de estudos de insetos sociais, Instituto de Biociência, UNESP, Av. 24-A, nº1515, Rio Claro-SP, Brazil.

Leafcutter ants remain among the most damaging agricultural pests in South America, causing severe economic losses in pinus and sugarcane crops. In the search for new approaches to integrated pest management and to reduce the environmental impact of conventional pesticides on non-target organisms, natural products with specific insecticidal activity have gained increasing attention. *Nectandra rigida* (Lauraceae), is a cerrado vegetal species, known as a notable font of alkaloids and lignans of insecticidal potential. This work aimed to investigate the insecticidal potential of methanolic stem extract of *Nectandra rigida* against the leafcutter ant (*Atta sexdens*), and the symbiotic fungi *Leucoagaricus gongilophorus*. The effect of the metabolites in the acetylcholinesterase enzyme (AsAChE) was evaluated as well as the proposed of specific action of natural-based insecticides. Stem extracts were evaluated through laboratory bioassays with worker ants, showing 98% of mortality within 9 days. Additionally, AsAChE inhibition assays were carried out using biosensors to explore a possible mechanism of action, as indicated by the inhibition of 31% of the activity at a 5 mg/mL concentration. Thus, the stem extract induced a 16 mm halo of inhibition of the symbiotic fungi, suggesting a multi-target insecticidal effect. Ongoing spectroscopic and chromatographic analyses aim to characterize the chemical profile of the extract and identify the secondary metabolites responsible for the observed activities. These findings highlight *Nectandra rigida* as a promising natural source of bioinsecticides, for the management of leafcutter ants.

Keywords: Leafcutter ants, *Nectandra Rigida*, acetylcholinesterase, *Leucoagaricus gongilophorus*





SEASONAL EFFECT ON CHEMICAL COMPOSITION AND CYTOTOXIC
EFFECT OF THE ESSENTIAL OIL OF *Vitex agnus-castus* L.

Rayane Correa Souza^{1*}, Lucas Botelho Jerônimo², Laine Celestino Pinto³, Pablo Luís Baia Figueiredo²

Rayane.souza@icen.ufpa.br

1-UFPA, ICEN, Rua Augusto Corrêa, 66075, Belém, PA, Brasil. 2- UEPA, PPGCA, Tv. Dr. Enéas Pinheiro, 66095-015, Belém, PA, Brasil. 3- HUJBB, R. dos Mundurucus, 4487, 66073-000, Belém, PA, Brasil.

Cancer is a complex disease that evolves through multiple pathogenetic mechanisms, involving modifications in the function of several oncogenes and genes that act in tumor suppression. *Vitex agnus-castus* L (Lamiaceae), popularly known as Angolan rosemary, is a medicinal plant that produces essential oil (EO). This study aims to evaluate the seasonal effect on the chemical composition and cytotoxic activity of *V. agnus-castus* EO. The leaves were collected in Belém, between November 2023 and August 2024. A voucher was incorporated into the UEPA Herbarium (MFS-010520). The leaves were dried in a climate-controlled room, crushed, and subjected to extraction with a modified Clevenger extractor for 3 h. GC-MS analyzed the chemical composition. The in vitro cytotoxicity analysis of EOs was performed using the MTT assay. The rainy season occurred from December to May, with average precipitation of 456.7 ± 164.1 mm, and the dry season from November, June, July and August, with average precipitation of 108.5 ± 70.9 mm. The main chemical constituents (> 5%) were 1,8-cineole (2.07-16.93%), (*E*)- β -Farnesene (5.74-11.19%), Bicyclogermacrene (3.02-8.89%), Sabinene (0.27-7.48%), (*E*)-caryophyllene (3.02-7.45%). The EOs showed antiproliferative activity against the cancer cell lines: gastric ascites (AGP-01), glioblastoma (AHOL), lung carcinoma (A549) and against the healthy murine macrophage cell line (RAW-264). The months with the highest cytotoxic activity against AGP-01 cells were April (IC₅₀ 4.15 mg/mL), November (IC₅₀ 4.23 mg/mL), and December (IC₅₀ 5.71 mg/mL). For AHOL and A549 cells, November (IC₅₀ 4.21 and 10.41 mg/mL) and December (IC₅₀ 4.75 and 11.80 mg/mL) were the months with the highest cytotoxic activity. Furthermore, anticancer activity was demonstrated in January (IC₅₀ 12.51 mg/mL) for A549. Thus, the months with the greatest toxicity for RAW-264 were November (IC₅₀ 5.47 mg/mL), April (IC₅₀ 5.54 mg/mL), and July (IC₅₀ 9.17 mg/mL). *Vitex agnus-castus* is a plant that produces biologically active molecules against cancer.

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Keywords: Terpenos, Anticâncer, Amazônia.





ANTIMICROBIAL PROPERTIES OF *EUGENIA* SPP.: ACTIVITY AND MECHANISMS AGAINST BACTERIAL AND FUNGAL PATHOGENS

Patryne L. da S. Dantas^{1*}, Leticia Bachmann¹, Alysson C. Blaese², Raquel Oppermann¹; Adrielli Tenfen²; Tatiani K. R. Botelho¹, **Michele D. Alberton^{1,2}**

michele@furb.br

1- Programa de Pós-Graduação em Biodiversidade, Universidade Regional de Blumenau. 2- Programa de Pós-Graduação em Química, Universidade Regional de Blumenau, Rua Antônio da Veiga 140, Blumenau, SC, Brazil, 89030-903.

The antimicrobial activity of the hydroalcoholic extracts of *Eugenia mattosii*, *E. astringens*, *E. catharinensis*, *E. involucrata*, *E. brasiliensis*, and *E. platysema* was evaluated against *S. aureus*, *E. coli*, *K. pneumoniae*, *P. aeruginosa*, *Salmonella* sp. (clinical strain), *S. aureus* MRSA (clinical strain), *S. epidermidis* (clinical strain), *C. albicans*, *C. parapsilosis*, and *C. krusei* (clinical strain), following CLSI (2012) and CLSI (2017) protocols. The project is registered in SISGEN under number A7519AA. *E. astringens* showed the most potent antimicrobial activity, with MIC values of 14 µg/mL against *S. aureus*, MRSA, and *S. epidermidis*. *E. brasiliensis* and *E. mattosii* also exhibited activity, particularly against Gram-positive strains (MIC 125–250 µg/mL). Among the tested yeasts, *E. astringens*, *E. brasiliensis*, and *E. mattosii* displayed the strongest antifungal effects, notably against *C. parapsilosis* (MIC 31, 31, and 62 µg/mL, respectively). The fractionation of *E. astringens* and *E. mattosii* confirmed their antimicrobial potential. For *E. astringens*, the insoluble fraction exhibited the strongest activity against *S. aureus* and MRSA (MIC < 7 µg/mL), while the aqueous fraction was highly active against *S. epidermidis* (MIC < 7 µg/mL). The aqueous fraction of *E. mattosii* was the most active, with MIC of 31 µg/mL against *C. parapsilosis*. The ethyl acetate and insoluble fractions also presented activity, with MIC values ranging from 62 to 125 µg/mL against *S. aureus* and *C. parapsilosis*. The addition of exogenous ergosterol markedly increased the MIC or completely abolished the antifungal activity of *E. astringens* and *E. mattosii* against *C. parapsilosis*. This behavior parallels the control amphotericin B, whose MIC increased from 3.9 µg/mL to 500 µg/mL when ergosterol was present. Together, these findings strongly suggest that the antifungal action of *E. astringens* and *E. mattosii* is associated with interactions at the fungal cell membrane, likely involving ergosterol binding. No evidence of fungal cell wall involvement was observed in the sorbitol assay. The study is ongoing with the phytochemical characterization of the evaluated extracts.

Keywords: *Eugenia*; Antimicrobial activity; Fungal Cellular Membrane





**PHYTOCHEMICAL AND BIOLOGICAL INVESTIGATION OF *XYLOPIA SERICEA*
(ANNONACEAE) BARK EXTRACTS**

Rubens Sousa Soares^{1*}, Lucas Tavares dos Santos¹, Francisca Maria Macêdo Pereira¹,
Jurandy do Nascimento Silva¹, Sâmya Danielle Lima de Freitas¹

soares@ufpi.edu.br

1- Department of Chemistry, UFPI, Teresina, PI, 64049-550, Brazil.

Xylopia sericea St. Hil. (Annonaceae) is an aromatic species native to Brazil, popularly known as “embiriba,” and traditionally used in folk medicine as an analgesic, anti-inflammatory, and for the treatment of gastrointestinal disorders¹. The species occurs across several Brazilian biomes, including Cerrado, Amazon, Caatinga, and Atlantic Forest². Given the scarcity of studies on *X. sericea*, this work aimed to perform the phytochemical and biological investigation of the ethanol extract from stem bark and its fractions. The ethanol extract (EX) was obtained by exhaustive extraction with ethanol, and the hexane (FH), ethyl acetate (FA), and methanolic (FM) fractions were obtained through column filtration chromatography. EX, FA, and FM were analyzed by HPLC-DAD to estimate the classes of compounds present, revealing intense absorption bands at 290 nm, indicative of phenolic compounds, in addition to broad bands between 15 and 45 minutes, characteristic of polyphenols belonging to the tannin class. The antioxidant activity of the extracts EX, FH, FA, and FM

SAMPLE	EC ₅₀ (µg mL ⁻¹)	Total phenolics (µg GAE mL ⁻¹ of sample ± SD)
EX	7.13 ± 0.09	333.84 ± 1.26
FH	> 4000 (no response)	3.83 ± 1.24
FA	4.24 ± 0.02	337.46 ± 1.66
FM	3.66 ± 0.01	337.83 ± 1.09
Ascorbic acid	22.72 ± 0.13	-
Trolox®	14.92 ± 0.41	-

Table 1. Average efficient concentration (EC₅₀) and total phenolics of samples

was evaluated using the DPPH radical scavenging assay, with ascorbic acid and Trolox® as controls. All samples, except FH, showed EC₅₀ values lower than the standards, confirming high antioxidant potential. The total phenolic content, determined by the Folin-Ciocalteu method and expressed as gallic acid equivalents (GAE), ranged from 333.84 to 337.83 mg GAE mg⁻¹ and correlated with the antioxidant activity observed and the HPLC results. These findings highlight not only the abundance of phenolic compounds but also their functional efficiency against the DPPH radical, emphasizing the remarkable chemical and biological potential of *Xylopia sericea*. The authors thank the Natural Products Laboratory, the Ecobiomaterials Laboratory, and the Federal University of Piauí.

¹MENDES, R. F. et al. **J. Pharm. Pharmacol.**, v. 69, n. 3, p. 341–348, 2017. ²EMBRAPA. *Xylopia sericea* A. St.-Hil. Brasília, DF: Embrapa, [s.d.].

Keywords: *Xylopia sericea*, biological activities e phenolic compounds





EVALUATION OF VOLATILE COMPOUNDS FROM *Trichoderma* STRAINS IN THE BIOCONTROL OF PHYTOPATHOGENS

Ana Paula Alfaia Castro^{1*}, Emerson Freires Viana¹, Ester Barroncas de Souza Teixeira¹, Rafael de Souza Rodrigues¹, Gilvan Ferreira da Silva¹

ana.alfaia@ufam.edu.br

1-Embrapa Amazônia Ocidental, Rodovia AM-010, Km 29, s/n, 69010-970, Manaus-AM, Brasil.

In different areas of the Amazon, important structures for conservation and sustainable use can be found, such as the Rio Negro Sustainable Development Reserve (RDS-RN) in Manaus (AM) and the Pico da Neblina National Park (PNPN) in São Gabriel da Cachoeira (AM). Both may be strategic for the isolation of microorganisms with a focus on molecule prospecting; among fungi, the genus *Trichoderma* stands out, recognized for producing volatile organic compounds (VOC's), which are important in the control of phytopathogens and in promoting plant growth¹. Although ecologically important, the soils of these areas still present gaps in microbial diversity, highlighting the need for further scientific and biotechnological studies. In this context, the present work evaluated three *Trichoderma* strains (CPAA TC66, CPAA EBST18, and CPAA EBST20), isolated from Amazonian soils (PNPN and RDS-RN), regarding VOC's production and inhibition of mycelial growth of the phytopathogen *Agroathelia rolfsii* INPA 2941, aiming to understand their bioactive potential and biotechnological applications. The strains were previously cultivated in PDA medium (potato-dextrose-agar), and 5×5 mm disks of the *Trichoderma* strains and the phytopathogen were inoculated in 60 mm plates. For VOC's assays, the "sandwich" system was used, in which the bases of two plates were juxtaposed: the lower containing *Trichoderma* and the upper the phytopathogen, sealed and incubated at 28 ± 1 °C for five days. Antagonistic activity was quantified by the percentage of mycelial growth inhibition ($PGI = [(control - treatment) / control] \times 100$), in triplicate. Preliminary results indicated high inhibitory activity of the three strains. In the VOC's assay, CPAA TC66, CPAA EBST18, and CPAA EBST20 inhibited the growth of *A. rolfsii* by 80.90%, 78.57%, and 57.14%, respectively. In addition to the reduction in mycelial growth, no sclerotia formation was observed compared to the control. These results suggest that *Trichoderma* VOC's suppress both growth and the formation of resistance structures of *A. rolfsii*, reinforcing the potential of these strains for biotechnological applications in phytopathogen management.

Keywords: Amazonian *Trichoderma*, biocontrol, volatile organic compounds (VOC's).

1-Trichoderma agriamazonicum sp. nov. (Hypocreaceae), a new ally in the control of phytopathogens. *Microbiological Research*, v. 275, p. 127469, 2023.





PHENOLIC PROFILE AND IN VITRO ACETYLCHOLINESTERASE AND α -GLUCOSIDASE INHIBITION OF *Myrcia tijuensis* EXTRACTS

Diogo A. Siebert¹, Camila J. Paganelli¹, Camila P. Valcanaia¹, Michele D. Alberton^{1*}

dsiebert@furb.br

1–Laboratory of Research on Natural Products, Department of Pharmaceutical Sciences, Universidade Regional de Blumenau, Rua São Paulo 2171, Blumenau, SC, 89030-001, Brazil.

Alzheimer's disease (AD) is a progressive neurodegenerative disorder whose global prevalence is expected to almost triple by 2050, and current therapies are limited by high failure rates and adverse effects. Type 2 diabetes mellitus, accounting for about 90% of diabetes cases worldwide, also poses a major public health problem. Synthetic drugs used for these conditions often cause side effects, and plant-derived compounds are considered for their therapeutic potential. The genus *Myrcia* is traditionally used in diabetes management. This study aims to evaluate, for the first time, *Myrcia tijuensis* Kiaersk. extracts for acetylcholinesterase and α -glucosidase inhibition and their chemical profile by HPLC-ESI-MS/MS. Aerial parts of *M. tijuensis* were collected in Blumenau (SC, Brazil) in August 2018. A voucher specimen was deposited at FURB Herbarium (no. 02089), and the project is registered in SISGEN under number A7519AA. Leaves and stems were dried, milled and macerated for seven days with dichloromethane, ethyl acetate or 70% ethanol to obtain crude extracts. Infusions were prepared by adding leaves or stems in 400 mL of boiling water for 15 min and lyophilized. Secondary metabolite classes were screened by colorimetric assays. Phenolic compounds were quantified by HPLC-ESI-MS/MS using 47 standards. Acetylcholinesterase and α -glucosidase inhibitory activities were evaluated *in vitro* following Ellman's and pNPG-based methods, respectively. Hydroalcoholic, ethyl acetate and dichloromethane extracts from leaves and stems of *M. tijuensis*, as well as their infusions, were obtained with variable yields. Hydroalcoholic extracts showed the highest recovery. Preliminary phytochemical screening revealed phenols, tannins, anthocyanins, flavonoids, catechins, steroids, triterpenoids and saponins, especially in leaf infusions and stem hydroalcoholic extracts. HPLC-ESI-MS/MS identified 17 phenolic compounds, including quercetin, ellagic acid, syringaldehyde and several phenolics reported for the first time in the genus. Enzymatic assays demonstrated potent α -glucosidase inhibition, with dichloromethane stem extract exhibiting the lowest IC₅₀ (0.05 mg/mL), and strong acetylcholinesterase inhibition in ethyl acetate leaf extract, dichloromethane stem extract and stem infusion (< 0.007 mg/mL), suggesting relevant antidiabetic and neuroprotective potential. This study demonstrates that *M. tijuensis* contains diverse phenolic compounds and shows significant *in vitro* inhibition of acetylcholinesterase and α -glucosidase, supporting its potential as a source of bioactive molecules for therapeutic development.

Keywords: *Myrcia tijuensis*, phenolic compounds, acetylcholinesterase inhibition, α -Glucosidase inhibition.





***INSECTICIDAL POTENTIAL OF Parahancornia amapa (Apocynaceae)
AGAINST Atta sexdens: ISOLATION AND CHARACTERIZATION OF
BIOACTIVE COMPOUNDS***

Anderson do Rego Pires^{1*}, Sean dos Santos Araujo¹, Gabriele Fernanda da Silva¹, Eduarda Oliveira dos Santos¹; Luis Guillermo Cuadrado Durango¹; Dorai Perioto Zandonai¹, Odair Correa Bueno², João Oiano Neto³; Maria Fátima das Graças Fernandes da Silva¹; João Batista Fernandes¹

*andersonrp@estudante.ufscar.br

¹-Chemistry Department, UFSCar, Rod. Washington Luís, Km 235 - Monjolinho, São Carlos, SP, 13565-905, Brazil. ²- Center for Social Insect Studies, UNESP, Avenida 24-A, 1515, Bela Vista, Rio Claro, SP, 13.506-900, Brazil. ³- Embrapa Pecuária Sudeste, Rod. Washington Luiz, km 234 s/nº, Fazenda Canchim, São Carlos, SP, 13560-970, Brazil.

Leaf-cutter ants of the genera *Atta* and *Acromyrmex* rank among the most destructive agricultural pests due to their aggressive herbivory. The widespread and indiscriminate use of synthetic pesticides to control these insects has led to severe environmental impacts, threatening ecosystem integrity and posing significant public health risks. In this context, Natural Products Chemistry emerges as a sustainable and promising approach, enabling the isolation of secondary metabolites with potential insecticidal activity. The Amazonian species *Parahancornia amapa* (Huber) Ducke is traditionally used as a natural insecticide, was investigated through exhaustive extraction, followed by chromatographic fractionation using silica gel (230–400 mesh), high-performance liquid chromatography (HPLC), LC coupled with mass spectrometry (LC-MS/MS), and nuclear magnetic resonance (NMR), enabled the isolation of previously unreported compounds in this species. Toxicity bioassays conducted with extracts and fractions from the twigs and leaves of *P. amapa* against medium-sized worker ants of *Atta sexdens* guided the isolation of bioactive metabolites. From the twig fraction, two novel alkaloids, a new pterocarpan derivative, and a previously unreported benzopyran were isolated. From the leaf fraction, three compounds were identified: an aryl-naphthalene lactone Justicidin B and two known flavonoids catechin and quercetin. The bioactive fractions from both twigs and leaf, from which these compounds were isolated, induced 100% mortality ($p < 0.05$) of *A. sexdens* worker ants within 12 and 14 days, respectively. Furthermore, the twig fraction exhibited inhibitory activity against *A. sexdens* acetylcholinesterase (AsAChE), with IC₅₀ values of 12.96 mg·L⁻¹ (± 1.02) for isoform A and 9.51 mg·L⁻¹ (± 0.35) for isoform B, suggesting a neurotoxic mechanism of action. These findings highlight *P. amapa* as a promising natural source of insecticidal compounds, reinforcing its potential as an eco-friendly alternative to conventional synthetic pesticides for the control of leaf-cutter ants.

Keywords: Natural Products, *P. amapa*, Insecticide, *Atta sexdens*, AsAChE.





ISOLATION, STRUCTURAL ELUCIDATION, AND POTENTIAL ANTIDIABETIC ACTIVITY OF α -GALLOYLPUNICALAGIN FROM THE LEAVES OF *Terminalia phaeocarpa*

José Hugo de S. Gomes^{1*}, Rodrigo M. de Pádua¹, Steyner de F. Cortês², Fernão C. Braga¹

josehugoufmg@gmail.com

1-Faculdade de Farmácia, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 2-Instituto de Ciências Biológicas, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Diabetes is a highly prevalent chronic disease, affecting approximately 830 million people worldwide¹. Despite therapeutic advances, current treatments remain of limited effectiveness, and bioactive natural products have emerged as an important source of therapeutic innovation. Species of *Terminalia* have different ethnomedicinal uses, and the potential antidiabetic activity of some species has been demonstrated in various experimental models. *T. phaeocarpa* is an endemic tree distributed across the Brazilian Cerrado and Atlantic Forest biomes, whose chemical composition and biological activities have never been investigated. The present study aimed to perform a phytochemical investigation of *T. phaeocarpa* leaves and to assess their potential antidiabetic activity through *in vitro* inhibition of the α -glucosidase enzyme². An ethanolic extract was prepared by percolation with 96 °GL EtOH, followed by fractionation between immiscible solvents. The extract induced significant α -glucosidase inhibition (pIC_{50} = 5.46 ± 0.05), as did the derived ethyl acetate (FrEtOAc; pIC_{50} = 5.79 ± 0.11) and methanol/water (7:3) (FrMeOH:H₂O; pIC_{50} = 5.74 ± 0.05) fractions. UHPLC-ESI-MS/MS analysis of the extract, FrEtOAc, and FrMeOH:H₂O led to the identification of 38 phenolic compounds, including tannins, flavonoids, and organic acids. The obtained chromatograms revealed a major peak in FrEtOAc. To isolate this constituent, FrEtOAc was fractionated over a Sephadex LH-20 column, yielding a tannin-enriched fraction in MeOH/acetone (1:1). Subsequent preparative RP-HPLC purification afforded a single ellagitannin. Both the tannin-enriched fraction (pIC_{50} = 1.61 ± 0.04) and the isolated ellagitannin (IC_{50} = 1.56 ± 0.93 μ M; pIC_{50} = 5.95 ± 0.27) were evaluated for *in vitro* α -glucosidase inhibition, confirming that the biological activity was concentrated in these samples. The chemical structure of the ellagitannin was elucidated by UHPLC-MS together with extensive ¹H and ¹³C NMR analyses, including one- and two-dimensional experiments (HSQC, HMBC, and NOESY). The spectroscopic data allowed its unequivocal identification as 1- α -O-galloylpunicalagin, a compound not previously reported in *T. phaeocarpa*. This is the first report on the biological activity and chemical composition of *T. phaeocarpa*. Based on previous evidence of polyphenol activity in diabetes, it is feasible to suppose that other polyphenols identified in the species may also contribute to the observed biological effects.

Keywords: *Terminalia phaeocarpa*, ¹H NMR, α -galloylpunicalagin, *in vitro*, α -glucosidase, IC_{50}

¹ WHO - World Health Organization. Diagnosis and management of type 2 diabetes (HeartsD). Geneva, Switzerland: 2025. Disponível em <<https://apps.who.int/iris/handle/10665/331710>>>

² Gomes JHS et al., 2021. Hypoglycemic and enzyme inhibitory effects of *Terminalia phaeocarpa*. J. Ethnopharmacol.





***PREDATORY BEHAVIOR AND ANTIBACTERIAL POTENTIAL OF
MYXOBACTERIA ISOLATED FROM BRAZILIAN COASTAL ECOSYSTEMS***

Bruno Farah Mastrorosa Luquetti^{1*}, Renan da Silva de Oliveira¹, Paula Christine Jimenez¹

* bruno.luquetti22@unifesp.br

¹Instituto do Mar, Universidade Federal de São Paulo, Campus Baixada Santista, Santos, SP – Brazil

Myxobacteria are Gram-negative rod-shaped bacteria that exhibit complex social behaviors, including cooperative predation. This strategy relies on the secretion of hydrolytic enzymes and specialized metabolites, many of which display antibacterial, antifungal, and anticancer activities. Despite their recognized biotechnological potential, studies on myxobacteria from coastal ecosystems remain limited, leaving a largely unexplored microbial diversity. This study aimed to study the micropredatory behavior of Brazilian marine myxobacteria considering the production of secondary metabolites. In this context, 22 strains from the MyxoMarin collection, the first collection dedicated to the curation of culturable myxobacteria strains from Brazilian coastal environments, were cultivated in liquid VY/2 medium supplemented with XAD-16 resin (2%). Crude extracts were obtained by acetone:methanol (1:1) extraction and screened for antibacterial activity against *Escherichia coli* using the TTC assay at 250 µg/mL. A total of 13 strains produced extracts with noteworthy activity, with inhibition values ranging from 11.81% to 48.22%, highlighting BRX070 (48.22%) and BRX029 (41.64%) as the most active. Predation assays were carried out with the initial 22 strains in solid WCX medium containing *E. coli* DH5α as bait. While various strains revealed compelling predatory capacity, BRX070 and BRX029 displayed significant growth in such conditions accompanied by extensive lysis zones across *E. coli* inoculum, compared to the other strains. Therefore, these strains were selected for coculture with *E. coli* DH5α in liquid medium followed by extract production. Crude extracts were analyzed by HPLC-DAD, which revealed clear differences in chemical profiles between those obtained by myxobacteria in coculture or in axenic conditions. However, no increase in antibacterial activity was observed. Although coculture did not enhance antibacterial activity, the observed chemical shifts suggests differential activation of biosynthetic pathways, highlighting the need for further studies focusing on the elucidation and function of these compounds induced in coculture conditions. Moreover, further studies must also focus on investigating hydrolytic enzyme production, which play a central role in predation, to better understand the mechanisms underlying prey degradation. Together, these findings underscore the promise of myxobacteria as valuable sources for the discovery of new antibiotics and hydrolytic enzymes of biotechnological relevance.

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Keywords: Marine biotechnology; marine natural products; micropredators; enzymatic activity; antibiotics.





CHEMICAL CHARACTERIZATION, ANTIOXIDANT ACTIVITY AND IN VITRO CYTOTOXICITY OF BACABA PULP EXTRACT (*Oenocarpus bacaba* Mart.)

Raphael Oliveira de Figueiredo², Matheus da Costa de Almeida¹, Daniel Barbosa Santos¹,
Laine Celestino Pinto², Paulo Wender Portal Gomes², Joyce Kelly da Silva², Pablo Luis Baia
Figueiredo^{1*}

Email: pablo.figueiredo@uepa.br

¹Universidade do Estado do Pará, ²Universidade Federal do Pará,

Oenocarpus bacaba Mart. (Arecaceae) is native to Brazil and abundant in the Amazon region. The fruit is rich in several bioactive compounds with antioxidant and antimicrobial properties¹. This work aimed to characterize the chemical composition of fruit pulp hydroethanolic extract of *O. bacaba* (BHE), evaluate its antioxidant capacity, estimate the total phenolics (TF) and the cytotoxicity. The fruit pulp was freeze-dried, and 10 g of dried pulp was exhaustively extracted with hexane, followed by a hydroethanolic solution (70% ethanol). Chemical composition analysis was performed by liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS), and the spectra were compared to the GNPS and MoNA libraries. In vitro antioxidant assays were evaluated using the DPPH and β -carotene/linoleic acid methods². The cytotoxicity (MTT assay) was evaluated against breast cancer (Sk-MEL-19), gastric ascites (AGP01), lung cancer (A549), and normal human lung fibroblasts (MRC5). BHE showed relative predominance of the flavonoids isoquercitrin and isorhamnetin-3-glucoside-4'-glucoside, followed by quinic acid, ferulic acid and caffeic acid. BHE inhibited $56.8 \pm 2.9\%$ of DPPH radicals, approximately twice as active as the trolox (633.7 ± 32.2 mg.TE/g). In the lipid peroxidation assay, BHE inhibited β -carotene oxidation by $36.3 \pm 0.8\%$, indicating good antioxidant capacity. The BHE presented a moderate classification for FT (2.54 ± 0.21 mg.GAE/g). In the study by Neves et al. (2015)³, the aqueous extract presented a low classification (0.081 to 0.11 mg GAE/g), possibly associated with the extraction method (water at 50°C). Another study identified a high phenolic content of 42.07 mg GAE/g in the bacaba peel. The BHE showed moderate cytotoxicity in the tumor lines Sk-MEL-19 (IC₅₀ = 91.04 μ g/mL, SI = 0.41), AGP-01 (IC₅₀ = 33.45 μ g/mL, SI = 1.13), and A549 (IC₅₀ = 43.67 μ g/mL, SI = 0.86), as well as in the healthy cell line MRC-5 (CI₅₀ = 37.80 μ g/mL), but without selectivity, Selective Index (SI) less than 2.0. Therefore, BHE have promising applications in the pharmaceutical and food industries.

¹Santos Filho, A. F., Toro, M. U., & Ferreira, I. C. (2020). Estudo fitoquímico, enzimático e capacidade antioxidante da polpa de bacaba (*Oenocarpus bacaba* Mart). *Cientific@ - Multidisciplinary Journal*, 7(2), 1–17; ²Carvalho, NCC, Monteiro, OS, da Rocha, CQ, Longato, GB, Smith, RE, da Silva, JKR, & Maia, JGS (2022). Análise Fitoquímica dos Extratos da Polpa do Fruto de *Annona crassiflora* Mart. e Avaliação de suas Atividades Antioxidante e Antiproliferativa. *Foods*, 11 (14), 2079; ³Neves, L. T. B. C., Campos, D. C. D. S., Mendes, J. K. S., Urnhani, C. O., & Araújo, K. G. M. D.. (2015). qualidade de frutos processados artesanalmente de açai (*Euterpe oleracea* Mart.) e bacaba (*Oenocarpus bacaba* Mart.). *Revista Brasileira De Fruticultura*, 37(3), 729–738.

Keywords: Flavonoids; isoquercitrin; LC-MS/MS.





ANTIMICROBIAL ACTIVITY OF PARTITIONS OF *Diplopterys pubipetala*

Veronica de Melo Sacramento^{1*}, Luis Henrique Rodrigues Rocha¹, Carla Jeane Marinho de Caires Nunes¹, Pedro Henrique Fonseca Veloso¹, Carlos Henrique Gomes Martins², Sara Lemes de Souza², Vanessa de Andrade Royo¹

veronica.sacramento.2014@gmail.com

1- Natural Products Laboratory, Center for Biological and Health Sciences, Unimontes, Av. Prof. Rui Braga, s/n – Vila Mauriceia, Montes Claros – MG, 39401-089 Brazil. 2-Antimicrobial Testing Laboratory, Institute of Biomedical Sciences, Federal University of Uberlândia, Uberlândia 38405-320, MG, Brazil

Native to the Cerrado, *Diplopterys pubipetala* (Malpighiaceae) has been investigated regarding the chemical composition of its leaves, which are rich in terpenes, phenolic compounds, and other secondary metabolites, with remarkable antioxidant activity. This study aimed to investigate leaf partitions of *D. pubipetala* against *Staphylococcus aureus* (ATCC 6538), *Escherichia coli* (ATCC 8739), and *Pseudomonas aeruginosa* (ATCC 27853). The minimum inhibitory concentration (MIC) was determined for the hexane and dichloromethane partitions using the broth microdilution method in 96-well plates, according to the Clinical and Laboratory Standards Institute guidelines. MIC values for all samples tested against *E. coli* and *P. aeruginosa* were equal to or higher than 2000 µg.mL⁻¹, classifying them as inactive. The observed limited antibacterial activity may result from the extract type or plant material quality; nevertheless, *D. pubipetala* remains promising for future targeted studies. The authors thank FAPEMIG (Foundation for Research Support of the State of Minas Gerais), Process APQ 03057-22.

Keywords: *Diplopterys pubipetala*, antibacterial activity, bioactive compounds

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ISOLATED FLAVONOIDS AND QUASSINOIDS AND ANTIPLASMODIAL ACTIVITY OF FRACTIONS FROM *HOMALOLEPIS CEDRON* (SIMAROUBACEAE)

Ronei de Souza Negreiros^{1*}, *Lais Garcia Jordão*², *Janaina Yasmim Ferreira da Silva*³, *Adrian Martin Pohlit*⁴

roneidesouzanegreiros@gmail.com

1- Post-Graduate Program in Chemistry, Universidade Federal do Amazonas (UFAM), Manaus – AM; 2- Post-Graduate Program in Biotechnology, UFAM, Manaus – AM; 4- Institutional Scientific Initiation Scholarship Program (PIBIC), Instituto Nacional de Pesquisas da Amazônia (INPA), Manaus – AM; 4- Coordenação de Tecnologia e Inovação (INPA), Manaus – AM.

Malaria is the best-known parasitic disease in the world. It is caused by a group of protozoa from the genus *Plasmodium* and transmitted through the bite of female mosquitoes of the genus *Anopheles*. The increasing resistance of malaria parasites to currently available antimalarials motivates the search for secondary metabolites from plants with antiplasmodial properties. *Homalolepis cedron* (Simaroubaceae) is popularly known as “pau-para-tudo”. This species is used for the treatment of malaria by different peoples of the Amazon region, such as Afro-Brazilian communities descended from quilombos in the municipality of Oriximiná-PA. From *H. cedron*, the antiplasmodial quassinoids cedronin, chaparrinone and simalikalactone D have been isolated in work by others. This work aims to identify new substances from *H. cedron* with antiplasmodial potential. Antiplasmodial tests against the multidrug resistant K1 strain of *Plasmodium falciparum* from continuous *in vitro* culture were conducted at the Malaria and Dengue Laboratory/INPA). Decoction of *H. cedron* leaves followed by liquid-liquid partitioning of the resulting H₂O extract provided CHCl₃ (1RNFCI09), EtOAc (1RNFAc09) and H₂O (1RNFAqS09) fractions that showed significant inhibitory/antiplasmodial activity (IC₅₀ = 3.72, 1.03 and 1.88 mg/mL, respectively). The leaf H₂O-acetone extract was chromatographed on sephadex-LH-20 and then reverse-phase silica (C-18) which led to the isolation of the flavonoids isovitexin, kaempferol-3-*O*-glucoside, quercetin-3-*O*-glucoside and vitexin. Normal phase column chromatography on the CHCl₃ extract of the root wood provided the quassinoids cedronin and brucein D. All substances were identified based on their 1D and 2D NMR, HRMS and MS/MS spectrometric properties and comparison with literature data. The four flavonoids and brucein D were isolated for the first time from *H. cedron*. This is also the first report on the antiplasmodial activity of fractions of *H. cedron* leaves. The authors thank the support of their institutions and the financial support of CAPES, CNPQ, and FAPEAM-Ed. 13/2022 Produtividade C, T & I.

Keywords: brucein D, cedronin, isovitexin, kaempferol-3-*O*-glucoside, quercetin-3-*O*-glucoside, vitexin.





Bioprospecting the anticancer potential of marine myxobacteria from the Brazilian coast

Isolda de Sousa Monteiro^{1*}, Renan S. Oliveira¹, Elthon G. Ferreira², Letícia V. Costa-Lotuf² e Paula C. Jimenez¹.

isolda.monteiro@unifesp.br

¹Instituto do Mar, Universidade Federal de São Paulo, Santos-SP, Brazil; ²Instituto de Ciências Biomédicas, Universidade de São Paulo, São Paulo-SP, Brazil.

Marine microorganisms are promising sources of bioactive compounds for human health. Among them, myxobacteria remain underexplored, especially in tropical and subtropical regions like Brazil, despite being prolific producers of secondary metabolites and widely distributed from non-saline soils to saline sediments. They are characterized by multicellular organization and the ability to synthesize structurally diverse metabolites, many of which have been recognized as potent anticancer agents. This study aimed to prospect marine myxobacteria from sediments collected along the Northern Coast of São Paulo (Ubatuba and São Sebastião) to evaluate their potential as producers of anticancer compounds. Sediment samples were plated on nutritionally poor media (WCX with *E. coli* as bait and St21 with sterile filter paper) at two salinity levels (0% and 60%). Sixteen strains were isolated, purified, and deposited in the MyxoMarin strain bank. Acetone:methanol extracts were obtained from the liquid culture of each strain and tested for cytotoxicity (MTT assay) against HCT-116 human colorectal cancer cells and HaCaT keratinocytes, and for inhibitory activity against the protease trypsin. Three extracts presented IC₅₀ values below 50 µg/mL against HCT-116, and were considered active: BRX-075 (6.43 µg/mL), BRX-076 (1.56 µg/mL), and BRX-079 (41.3 µg/mL). In trypsin inhibition at 50 µg/mL, extracts BRX-076 (17.20%), BRX-079 (19.61%), BRX-080 (22.68%), BRX-083 (33.07%), BRX-084 (33.50%), BRX-090 (25.03%), BRX-094 (30.49%), BRX-096 (23.97%), BRX-097 (11.08%), and BRX-098 (13.54%) showed activity, suggesting multifunctional bioactivity. Selected extracts were analyzed by HPLC, revealing distinct chemical profiles at 254 and 280 nm, and potential for further taxonomic and metabolite characterization. These findings highlight Brazilian marine myxobacteria as a promising source of novel bioactive compounds and reinforce the importance of exploring marine microbial diversity for anticancer drug discovery.

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Keywords: marine microorganisms, cytotoxicity, protease inhibitors, blue biotechnology, marine natural products.





ANTIPLASMODIAL C-AND O-GLYCOSYL FLAVONES AND OTHER COMPOUNDS FROM THE LEAVES AND BRANCHES OF *SIMABA PUBICARPA* DEVECCHI, W. W. THOMAS & FRANCESCH. (SIMAROUBACEAE)

Ana Carolina Arcos de Figueiredo¹, Djalma da S. Pereira^{2,*}, Laís G. Jordão³, Marlene R. M. Camargo³, Beatriz Iasmim da S. Cardoso¹, Ana Ketlenn M. Almeida¹, Ronei de S. Negreiros², Edizon V. Lopes⁴, Tiago B. Pereira⁴, Felipe Moura A. da Silva^{2,5} e Adrian M. Pohlit^{2,3,4}

ana.figueiredo@ufam.edu.br

1-Programa Institucional de Bolsas de Iniciação Científica, Instituto Nacional de Pesquisas da Amazônia, 69067-375, Manaus-AM, Brasil 2- Programa de Pós-graduação em Química, Universidade Federal do Amazonas, 69080-900, Manaus-AM, Brasil 3- Programa de Pós-graduação em Biotecnologia, Universidade Federal do Amazonas, 69080-900, Manaus-AM, Brasil 4- Coordenação de Tecnologia e Inovação, Instituto Nacional de Pesquisas da Amazônia, 69067-375, Manaus-AM, Brasil 5-Centro de Apoio Multidisciplinar, Universidade Federal do Amazonas, 69077-000, Manaus-AM, Brasil

The aim of this work was to investigate the chemical composition and antiplasmodial activity of the Amazon forest tree *Simaba pubicarpa*. Branch wood and branch bark hexane and EtOAc extracts were prepared by sequential maceration. Sequential normal-phase column chromatography (CC) on the hexane branch wood extract yielded the triterpenes niloticin (1) and piscidinol A (2). Aqueous acid extraction of the CHCl₃ soluble fraction of the MeOH branch wood extract followed by basification of the acidic extracts, extraction with CHCl₃ and semipreparative HPLC yielded 9-methoxycanthin-6-one (3). *p*-Salicylic (4) and vanillic (5) acids were obtained after reverse phase CC, then normal phase CC performed on the branch bark EtOAc extract. Pulverized leaves were macerated in hexanes, then MeOH/H₂O. After partial evaporation, the resulting MeOH/H₂O extract was partitioned with hexanes, then EtOAc. Sequential reverse-phase CC on the EtOAc fraction, followed by semipreparative HPLC provided methyl gallate (6) and the flavonoids epicatechin (7), afzelin (8) and quercitrin (9). The leaf MeOH/H₂O extract was suspended in 1% HCO₂H in MeOH, then filtered. The filtrate was evaporated and underwent serial reverse-phase CC, then semipreparative HPLC, yielding isovitexin (10) and vitexin (11). Compounds 4 and 7–11 are reported for the first time in the genus *Simaba*. Extracts and compounds 6–11 were evaluated *in vitro* against the human malaria parasite *Plasmodium falciparum* K1 strain. Extracts of all parts and afzelin were active and compounds 6, 9–11 were moderately active, demonstrating the antiplasmodial potential of *S. pubicarpa* extracts and chemical constituents.

Keywords: Afzelin; isovitexin; vitexin; *Plasmodium falciparum*; Amazon rainforest.





ISOLATION OF ERGOSTEROL PEROXIDE WITH ANTIMICROBIAL POTENTIAL FROM *DIAPORTHE HONGKONGENSIS*

Andrei da Silva Alexandre^{1,2*}, David Ribeiro da Silva¹, Cecilia Veronica Nunez^{1,2}

and.alexandre36@gmail.com

1-Laboratório de Bioprospecção e Biotecnologia, INPA, Av. André Araújo, 69067-375, Manaus, AM, Brazil. 2-Programa de Pós-graduação em Biotecnologia e Recursos Naturais da Amazônia, UEA, 69050-010, Manaus, AM, Brazil

Endophytic fungi of the genus *Diaporthe* are prolific producers of bioactive metabolites, including sterols, terpenoids, and polyketides. In this context, this study aimed to investigate the antimicrobial potential of *D. hongkongensis* isolated from *Minquartia guianensis* (Coulaceae), focusing on the isolation and characterization of bioactive constituents. The fungus was reactivated on Sabouraud Dextrose Agar (30 °C, 7 days) and subjected to submerged fermentation in Erlenmeyer flasks totaling 6.5 L of Sabouraud Dextrose Broth with 0.2% yeast extract at 30 °C for 21 days under agitation (120 rpm). Post-fermentation biomass was extracted sequentially using dichloromethane (DCM), ethyl acetate (EtOAc), and methanol (MeOH). The resulting crude extracts were screened for antibacterial and antifungal activities against reference strains. The EtOAc and DCM extracts selectively inhibited *Staphylococcus aureus* (MIC 500–1000 µg/mL), while no significant activity was observed against *Escherichia coli* or *Pseudomonas aeruginosa*. The MeOH extract showed moderate antifungal activity against *Candida albicans* and *Cryptococcus gattii* (MIC 800 µg/mL). Guided by these results, the DCM–EtOAc extract was subjected to chromatographic separation, affording the isolation of ergosterol peroxide. The compound was identified by NMR spectroscopic analyses (¹H and ¹³C NMR, DEPT-135, COSY, HSQC, HMBC), confirming its structure as 5 α ,8 α -epidioxyergosta-6,22-dien-3 β -ol. The compound's distinctive 5 α ,8 α -peroxide bridge functions as a pharmacophore that mediates its antimicrobial activity by interacting with membrane sterols, destabilizing lipid bilayers, and inducing reactive oxygen species that disrupt microbial homeostasis. Isolated from fungi and plants, ergosterol peroxide exhibits broad-spectrum bioactivity, with antifungal and antitubercular activities among the most consistently documented. Its identification in *D. hongkongensis* is notable, marking the first report of this metabolite from the species and underscoring the ecological versatility and metabolic richness of the genus *Diaporthe*, while reinforcing evidence that endophytic strains from biodiverse ecosystems are valuable reservoirs of pharmacologically active sterols. The authors would like to thank CAPES, CNPq, FAPEAM, FINEP and LTQPN-INPA.

Keywords: sterol, endophytic fungi, submerged fermentation, bioprospecting, NMR





**BIOPROSPECTION OF SECONDARY METABOLITES FROM *Eugenia uniflora* L.
AND EVALUATION OF ANTIOXIDANT ACTIVITY AND TOXICITY AGAINST
*Artemia salina***

Júlia Menezes Silva^{1*}, Raphael Amancio de Jesus², Natália Nogueira Saraiva¹

menezessju2@gmail.com

1-LabQGO, Departamento de Farmácia de Lagarto, UFS, Av. Gov. Marcelo Déda 13, Lagarto, SE, Brazil. 2-LABORGANICS, Departamento de Química, UFS, Avenida Marcelo Deda Chagas, São Cristóvão, SE, Brazil.

The excessive production of reactive oxygen species (ROS) is associated with inflammation in diseases such as cancer, diabetes, and arthritis. Thus, exploring new sources of natural antioxidants is a promising strategy for developing therapeutic alternatives. *Eugenia uniflora* L. is a plant traditionally used in folk medicine due to its antioxidant and anti-inflammatory properties; however, studies are needed to validate its pharmacological effects and assess its toxicity. This study aimed to perform the bioprospecting of secondary metabolites from *E. uniflora* L. cultivated in Lagarto – SE and evaluate its antioxidant activity and toxicity against *Artemia salina*. From the leaves of *E. uniflora*, the organic extract was obtained by maceration (83% ethanol), followed by turbolysis and liquid-liquid partitioning using petroleum ether, dichloromethane, and ethyl acetate. The extract and fractions were analyzed by High-Performance Liquid Chromatography (HPLC) under exploratory gradient conditions, using flavonoid chemical standards. Assays were performed to determine Total Flavonoid Content (TFC) and Total Phenolic Content (TPC). The antioxidant potential was evaluated using 2,2-diphenyl-1-picrylhydrazyl (DPPH) and Ferric Reducing Antioxidant Power (FRAP) assays. The toxicity of the extract and fractions was tested against *Artemia salina* larvae at different concentrations (1000 – 0.1 µg/mL), using a 1% potassium dichromate solution (positive control) and a 1% dimethyl sulfoxide solution (negative control). The flavonoid quercetrin was identified in the dichloromethane fraction (DF) and the ethyl acetate fraction (EAF). The EAF showed the highest TPC (416.01 mg GAE/g) and TFC (39.16 mg QE/g) values, followed by the organic extract with 273.32 mg GAE/g and 17.40 mg QE/g. Both the EAF and the organic extract exhibited the highest antioxidant activity, with 95% and 73% DPPH inhibition and 565.27 and 500.93 µmol TE/g in the FRAP assay, respectively. The organic extract and petroleum ether fraction were classified as non-toxic (LC₅₀ > 1000 µg/mL), while the dichloromethane fraction (LC₅₀ 732.1 µg/mL) and EAF (LC₅₀ 961 µg/mL) showed low toxicity. Based on the results, the presence of flavonoids and phenolic compounds was confirmed in the extracts and fractions of the plant species from the region, along with antioxidant activity and low toxicity, making it a promising candidate for future studies.

Keywords: Pitanga; TFC; TPC; DPPH; FRAP; *Artemia salina*.





**CHEMICAL CHARACTERIZATION OF VOLATILE ORGANIC COMPOUNDS FROM
Bacillus velezensis LGMB12 AND THEIR ANTIFUNGAL POTENTIAL**

Jéssica Alionso Huk¹, Marcela Naomi O. da Silva², Vanessa Merlo Kava², Beatriz Helena L.N. Sales Maia^{1*}

jessica.huk@ufpr.br

1-LAPNEQ, Department of Chemistry, UFPR, Av. Cel. Francisco H. dos Santos, 100, Curitiba, PR, Brazil. 2-LabGeM Department of Genetics, Rua Cel. Francisco H. dos Santos S/N, Curitiba - Paraná, Brazil. Biological Sciences Sector.

Endophytic bacteria, known as Plant Growth Promoting Bacteria (PGPB), play a key role in sustainable agriculture, acting as biological agents of protection against pathogens. This protection occurs through the production of secondary metabolites such as the synthesis of phytohormones, volatile organic compounds (VOCs), non-volatile compounds, and facilitation of biological fixation of atmospheric nitrogen, which contribute to improving soil fertility. *Bacillus velezensis* is a rhizobacterium that has been gaining prominence as a biocontrol agent through the production of VOCs, and a new strain of *Bacillus velezensis* (LGMB12) was isolated from a collection of 217 endophytic bacteria from the roots of four lines and three hybrid genotypes of corn. The genome was sequenced by LabGeM. This study aims to extract and identify the VOCs from this new strain and evaluate its antifungal potential against the phytopathogens *Sclerotinia sclerotiorum* and *Monilinia fructicola*, both considered pests in crops such as soybeans and stone fruits. The bacterium *B. velezensis* LGMB12 was cultured in NA medium, the vials were prepared with solid medium, and the bacteria were incubated in an oven at 30°C. VOC collection was performed using headspace solid-phase microextraction (HS-SPME), and analysis was performed using gas chromatography coupled with mass spectrometry (GC-MS). The major compounds identified were 2-nonadecanone, 6,10,14-trimethyl-2-pentadecanone, 6,10-dimethyl-2-undecanone, *n*-pentadecanoic acid, and *n*-octadecanoic acid. Their antifungal potential was evaluated using paired plates (PDA medium) and Petri dishes with dividers (NA medium) against the two phytopathogens. In the plates without dividers, the colonies of both fungi were smaller ($p < 0.05$; inhibition >98%) compared to the control, suggesting significant antagonism by diffusible metabolites. In the evaluation of volatile metabolites, the fungus *S. sclerotiorum* had its growth restricted in PDA medium, without invasion of the bacterial compartment, while in the control, total colonization of the plate was observed, exceeding the barrier (PDA and NA). Tests with *M. fructicola* showed changes in the morphology of the fungal colony in the presence of bacteria, indicating antagonist-pathogen interactions. The results reinforce the potential of the *B. velezensis* LGMB12 strain as a bioagent and its applicability in the development of bioinputs aimed at the sustainable management of phytopathogens in different agricultural crops.

Keywords: Endophytic bacteria, antagonism, in vitro test, secondary metabolites.





BENZYL TETRAHYDROISOQUINOLINE ALKALOIDS FROM *Nectandra membranacea* (LAURACEAE)

Vinicius C. Rocha^{1,2*}, Felipe da S. Sales², Andre G. Tempone³, João Henrique G. Lago²

vc.rocha@unifesp.br

¹Department of Chemistry, UNIFESP, Diadema, Brazil; ²Center for Natural and Human Sciences, UFABC, Santo André, Brazil. ³Laboratory of Pathophysiology, Butantan Institute, São Paulo, Brazil

Chagas disease, which is caused by the protozoan *Trypanosoma cruzi*, affects millions of people worldwide, particularly in South and Central America. The available treatments, benznidazole and nifurtimox, have several adverse effects.¹ Therefore, it is necessary to search for new compounds with anti-*T. cruzi* activity, especially those based on the structures of natural products. In this context, the Brazilian floral biodiversity is an inexhaustible source of new bioactive compounds. Previous studies on *Nectandra membranacea* (Lauraceae) revealed alkyl γ -lactones with anti-*T. cruzi* activity. As a continuation of our studies on this plant, we subjected the MeOH extract from its branches to a chemically active procedure to afford an alkaloidal phase. This phase exhibited *in vitro* activity against *T. cruzi*, resulting in 100% death of trypomastigote forms of the parasite at 300 μ g/mL. Thus, it underwent several chromatographic steps over silica gel and Sephadex LH-20, yielding alkaloids **1–4**. NMR analysis and comparison with literature data^{2,3} identified **1** and **2** as the diastereomers (*R*)- and (*S*)-*O,O*-dimethylcoclaurine, while **3** was characterized as velucryptine. The NMR spectra of compound **4** showed, in addition to the signals attributed to benzene rings and methoxy groups, peaks at δ_H 8.35 (d, *J* = 5.5 Hz) / δ_C 138.6 and δ_H 7.52 (d, *J* = 5.5 Hz) / δ_C 119.5 assigned to hydrogens and carbons from positions 2 and 3, respectively. Additionally, these spectra showed also signals at δ_H 6.08 (s) / δ_C 72.5 attributed to an oxymethine carbon at α position. Therefore, the structure of compound **4** was elucidated as depicted on Figure 1. The discovery of alkaloids **1–4** expands the knowledge of the chemical diversity biosynthesized by *N. membranacea* and contributes to the chemosystematics of the genus *Nectandra* in addition to identifying new bioactive compounds against *T. cruzi* (CNPq, FAPESP, CAPES)

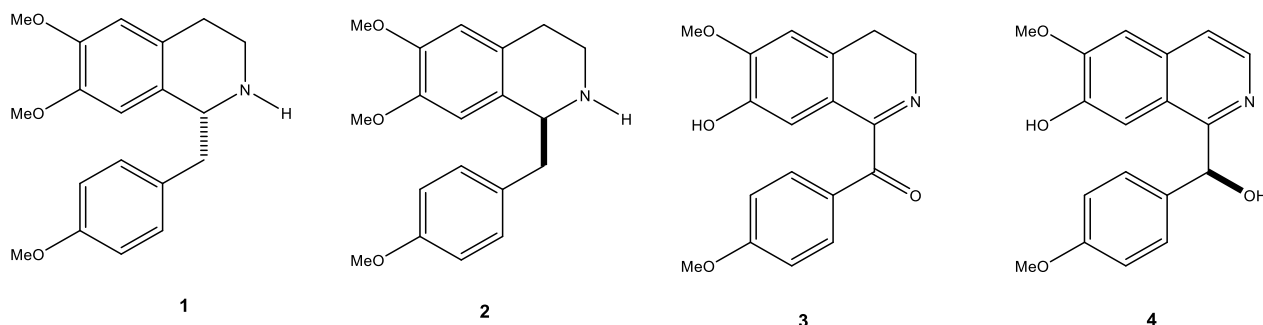


Figure 1. Structures of alkaloids **1 – 4** from *Nectandra membranacea*.

Keywords: *Nectandra membranacea*; alkaloids; benzylisoquinoline

References: ¹Pérez-Molina et al., *The Lancet* **2018**, 10115, 82; ²Werner et al., *Eur. J. Org. Chem.* **2007**, 3911;

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**DEVELOPMENT OF OPHTHALMIC FORMULATIONS WITH GREEN PROPOLIS
STANDARDIZED EXTRACT FOR THE TREATMENT OF ALKALI-INDUCED
SUPERFICIAL CORNEAL ULCERS**

Giulia Stavrakas Miranda^{1*}, Daniela Gracia Zoca², Fernanda Gosuen Gonçalves Dias²,
Pedro Sandoval dos Santos Ribeiro Cavallari², Wilson Cunha², Márcio Luíz Andrade e
Silva², Mario Ferreira Conceição Santos¹

giustavrakas@gmail.com

1-Programa de Pós-Graduação em Genética e Melhoramento, UFES, Alto Universitário, S/N, Alegre,
ES, Brazil. Departamento de Física e Química, UFES, Alto Universitário, S/N, Alegre, ES, 29500-
000, Brazil. 2-Núcleo de Pesquisa em Ciências Exatas e Tecnológicas, Universidade de Franca,
Parque Universitário, Franca, São Paulo, 14404-600, Brazil.

Corneal ulcers induced by alkali occur due to the saponification of triglycerides upon contact with hydroxyl ions, leading to lyses of cell membrane. Green propolis (GP), which main compound is Artepillin C, presents a variety of biological activities, including healing activity. The GP derived from plant species *Baccharis dracunculifolia* was provided by Apis Flora Comercial Ltda. (lot: 65400918). The hydroalcoholic extract was produced by maceration with ethanol:water (7:3 v/v). Artepillin C was obtained by filtration of GP with ethyl acetate. The content of Artepillin C was settled by RP-HPLC-PDA. The mobile phase was composed of a gradient system with Solvent A (acetic acid:water, 0.1:Solvent A) and Solvent B (acetonitrile), applied as follows: 30% B (0-10 min), 30-55% B (10-11 min), 55% B (11-32 min), 55-30% (32-33 min) and 30% B (33-42 min). The total content of Artepillin C was 266,86 µg/mL (21,05%). The ophthalmic formulations containing the standardized extract were prepared using polyethylene glycol 400 (PEG400), polysorbate 80 (Tween 80®), and distilled water (8:2:90 v/v/v). The final concentrations were 5, 10, and 15 mg/mL. *In vivo* tests were conducted with rats. The animals were randomly organized in 8 groups according to the treatment: GP5 (5 mg/mL formulation); GP10 (10 mg/mL formulation); GP15 (15 mg/mL formulation); SC (solvent control); PC (positive control with commercial drug); UC (untreated ulcers), PCT (positive control for genotoxicity); and NC (negative control). Histopathological, biochemical, and genotoxicity analyses were performed. The results revealed that groups treated with GP extract formulations exhibited significant reduction in ulceration compared to UC group. No significant differences were observed among the treated groups, indicating similar healing activity between the formulations and the commercial drug. Notably, GP5 achieved complete ulcer healing within 48h. Histopathological, genotoxicity, and biochemical analyses revealed no significant differences compared to NC group, confirming the absence of genotoxic, cytotoxic, hepatotoxic, of nephrotoxic effects. Overall, GP extract proved effective for the treatment of superficial chemical keratitis, representing a promising and cost-effective alternative

Keywords: Artepillin C; healing activity; *in vivo*; hydroalcoholic extract; propolis.





IN VITRO CYTOTOXIC E ANTI-INFLAMMATORY ACTIVITY OF *Ayapana triplinervis* ESSENTIAL OIL

Lucas Gabriel Viana Barbosa^{1*}, *Daniel Barbosa Santos*¹, *Alexandre Motta da Silva*¹, *Ellen Nayara Silva de Jesus*¹, *Luana Sousa Peixoto Barros*¹, *Leandra Feliz Santos*¹, *Renata Cunha Silva*¹, *Laine Celestino Pinto*², *Pablo Luis Baia Figueiredo*¹

Danielbsantos086@gmail.com

1-Laboratório de Químicas dos Produtos Naturais, Universidade do Estado do Pará, 66095-015, Belém, PA, Brazil. 2-Laboratório de Neuropatologia Experimental, Hospital Universitário João de Barros Barreto, Universidade Federal do Pará, 66073-000, Belém, PA, Brazil.

Ayapana triplinervis (Asteraceae) is an aromatic species from the Amazon region found under the morphotypes "white japana" and "purple japana". The aim of this study was to evaluate the *in vitro* cytotoxic and anti-inflammatory activity of *Ayapana triplinervis* essential oil (AtEO). The specimen was collected in Mirasselas, Pará, extracted by hydrodistillation in a modified Clevenger (3 hours). A voucher (MG-241933) was incorporated into the Herbarium of Universidade do Estado do Pará, and registered in SISGEN (A090EB2). The chemical composition was analyzed by gas chromatography coupled to mass spectrometry (GC-MS). The oils were evaluated (MTT assay) against gastric ascites (AGP01), glioblastoma (AHOL), lung cancer (A549), and non-malignant murine macrophages (RAW 264.7). The MTT assay was performed to evaluate cell viability, and the nitrite method was used to evaluate the anti-inflammatory activity. A total of 23 chemical constituents were identified; the main compounds were the oxygenated monoterpene 2,5-dimethoxy-*p*-cymene (45.0%) and the hydrocarbon sesquiterpenes β -selinene (19.2%) and (*E*)-caryophyllene (18.4%). AtEO showed cytotoxicity in all cell lines, AHOL1 (IC₅₀ 5.75 μ g/mL), AGP-01 (IC₅₀ 12.53 μ g/mL), A549 (IC₅₀ 6.56 μ g/mL), RAW 264.7 (IC₅₀ 13.41 μ g/mL), with twice as much selectivity in AHOL1 and A549 strains (Seletive index of 2.75 and 2.04, respectively), compared to macrophage strains, demonstrating its antiproliferative action. AtEO showed regulation in nitrite levels (116.7 $\pm$ 12.66, 89.44 $\pm$ 1.77, 128.4 $\pm$ 5.33 nM), highlighting the anti-inflammatory effect of the oil. The results show significant *in vitro* cytotoxic and anti-inflammatory activities. These findings endorse the therapeutic potential of AtEO in therapeutic strategies against cancer and inflammation.

Keywords: japana; antiproliferation; inflammation; monoterpenes.

Acknowledgments: UEPA, UFPA, CAPES, CNPq





***Lippia lacunosa* AS A PROMISING SOURCE OF PHENYLETHANOID GLYCOSIDES WITH INHIBITORY ACTIVITY AGAINST SARS-COV-2 PROTEASES**

Thamirys Silva da Fonseca^{1*}, Beatriz Graziela Martins de Mattos², Larissa Esteves Carvalho Constant³, Diego Allonso^{2,3}, Simony Carvalho Mendonça², Gilda Guimarães Leitão^{1,4}, Suzana Guimarães Leitão^{1,2}

thamirysfonseca@ufrj.br

1-Programa de Pós Graduação em Ciências Farmacêuticas, UFRJ, Brazil. 2- Faculdade de Farmácia, UFRJ Janeiro, Brazil. 3- Laboratório de Biotecnologia e Bioengenharia Estrutural, UFRJ Brazil. 4- Instituto de Pesquisas de Produtos Naturais, UFRJ, Brazil

Lippia lacunosa Mart. & Schauer (Verbenaceae) is a native and endemic species of Brazil, traditionally used to treat respiratory disorders^{1,2}. Considering that SARS-CoV-2 primarily affects the respiratory system, this species represents a promising candidate for COVID-19-related studies. Phytochemically, *L. lacunosa* is rich in phenolic metabolites, particularly phenylpropanoid glycosides (PhGs). Previous reports highlight the inhibitory potential of these compounds against viral targets such as the SARS-CoV-2 proteases 3CLpro and PLpro³, which are essential for viral replication. Thus, this study aimed to evaluate the inhibitory activity of *L. lacunosa* extracts against these proteases, followed by metabolite fractionation using Countercurrent Chromatography (CCC) and chemical characterization by LC-MS/MS. Ethanolic and ethyl acetate (EtOAc) extracts were tested at 100 µg/mL in FRET-based enzymatic assays using recombinant SARS-CoV-2 proteases (3CLpro and PLpro). The ethanolic extract inhibited over 90% of both proteases, while the EtOAc extract showed 100% inhibition of 3CLpro and 55% inhibition of PLpro. The EtOAc extract was selected for CCC fractionation, employing the biphasic solvent system ethyl acetate-butanol-water (1:0.05:1), yielding 9 fractions. LC-MS/MS combined with Feature-Based Molecular Networking (FBMN) confirmed PhGs like *m/z* 665 [M-H]⁻ (acetyl-verbascoside), *m/z* 755 [M-H]⁻ (forsythoside B), and other glycosylated flavonoids. Perspectives include testing all fractions against proteases and isolating the most active metabolites. Despite its extensive popular use, research on *L. lacunosa* is scarce; to our knowledge, this is one of the first investigations into its antiviral potential, especially against SARS-CoV-2, reinforcing the importance of exploring Brazilian native plants as sources of bioactive compounds. The authors thank the support from their institutions and the financial support of FAPERJ, Capes and CNPq.

Keywords: Verbenaceae, 3CLpro, PLpro, chemometrics, HSCCC, LC-MS/MS.

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Evaluation of the biological activity of mangiferolic acid isolated from geopropolis from Bahia - Brazil

Raqueline Pastor de Santana e Santana^{1*}, Adrienne Bastos Ferreira¹, Nelson Gonçalves Mortágua Gomes², Clayton Queiroz Alves¹, Hugo Neves Brandão¹

raquelinpastor@gmail.com

¹ Graduate Program in Plant Genetic Resources, UEFS, Avenida Transnordestina, S/N, Feira de Santana-BA, Brazil.

² REQUIMTE/LAQV, Laboratory of Pharmacognosy, Department of Chemistry, Faculty of Pharmacy, University of Porto, R. Jorge Viterbo Ferreira, n° 228, 4050-313 Porto, Portugal

Geopropolis is a natural substance produced by stingless bees, traditionally employed in the therapeutic management of various human pathologies. (Coutinho et al., 2023). This study aimed to isolate and evaluate the biological activity of metabolites present in extracts of geopropolis produced by *Melipona scutellaris*. For this purpose, geopropolis collected in the city of Cruz das Almas, Bahia (Brazil), was subjected to maceration in methanol (3 × 24 h), yielding a crude extract, which was then partitioned with organic solvents (hexane, chloroform, and ethyl acetate). The chloroform phase was subjected to column chromatography using silica gel as the stationary phase and organic solvents of increasing polarity as the mobile phase. Through these procedures, a compound was isolated and identified as mangiferolic acid (Figure 1) by analysis of ¹H and ¹³C Nuclear Magnetic Resonance (1D and 2D) spectra, in addition to comparison with data previously reported in the literature (Jong et al., 2013). Mangiferolic acid exhibited significant antioxidant activity against the superoxide radical, with a dose-dependent response (IC₅₀ = 92.1 µM/mL), and showed no cytotoxicity in murine macrophages (RAW 264.7). The results demonstrated the biological potential of geopropolis from *Melipona scutellaris*, as evidenced by the isolation of mangiferolic acid with noteworthy antioxidant activity and low cytotoxicity. These findings highlight the importance of investigating Brazilian natural products as a source of promising bioactive molecules. Acknowledgments. The authors thank CAPES, the State University of Feira de Santana (UEFS), and the Graduate Program in Plant Genetic Resources for financial support.

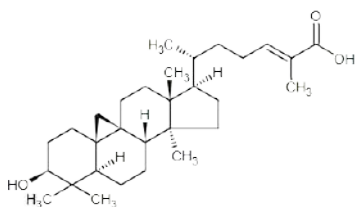


Figure 1: Chemical structure of mangiferolic acid

Keywords: Bioactive Potential, Geopropolis, *Melipona scutellaris*, Mangiferolic Acid, Bees, Triterpene.



EVALUATION OF THE INSECTICIDAL ACTIVITY OF *Parahancornia amapa* IN THE CONTROL OF LEAF-CUTTER ANTS

Lulliana Thalita Franco^{1*}, Anderson do Rego Pires¹, Janaina Brandão Seibert¹, Maria Fátima das Graças Fernandes da Silva¹, Jéssica Cristina Amaral², João Batista Fernandes¹.

lulli.tfranco@gmail.com

1- Laboratory of Natural Products, Chemistry Department, Federal University of São Carlos (UFSCar), Rod. Washington Luis s/n km 235, São Carlos, SP, 13565-905, Brazil. 2- Department of Plant Pathology and Nematology, University of São Paulo (USP)/Luiz de Queiroz College of Agriculture (ESALQ), Av. Pádua Dias, 11, Piracicaba, SP, 13418-900, Brazil.

Leaf-cutting ants of the genera *Atta* and *Acromyrmex* are considered the main pests of *Pinus* and *Eucalyptus* plantations, causing significant economic losses. Various strategies have been employed to control these pests, with synthetic insecticides being the most commonly used method. However, the continuous and indiscriminate use of these products over the years has led to serious environmental consequences and health risks^{1,2}. In this context, natural products have emerged as promising alternatives, with special emphasis on plant extracts, particularly those from *Parahancornia amapa*, a species native to the Amazon. Extraction processes were carried out using hexane and ethanol on the leaves and bark, from which the hexane extract of the leaves and the ethanolic extract of the bark exhibited significant insecticidal activity against *Atta sexdens* workers. This study enabled the isolation of three compounds, reported for the first time for this species, and their characterization by nuclear magnetic resonance (NMR) spectroscopy. Furthermore, a phytochemical investigation was conducted to annotate the metabolites present using UHPLC-QToF/MS-MS analyses. The data obtained were processed and refined with the support of spectral databases such as GNPS, MSFinder, and MSDial, allowing the annotation of several secondary metabolites, including flavonoids, coumarins, pterocarpanes, terpenes, and iridoids. The presence of these chemical groups, widely recognized for their biological properties, reinforces the bioactive potential of *P. amapa* and highlights its relevance as a source of natural products for sustainable pest management.

Keywords: Leaf-cutting ants, insecticides, natural products, *Parahancornia amapa*.

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EVALUATION OF THE ANTIFUNGAL ACTIVITY AND MECHANISM OF ACTION OF THE CRUDE HYDROALCOHOLIC EXTRACT OF *MYRCIA EUGENIOPSOIDES* AGAINST DERMATOPHYTES.

Patrícia Helena Arrabal^{1*}, Carolina Juliane Francisco², Leticia Bachmann², Patryne L. da Silva Dantas², Michele D. Alberton², Tatiani K. R. Botelho².

¹PIBIC-CNPQ scholarship holder, Pharmacy course, Regional University Foundation of Blumenau.

²Graduate Program in Biodiversity, Regional University Foundation of Blumenau. tatianibotelho@furb.br

The increasing resistance of dermatophytes to conventional antifungals has driven the search for alternative treatments, particularly those based on natural products. Antifungal activity has been reported in the *Myrcia* genus; however, *Myrcia eugeniopsoides* remains scarcely studied in this context. This study aimed to evaluate the minimum inhibitory concentration (MIC), minimum fungicidal concentration (MFC), mechanism of action, and inhibition of conidial germination of *M. eugeniopsoides* extract against *Nannizzia gypsea*, *Trichophyton mentagrophytes*, *Microsporum canis*, and *Trichophyton interdigitale*. The crude hydroalcoholic extract was obtained by maceration in a 70% hydroalcoholic solution, followed by filtration and drying. Dermatophytes were identified by mass spectrometry (MALDI-TOF) and VITEK MS (bioMérieux) and cultured on selective agar at 35 °C for seven days. The MIC was determined by broth microdilution in 96-well plates using RPMI 1640 medium, with itraconazole as a positive control. The MFC was determined from MIC results by plating on selective agar corresponding to MIC, MIC ×2, and MIC ×4. To investigate the mechanism of action, MIC assays were performed with sorbitol or ergosterol added to the RPMI medium. Agents that interact with ergosterol or sorbitol are identified when MIC values increase compared with the control without additives. In the conidial germination inhibition assay, 10 µL of the MIC, MIC ×2, and MIC ×4 concentrations were plated on sterile slides, followed by a drop of lactophenol blue, and readings were taken in five random fields. The extract showed strong antifungal activity against several dermatophytes tested, with MIC values ranging from 62.5 to 250 µg/mL, particularly *T. interdigitale* (62.5 µg/mL). MFC assays indicated fungicidal activity. In the mechanism of action evaluation, increased growth was observed with sorbitol, but no growth occurred in the ergosterol assay, requiring further analysis. Complete inhibition of conidial germination was also recorded. These findings suggest strong antifungal potential of *M. eugeniopsoides* extract against dermatophytes, with probable action on the fungal cell wall and fungicidal activity. The results highlight the need for further studies to better characterize its antifungal and cytotoxic properties. **Keywords:** Tinea; Microbial Sensitivity Tests; Antifungal Drug Resistance.



PRECLINICAL SAFETY EVALUATION OF *Cyperus articulatus* L. ESSENTIAL OIL

Tânia Mara Pires Moraes¹, Brayan Almeida Ferreira^{1*}, Jacqueline Parente de Sousa¹, José Sousa de Almeida Júnior¹, Patrícia Gabrielly da Silva Pires¹, Priscila Bezerra Lima¹, Waldiney Pires Moraes¹

tania.moraes@ufopa.edu.br

1- Pharmacology Laboratory, ISCO, Federal University of Western Pará, UFOPA, Santarém, Pará, 68040-255, Brazil.

INTRODUCTION: Phytotherapy, an ancient practice, uses medicinal plants for health treatments. Priprioca (*Cyperus articulatus* L.) is a medicinal plant whose essential oil is valued in the food industry and has several therapeutic properties, such as analgesic, antioxidant, anticonvulsant and antimicrobial. Therefore, given its high popular consumption, studies that guarantee the safety and efficacy of its use are essential. **OBJECTIVE:** To evaluate the safety of *Cyperus articulatus* L. essential oil (CAEO) through hemolytic activity. **METHODOLOGY:** The Red Blood Cells (RBC) test was performed. RBC 2% (v/v) were incubated with test drugs at concentrations of 2,000 to 15.6 µg/mL. Hemoglobin release was measured by absorbance at 450 nm. The positive and negative controls were 1% Extran and 1% dimethyl sulfoxide, respectively. Cytotoxicity was evaluated based on the hemolysis rate, classifying the activity as: 0-9% (non-toxic), 10-49% (slightly toxic), 50-89% (toxic) and 90-100% (highly toxic). Data analysis was performed by the variance test (ANOVA) and Newman-Keuls post-test ($p < 0.05$), using Graph Pad and Microsoft Excel software. **RESULTS AND DISCUSSION:** The RBC showed low hemolysis rates of CAEO, below the values observed in the positive control. The highest concentration (2,000 mg/mL) caused 7.5% ($\pm 0.30\%$) hemolysis, reducing to 0.31% ($\pm 0.07\%$) at the lowest concentration (15.625 mg/mL), compared to the positive control with Extran (100% hemolysis). No studies on the hemolyzing effect or any post-clinical safety tests for the use of CAEO recommended by the National Health Surveillance Agency were found. However, in vitro studies of the hemolytic evaluation of the ethanolic extract of *Cyperus articulatus* var. nodosus residue indicate the feasibility of cytotoxicity tests to support the dosage used. **CONCLUSIONS:** CAEO demonstrated low cytotoxicity at the concentrations tested, suggesting safety for its use with hemolysis rates lower than the positive control. **Acknowledgements:** FAPESPA – Amazon Foundation for Support of Studies and Research, UFOPA – Federal University of Western Pará.

Keywords: Cytotoxicity, *Cyperus articulatus*, Essential oil, Priprioca





ASSESSMENT OF ANTIOXIDANT AND ANTIBACTERIAL ACTIVITIES OF ALGAL RESIDUES AND BREWER'S YEAST

Daniel de Oliveira Nogueira^{1*}, Alessandra da Silva Correia², Marília dos Reis N. Chen¹,
Ana Luisa Motta L. Martins¹, Camila Adão Malafaia³, Daniel Weingart Barreto³, Denise
Maria Guimarães Freire², Ivana Correa R. Leal¹

daniel.o.nogueira@gmail.com

1-LaProNeb, Faculdade de Farmácia, UFRJ, Av. Avenida Carlos Chagas Filho, 373, Cidade
Universitária, RJ, Brazil. 2-Labim, Instituto de Química, UFRJ, Av. Athos da Silveira Ramos 149,
Cidade Universitária, RJ, Brazil. 3- Assessa Industria, Comercio e Exportação Ltda, Est
Bandeirantes, 11742, Vargem Pequena, RJ, Brazil.

The growing concern for the environment and the adoption of the circular economy model have driven the search for innovative solutions for the valorization of agro-industrial residues. In this context, brewer's yeast and algal biomass represent promising sources of bioactive compounds with potential applications in several areas, such as food, pharmaceuticals, and cosmetics. The utilization of these residues not only contributes to mitigating environmental impacts but also adds value to by-products that would otherwise be discarded, promoting a more sustainable production cycle. For the present study, residues of the algae *Hypnea musciformis* and *Sargassum filipendula* were kindly provided by ASSESSA, while residual yeasts were obtained from the production of Ale beer (Angel A-01, *Saccharomyces cerevisiae*) and Lager beer (W 34/70, *Saccharomyces pastorianus*) supplied by Colonus Brewery (RJ). The objective of this study is to evaluate the antioxidant and antimicrobial potential of extracts from algal and brewer's yeast residues, aiming valorization as high-value-added ingredients, especially as cosmetics and biosurfactants products. Initially, proximate composition analysis was performed to identify the components of the residues in addition to the total phenolic content, that was determined using the Folin–Ciocalteu method. Subsequently, the residues were frozen, lyophilized and extracted with three different solvent systems: distilled water, 70% ethanol, and rhamnolipid. As results, proximate composition revealed high levels of carbohydrates and proteins in the residues analyzed, supporting their valorization not only as sources of compounds with antioxidant and antibacterial activity, but also as substrates in biotechnological processes. The three extracts obtained are being analyzed concerning their chemical composition by UHPLC-DAD-MS/MS. In the next step, antioxidant activity of the extracts will be assessed *in vitro* using the DPPH, FRAP, and ABTS assays and the antimicrobial activity will be evaluated through the broth microdilution method to determine the Minimum Inhibitory Concentration (MIC) against the anaerobic bacterium *Cutibacterium acnes* that causes acne. The authors gratefully acknowledge ASSESSA and Colonus Brewery for providing the biological materials, and CAPES, CNPq, and FAPERJ for financial support.

Palavras chave: Sustainability, Cosmetics, Algal residues, brewer's yeast, antioxidante and antibacterial activities





ANTARCTIC LICHENS AS A PLATFORM TO DISCOVER BIOACTIVE MOLECULES WITH NEUROPROTECTIVE AND ANTI-INFLAMMATORY POTENTIAL

Cristian Cordero¹, Gerald Zapata ², Karem Henriquez ³, Iván Opazo-Aballay¹, Mario Aranda⁴

cristiancordero07@gmail.com

1 Laboratorio de Investigación de Alimentos y Medicamentos (LIFA). Facultad de Química y Farmacia. Pontificia Universidad Católica de Chile. Santiago, Chile. 2 Molecular Graphics Suite, Facultad de Ciencias Químicas y Farmacéuticas, Universidad de Chile, Santiago, Chile. 3 Laboratorio de Biotecnología y Genética de Alimentos (BGA), Facultad de Ciencias, Universidad del Bío-Bío. Chillán, Chile.

Antarctic lichens endure extreme cold, intense UV radiation, strong winds, and chronic nutrient scarcity—pressures that drive distinctive secondary metabolism. We investigated eight Antarctic lichens as a source of bioactive molecules with neuroprotective and anti-inflammatory potential. To link chemistry with function, we applied an **effect-directed analysis (EDA)** integrating **HPTLC bioassays**, **LC-MS profiling**, and **molecular docking**, enabling the pinpointing and characterization of **COX-2** and **acetylcholinesterase (AChE)** inhibitors. Chemical profiling revealed a landscape dominated by depsides, depsidones, dibenzofurans (notably usnic acid), naphthoquinones, and fatty acids. Functional assays demonstrated COX-2 inhibition, AChE inhibition, and antioxidant activity, consistent with mechanisms relevant to neuroinflammation and oxidative stress. Docking supported plausible binding of representative metabolites within the catalytic sites of COX-2 and AChE, indicating concordance between structure and mechanism. A salient observation was **polypharmacology**. Several metabolites were active across more than one readout: **usnic acid** and **sphaerophorin** consistently exhibited dual antioxidant and enzyme-inhibitory behavior. In addition, an **unusual fatty acid**, **pentahydroxyoxoheptacosanoate**, detected in multiple species, showed **remarkable anti-inflammatory activity**, highlighting underappreciated lipophilic contributors to lichen bioactivity. Collectively, these findings expand the chemical and functional map of Antarctic lichen chemodiversity and underscore their value as reservoirs of drug-like natural products. The integrated **EDA–HPTLC/LC-MS–docking** strategy provides a rapid, efficient route to identify mechanism-anchored leads from complex matrices and prioritizes candidates for cell-based validation in **neuroprotection** and **inflammation** research.

Keywords: lichen, bioactive molecules, neuroprotection, inflammation, COX-2, acetylcholinesterase (AChE)





Isolation and characterization of novel limonoids in *Trichilia pallida* (Meliaceae) guided by LC-MS/MS

Carlos André Ferreira Moraes^{1*}, Jéssica Cristina Amaral², Luis Guillermo Cuadrado Durango¹, João Batista Fernandes¹, João Batista Fernandes¹, Maria Fátima das Graças Fernandes da Silva¹

carlosmoraes@estudante.ufscar.br

1- Laboratory of Natural Products, Department of Chemistry, UFSCar. Rod. Washington Luís, s/n - Monjolinho, São Carlos - SP, 13565-905, Brazil. 2- Department of Plant Pathology and Nematology, University of São Paulo (USP)/Luiz de Queiroz College of Agriculture (ESALQ), Piracicaba-SP, Brazil.

The Meliaceae family is widely recognized not only for the quality of its timber but also for its ability to biosynthesize tetranortriterpenes (limonoids), a class of secondary metabolites that exhibit a broad spectrum of biological activities, including insecticidal, bactericidal, antifungal, and anticancer properties. Several genera within this family have been extensively investigated owing to the bioactive potential of their constituents, with particular emphasis on *Melia* L., *Toona* (Endl.) M. Roem., *Azadirachta* A. Juss., and *Trichilia* P. Browne^{1,2}. In the present study, an analytical strategy was established based on the monitoring of diagnostic ions in tandem mass spectrometry (MS/MS) fragmentation spectra, with the aim of identifying putative limonoids and guiding the selection of *Trichilia pallida* extracts and fractions for metabolite isolation. All extracts and fractions were analyzed by ultra-high-performance liquid chromatography (UHPLC) coupled with high-resolution mass spectrometry (HRMS). MS/MS spectra displaying diagnostic ions were employed to direct fraction collection by high-performance liquid chromatography (HPLC), with monitoring at 215 nm. This approach enabled the isolation and structural elucidation—through one-dimensional (1D) and two-dimensional (2D) nuclear magnetic resonance (NMR) spectroscopy—of eleven limonoids and two norlimonoids. Three isolated limonoids were further evaluated for their cytotoxic potential using the MTT assay against the MRC-5 (non-tumoral), A549 (lung cancer), A2780 (ovarian cancer), and B16F10 (murine melanoma) cell lines. Notably, promising activity was observed against B16F10 cells, in which the limonoids induced the expression of the *Caspase-3* gene, a key effector directly associated with apoptosis. Collectively, these results underscore the potential of limonoids as lead candidates for the development of novel antitumor agents, highlighting their relevance as promising scaffolds in oncological drug discovery.

Keywords: Limonoids, mass spectrometry, molecular network.

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TIBOUCHINA GRANULOSA: BEYOND ORNAMENTAL USE, A SOURCE OF ANTIOXIDANT BIOACTIVE COMPOUNDS

Melissa Gabriela Soares de Almeida Luz^{1*}, Sthefany Nolasco de Sena¹, Victor Campana Leite¹, Janaina de Carvalho Veríssimo¹, Stéfanie Caneschi Coelho de Souza¹, Nicolas de Castro Campos Pinto¹, Elita Scio Fontes¹

mellissa.almeida@estudante.ufjf.br

1- Instituto de Ciências Biológicas, Departamento de Bioquímica, UFJF, Rua José Lourenço Kelmer, s/n - São Pedro, Juiz de Fora - MG, 36036-900, Brazil.

Tibouchina granulosa (Melastomataceae), popularly known as “quaresmeira-roxa,” is native to Brazil and widely cultivated as an ornamental plant due to its striking flowers, rapid growth, and adaptability to diverse soil and climate conditions. Beyond its ornamental value, the species holds considerable potential, as its secondary metabolites may exert biologically relevant activities. Considering its abundance in the Atlantic Forest and the limited studies addressing its chemical composition and pharmacological properties, further investigation is highly warranted. This study aimed to quantify the phenolic and flavonoid content of the ethanolic leaf extract of *T. granulosa* (ETB) and to evaluate its antioxidant activity, given the well-established role of these metabolites in mitigating oxidative stress. ETB was obtained by ultrasound-assisted extraction in absolute ethanol at 45 °C for 1 hour, followed by filtration and rotary evaporation. Total phenolics were determined by the Folin–Ciocalteu method, while flavonoids were quantified using the aluminum chloride complexation assay. Antioxidant activity was assessed through DPPH radical scavenging and nitric oxide inhibition assays. The extract exhibited 185.29 ± 1.07 mg TAE/g (tannic acid equivalents), corresponding to total phenolic compounds, and 54.00 ± 4.41 mg QE/g (quercetin equivalents), corresponding to total flavonoids, confirming its richness in metabolites with recognized antioxidant potential. In the DPPH assay, ETB exhibited strong activity ($IC_{50} = 2.48 \pm 0.17$ µg/mL) compared with quercetin ($IC_{50} = 0.65 \pm 0.062$ µg/mL). In contrast, nitric oxide inhibition was lower ($IC_{50} = 241.63 \pm 6.70$ µg/mL) than that of rutin ($IC_{50} = 102.90 \pm 2.07$ µg/mL). The high activity observed, particularly in the DPPH assay, can be directly attributed to the elevated levels of phenolics and flavonoids, compounds known to neutralize reactive oxygen species. Overall, these findings highlight the potential of *T. granulosa* extract as a bioactive ingredient for cosmetic and phytotherapeutic applications targeting oxidative stress-related conditions, supporting further studies on its standardization and technological development. The authors thank the support from their institutions and the financial support of CAPES, CNPq, FAPEMIG e UFJF.

Keywords: Antioxidant potential, bioactive compounds, flavonoids, phenolic compounds, *Tibouchina granulosa*.



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ANTIBACTERIAL AND ANTIBIOFILM EFFECTS OF GREEN PROPOLIS EXTRACTS AGAINST BOVINE MASTITIS STRAINS: IN VITRO, IN VIVO AND ONE HEALTH PERSPECTIVES

Marilia dos Reis Nery Chen^{1*}, Débora Baptista Pereira², Carla Monteiro Leal¹, Otávio Augusto Leitão dos Santos¹, Carla Christine Lange³, Debora Foguel¹, Maria Isabel Sampaio dos Santos¹, Douglas Siqueira de Almeida Chaves²; Ivana Correa Ramos Leal¹.

marilia.nery@outlook.com

1. Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil. 2. Federal Rural University of Rio de Janeiro (UFRRJ), Rio de Janeiro, Brazil. 3. Embrapa Dairy Cattle, Juiz de Fora, Minas Gerais, Brazil.

Bovine mastitis is one of the main diseases that impairs dairy production, generating economic and social losses. Antibiotic therapy has become a growing concern due to bacterial resistance, which reinforces the need for safe, effective, and sustainable alternatives within the *One Health* framework. Brazilian green propolis (BGP) stands out for its biological potential, associated with the presence of phenolic and prenylated compounds. The objective of this study was to evaluate the antibacterial and antibiofilm potentials of BGP against multiresistant and sensitive strains isolated from bovine mastitis, comparing different extraction methods in order to develop a topical formulation for veterinary use. Ethanolic and methanolic extracts were obtained by maceration, percolation, and ultrasound, and were chemically characterized by HPLC-HRMS/MS and processed using MZmine 4.2. In parallel, feature-based molecular networking available on the GNPS2 platform were used to annotate substances present in the selected extracts. In addition, antimicrobial activity tests (MIC), antibiofilm activity, and scanning electron microscopy (SEM) analysis were also performed. The ethanolic extract obtained by percolation showed the highest yield (47.34%), while the methanolic extract achieved the best results in total phenolics (45.12 mg GAE/100 g). The chemical profile consisted in the annotation of 12 constituents, with artepillin C (*chemical marker*) reaching 33.062% and 30.839% in the percolated extracts, along with baccharin, drupanin, kaempferide, *p*-coumaric acid and other. All extracts demonstrated antibacterial activity against 11 out of 15 strains tested, including *Staphylococcus aureus* (MIC 256 µg/mL) and *S. auricularis* (MIC 64 µg/mL), being inferred as bactericide. Furthermore, all isolates were biofilm producers, with *Staphylococcus* and *Streptococcus* showing the strongest production (level 4). Ultrasound-treated methanolic extracts and ethanolic percolation extracts showed more than 80% inhibition of biofilm formations at subinhibitory concentrations, as evidenced by scanning electron microscopy through the formation of vesicles on the bacterial surface. In the *in vivo* assay stage, an infection model in the invertebrate *Tenebrio molitor* was established, determining sublethal concentrations of both extract and bacteria. To date, the results indicate a potent antibacterial, anti-biofilm, as well as good tolerance in larvae, supporting the continuation of the *in vivo* assays, now in the final stage, and the advancement of the topical nanoemulsion development. These findings strengthen green propolis as a promising candidate for the sustainable control of bovine mastitis, in line with the principles of *One Health*.

Keywords: Brazilian propolis, Natural product, One health, Biofilm, *Staphylococcus*, *Baccharis*.

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SEARCH FOR SECONDARY METABOLITES FROM BACURI FRUIT (*Platonia insignis*) WITH POTENTIAL ANTIPARASITIC ACTIVITY

Lutuima Ambrósio Capangue Neto^{1*}, Louis Pergaud Sandjo¹

mawynetho24@gmail.com

1- Departamento de Química, CFM, UFSC, Campus Universitário Trindade - C.P. 5094, 88035-972 Florianópolis, SC, Brazil.

The use of natural products as an original and valuable source of new active molecules can be very effective and important in the development of new drugs as a therapeutic strategy to improve the treatment of neglected tropical diseases. The incessant search for new drugs from plants has led scientists to the discovery of many metabolites with potential for drug development through the isolation, elucidation of structure, composition and evaluation of bioactivity based on phytochemical composition and uses in traditional medicine. Folk medicine describes the use of the plant *Platonia insignis* Mart., popularly known as "bacurizeiro", a member of the Clusiaceae family, found predominantly in the north and northeast regions of Brazil. The species *Platonia insignis* Mart. has been extensively studied and has gained prominence for its pharmacological potential as a source of products with healing, antimicrobial, antitumor, antioxidant, and anti-inflammatory properties, as well as for the treatment of skin diseases and diarrhea. Bacuri seeds are rich in fatty acids like triacylglycerols, and metabolites with potential therapeutic activity, such as xanthenes, biflavonoids and polyisoprenylated benzophenones. In this context, this work aims to develop a phytochemical study to identify and isolate bioactive compounds from shell and seeds of bacuri fruit, which are usually discarded, and evaluate their antiparasitic activities. To achieve these goals, the different parts of the fruit (shell: 1.56 kg and seed: 850 g) were separated, and the plant material was then subjected to extraction by maceration at room temperature in DCM:MeOH (1:1, v/v) in a closed container for up to 10 days. Subsequently, the extracts were filtered and concentrated under reduced pressure at 40°C. The crude extract of the shell and seed was suspended separately in water and partitioned using a liquid-liquid extraction process resulting in fraction in hexane, dichloromethane and n-butanol. The remaining aqueous fractions were frozen for later lyophilization. To improve the biological activity of the isolated compounds, molecular planning will be carried out to perform semisynthesis through low-complexity reactions to modify the molecules of the isolated compounds, in order to alter some important parameters in molecular activity, such as toxicity, selectivity, lipophilicity and bioavailability.

Keywords: Clusiaceae family, *Platonia insignis*, Bacuri, phytochemical, crude extract.





POLYPHENOLIC PROFILES AND ANTIFUNGAL POTENTIAL OF *Eugenia* SPECIES AGAINST *Candida auris*: in vitro AND in silico INSIGHTS

Camylla Janiele Lucas Tenório^{1,2*}, João Gabriel Câmara Monteiro¹, Janaína Carla Barbosa Machado^{1,3}, Máгда Rhayanny Assunção Ferreira^{1,3,4}, Luiz Alberto Lira Soares^{1,2,3}

camylla.tenorio@ufpe.br

1-NUDATEF, Departamento de Ciências Farmacêuticas, Universidade Federal de Pernambuco, Pernambuco, Brazil. 2-Programa de Pós-graduação em Inovação Terapêutica, Centro de Biociências, UFPE, Recife, Pernambuco, Brazil. 3-Programa de Pós-graduação em Ciências Farmacêuticas, Centro de Ciências da Saúde, UFPE, Recife, Pernambuco, Brazil. 4-Departamento de Engenharia Biomédica, Centro de Tecnologia e Geociências, UFPE, Recife, Pernambuco, Brazil.

The genus *Eugenia* is the largest neotropical representative of the *Myrtaceae* family. It is widely distributed in Brazil and recognized for its diversity of secondary metabolites with potential pharmacological applications. This study investigated the diversity of polyphenolic metabolites in leaf extracts of *E. uniflora*, *E. dysenterica*, *E. pyriformis*, and *E. stipitata*, correlating these profiles with their antifungal potential, and assessed whether molecular modelling could support the *in vitro* findings. Leaves were collected, identified, registered (A74AD6E), stabilized, and subjected to turbolysis (5% w/v) with 50% (v/v) ethanol. Phytochemical profiles were then obtained by LC-ESI(-)MS. Antifungal activity against *Candida auris* CDCP (11903) was evaluated using broth microdilution, while molecular modelling targeted lanosterol 14 α -demethylase (PDB 3LD6) with Autodock Vina. Distinct phytochemical profiles were observed among the species. *E. uniflora* was rich in glycosylated flavonoids of myricetin (myricitrin, myricetin-O-glucoside, myricetin-O-pentoside), quercetin derivatives (quercitrin, quercetin-O-deoxyoside), and hydrolysable tannins. *E. dysenterica* contained abundant procyanidins (dimeric and trimeric), catechin, and rutin. *E. pyriformis* presented epigallocatechin, procyanidin B, and quercetin, whereas *E. stipitata* showed catechin, quercetin-O-glucuronide, and ellagic acid derivatives. In antifungal assays, *E. uniflora* displayed the strongest activity (MIC: 62.5 μ g/mL), followed by *E. pyriformis* and *E. stipitata* (both 250 μ g/mL), while *E. dysenterica* showed the weakest effect. These results suggest that glycosylated myricetin and quercetin derivatives contribute to the stronger activity of *E. uniflora*, whereas species rich in procyanidins and ellagic acid derivatives displayed intermediate to lower activity. The *in silico* analyses supported these findings: quercetin-3-O-gallate (-11.5 kcal/mol), dismantin (-10.0), myricitrin (-9.7), myricetin-3-O-glucoside (-9.6), and epigallocatechin gallate (-9.5) showed strong binding affinities at the enzyme's active site. Therefore, the phytochemical, biological, and modelling data highlight the central role of polyphenolic compounds in the antifungal activity of *Eugenia* species, reinforcing their potential as sources of innovative antifungal molecules.

Keywords: flavonoids, pitanga, uvaia, cagaita, araçá-boi.





EFFECT OF FERMENTATION ON THE CHEMICAL PROFILE OF THE FRUITS AND SAP OF PLANT AND FUNGI NATIVE SPECIES OF CENTRAL CHILE AND ITS RELATIONSHIP WITH ANTIOXIDANT CAPACITY AND PHARMACOLOGICAL ACTIVITIES ASSOCIATED WITH METABOLIC SYNDROME

Javier Echeverría^{1*}, Cristina Villa¹, Michelle Morales¹, Loreto Carrasco¹, Francisco A. Cubillos^{2,3,4}; Cesar Echeverría^{5,6,7}

javier.echeverriam@usach.cl

1-Departamento de Ciencias del Ambiente, Facultad de Química y Biología, Universidad de Santiago de Chile, Santiago, Chile. 2- Departamento de Biología, Facultad de Química y Biología, Universidad de Santiago de Chile, Santiago, Chile. 3-ANID–Millennium Science Initiative–Millennium Institute for Integrative Biology (iBIO), Santiago, Chile. 4-ANID-Millennium Nucleus of Patagonian Limit of Life (LiLi), Valdivia, Chile. 5-Laboratorio de Biología molecular, Facultad de Medicina, Universidad de Atacama, Copiapó, Chile. 6-Instituto de Ciencias Naturales, Facultad de Medicina Veterinaria y Agronomía, Universidad de Las Américas, Santiago, Chile. 7-Centro de Investigación en Ciencias Biológicas y Químicas, Universidad de Las Américas, Santiago, Chile.

The fruits, saps, and bulbs of native Chilean plants and fungi have been traditionally used by pre-Hispanic cultures for their medicinal and nutritional benefits. They are used in the production of jams, syrups, and fermented beverages. This research aimed to determine the chemical profile (using HPLC-DAD and UPLC-MS, along with TAC, TFC, and TPC analyses) of five species (*Schinus areira* L., *S. latifolia* (Gill. ex Lindl.) Engler, and *S. polygama* (Cav.) Cabrera [Anacardiaceae], *Jubaea chilensis* (Molina) Baill. [Arecaceae], and *Cyttaria espinosae* Lloyd [Cyttariaceae]) before and after fermentation with *Saccharomyces cerevisiae* EC1118, also assessing their antioxidant capacity (*in vitro*: DPPH, FRAP, CUPRAC, ABTS, and ORAC; and cellular antioxidant capacity assays), cytotoxicity (HUVEC and HepG2 cell lines), and their impact on digestive enzymes related to metabolic syndrome (α -glucosidase, α -amylase, and pancreatic lipase). The results showed that fermentation significantly increased TAC, TFC, and TPC values, improved DPPH, FRAP, CUPRAC, ABTS, and ORAC values, and inhibited ROS. The extract did not exhibit cytotoxicity in non-tumor HUVEC cells ($IC_{50} > 100 \mu\text{g/mL}$) and showed antiproliferative activity against HepG2 and MCF-7 cell lines. Enzymatic inhibition was moderate. These findings emphasize the bioactive potential of traditional fermented beverages made from Chilean native species and highlight their importance in nutritional and pharmacological uses.

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Keywords: Chilean fermented beverages, alcoholic fermentation, chemical profile, antioxidant capacity, enzymatic activity, metabolic syndrome





BIOCATALYTIC APPROACHES TO WASTE VALORIZATION: ANTI-AGING AND ANTIOXIDANT ACTIVITIES FOR ACYLATED CITRUS DERIVATIVES

Nátalie Tavares Delgado^{1*}, Natalie Giovanna da Rocha Ximenes¹, Layla Theodoro da Conceição¹, Patrícia Homobono B. De Moura¹, Ivana Correa Ramos Leal¹

natalie.tdelgado@gmail.com

1 - 1 - Laboratory of Natural Products and Biological Assays (LaProNEB), UFRJ, Av. Carlos Chagas Filho, 373, Block A – 2nd Floor, Room 34, Department of Natural Products and Food, Federal University of Rio de Janeiro, University City, Rio de Janeiro, 21941-599, Brazil.

The process of skin photoaging, driven by the production of reactive oxygen species, leads to collagen degradation and the appearance of wrinkles. This study primarily aims to utilize waste from the citrus juice industry, rich in flavonoids, which exhibit anti-aging action due to their antioxidant capacity and inhibition of metalloproteinases, such as tyrosinase, important in the melanogenesis process. The application of these substances is limited due to their high hydrophilicity. To enhance their action, this project proposes the enzymatic synthesis of acylated derivatives of these extracts (Tundis et al., 2015), aiming for more hydrophobic matrices. The extraction of each part of the peels (albedo and flavedo of *Citrus sinensis*) was performed by static maceration at room temperature using EtOH:H₂O (8:2) as solvent system, stored for 24 h. Hesperidin and the crude extracts from albedo and flavedo were acylated by transesterification reaction using 22.5 mg of each sample in 1.5 mL of vinyl ester; 0.5 mL of solvent (isopropanol for esters with C2 to C4 carbon chains or *tert*-butanol for esters with C10 and C12 carbon chains). The reaction mixture was placed in an orbital shaker (60 °C – 180 rpm) for 5 min, and then 9 mg of the commercial enzyme N435 (40% relative to the substrate amount) was added for reactions with C2 to C4, and 22.5 mg of N435 (100% relative to the substrate) for reactions with C10 and C12 carbon chain esters. The crude extracts and the corresponding derivatized extracts, as well as commercial pure compounds annotated by mass spectrometry as majority in the extracts, such as hesperidin, quercetin, pectin and rutin, are being submitted to tyrosinase enzyme inhibition assays at concentrations ranging from 2 to 2000 µg/mL, according to the protocol established by Khatib et al. (2005), using the SpectraMax iD3 multimode microplate reader. The flavedo extract showed 20% inhibition at a concentration of 200 µg/mL, compared to 81% for the control kojic acid at the same concentration. Hesperidin, found in majority in *Citrus* extract, showed a potential of 30% inhibition also at 200 µg/mL. Studies are underway to determine the IC₅₀ of the extracts and acylated derivatives, aiming to increase the inhibitory potential against the anti-aging enzymes. Antioxidant assays are also in progress. The author acknowledges the support of UFRJ, FAPERJ, CNPq, and CAPES.

Keywords: Acylation, antioxidant, biocatalysis *Citrus*, tyrosinase



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***CABREUVANOLS A-C, THREE NEW CASSANE-DERIVED DITERPENES FROM
Myrocarpus frondosus AND THEIR ANTI-INFLAMMATORY EFFECTS***

Ana Caroline da Silva^{1*}, Eduardo M. Dalmarco², Beatriz Garcia Mendes Borba²,
Louis P. Sandjo¹

ana.caroline.s@posgrad.ufsc.br

1-LQPN, Department of Chemistry, CFM, UFSC, Campus Universitário Trindade, 88040-900,
Florianópolis, SC, Brazil. 2- Department of Clinical Analysis, CCS, UFSC, Campus Universitário
Trindade, 88040-970 Florianópolis, SC, Brazil

Myrocarpus frondosus (Fabaceae) is a species native to South America, popularly known as Cabreúva, and has been traditionally used for its medicinal properties, especially anti-inflammatory properties [1]. This study aimed to isolate and characterize new metabolites from the bark of this plant, in addition to evaluate their biological activity. Thus, seven compounds were obtained by using successive chromatographic techniques. Three were new cassane diterpenes, trivially named Cabreuvanols A, B, and C (2–4), while the four known compounds were ayapin (1), afromosin 7-O-β-D-apiofuranosyl-(1→2)-glucopyranoside (5), tyrsifloside (6), and afromosin 7-O-β-D-glucopyranoside (7). Their structure was assigned by the mean of 1D/2D NMR and HR-MS data, while the absolute configuration of cabreuvanol A (2) was confirmed by X-ray crystallography. The crude extract, the fractions, and compounds 1-3 were evaluated for their cytotoxicity against mouse J774 macrophages and for their anti-inflammatory effects through inhibition of nitric oxide (NOx) production [2,3]. The crude extract and fractions showed low cytotoxicity and high capacity to inhibit NOx production, with a significance of 70% inhibition at the tested concentrations, for ethyl acetate (EAF) and dichloromethane (DCMF) fractions. The extract and these two fractions were more potent than the reference drug, dexamethasone, at a dose of 2.75 µg/mL (20.65 ± 0.87 µg/mL). The new compounds, cabreuvanols A and B also showed inhibitory effects. Compound 3 was more cytotoxic than others. Furthermore, anti-inflammatory activity was demonstrated in a murine model of acute lung inflammation (ALI) caused by LPS. In this model, the crude extract and fractions significantly reduced NOx levels, while compounds 1 and 2 moderately reduced NOx by 58.6 ± 4.7% and 23.4 ± 8.8%, myeloperoxidase (MPO) activity, exudation, and cell migration in bronchoalveolar lavage fluid, confirming the anti-inflammatory effect in vivo. The results indicate that Cabreúva is a source of bioactive diterpenoids with potential application in the development of anti-inflammatory agents.

The authors would like to thank the institutions, CAPES and FAPESC for its funding support.

Keywords: *Myrocarpus frondosus*, Structure elucidation, Diterpenes, Anti-inflammatory activity

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**BRAZILIAN RED PROPOLIS AND ISOLATED PRENYLATED BENZOPHENONES
AS POTENTIAL ANTI-INFLAMMATORY MODULATORS MODULATING NETs AND
CYTOKINES**

Matheus Hikaru Tanimoto¹, Paulo Sérgio de Almeida Augusto², Ana Maria de Freitas
Pinheiro¹, Isabela Macêdo dos Santos¹, Jairo Kenupp Bastos¹

tanimoto@usp.br

1 - Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo (FCFRP-USP). 2 - Faculdade de Medicina de Ribeirão Preto – Universidade de São Paulo (FMRP-USP)

Previous studies have consistently reported the anti-inflammatory potential of compounds isolated from propolis, yet the mechanisms underlying these effects remain incompletely understood. Among the pathways involved in inflammation, neutrophil extracellular traps (NETs) formation and the release of pro-inflammatory cytokines are considered crucial events contributing to tissue damage and disease progression. To the best of our knowledge, this is the first study to evaluate the capacity of prenylated benzophenones isolated from Brazilian red propolis, as well as the crude extract, to modulate NETs release and cytokine production in human neutrophils. Human neutrophils were isolated from peripheral blood and pre-treated with guttiferone E, oblongifolin B, or the crude ethanolic extract of Brazilian red propolis for 1 hour at concentrations ranging from 100 to 0.03 μ M. Cells were subsequently stimulated with 5 μ M ionomycin to induce NET formation. NET release was quantified for 6 hours post-stimulation using SytoxGreen[®] as DNA extracellular probe, and cytokine levels were determined at the final time point. Treatment with higher concentrations (100 and 30 μ M) of both isolated compounds and the crude extract resulted in a significant reduction in NET release compared to controls. Furthermore, the same concentrations were associated with decreased secretion of pro-inflammatory cytokines TNF- α and IL-1 β , suggesting a dose-dependent inhibitory effect (oblongifolin B: reduced 67% TNF in the highest dose, and 60% in IL-1B; guttiferone B: reduced 45 % TNF in the highest dose, and a modest 5% in IL-1B; crude extract: reduced both TNF and IL-1B in 55% in the highest dose). These findings indicate that both isolated prenylated benzophenones and the whole extract of Brazilian red propolis possess relevant anti-inflammatory properties through the modulation of neutrophil activity. Importantly, these data highlight a potential mechanism of action that could contribute to the therapeutic effects attributed to propolis in inflammatory disorders. Nevertheless, additional studies are warranted to further characterize this concentration-dependent effect, to evaluate possible cytotoxicity in neutrophils, and to validate the results in *in vivo* models. Such investigations will be essential to support the pharmacological development of red propolis-derived compounds as potential anti-inflammatory agents.

Keywords: Brazilian Red Propolis, Prenylated Benzophenones, NET, cytokines, anti-inflammatory





HISTORICAL ETHNOBOTANY OF CANNABIS SATIVA L. IN BRAZIL: DOCUMENTARY EVIDENCE OF MEDICINAL USES BEFORE CRIMINALIZATION

Luiza Siqueira Pires^{1*}, Nina Cláudia Barboza da Silva², André Gonzaga dos Santos¹

ls.pires@unesp.br

1-São Paulo State University (UNESP), School of Pharmaceutical Sciences, Laboratory of Pharmacognosy, Araraquara, Brazil. 2-Universidade Federal do Rio de Janeiro (UFRJ), Faculdade de Farmácia, Laboratório de Botânica Aplicada, Rio de Janeiro, Brazil.

The historiography of cannabis in Brazil is often centered on prohibition and stigma, leaving its earlier medicinal uses underexplored. This research aims to recover historical evidence of its therapeutic applications in Brazil before prohibition, highlighting its role in medical and pharmaceutical practices. The methodology relies on systematic archival research in historical libraries and collections in Araraquara and São Paulo, with plans to expand to Rio de Janeiro, Belo Horizonte, Ouro Preto, and Salvador. Sources include pharmacopoeias, formularies, medical dictionaries, and therapeutic manuals, identified using keywords such as “Cannabis sativa,” “Cannabis indica,” “cânhamo,” and “hashish”. To date, 32 documents, from 1865 to 1953, have been analyzed. Cannabis references commonly cited flowers, leaves, and seeds, typically prepared as tinctures, alcoholic or oily extracts, emulsions, and cataplasms. Therapeutic indications focused on neurological and neuropsychiatric disorders, with cannabis used as a hypnotic, sedative, antispasmodic, stimulant, or calming agent. It was also employed in pain management related to gastric, menstrual, neuralgic, rheumatic, and migraine conditions, as well as in respiratory disorders like asthma and bronchitis. Gynecological and sexual uses included menstrual regulation, suppression of lactation, and aphrodisiac effects, with applications in digestive, urinary, dermatological, rheumatic, and ocular disorders. Partial results also revealed controversies in medical discourse: while some records highlight cannabis as an effective treatment for epilepsy, anxiety, or withdrawal syndromes, others describe toxic outcomes such as delirium, psychosis, or addiction. These apparent contradictions may reflect the complex regulatory role of the endocannabinoid system in maintaining physiological balance. This study indicates cannabis’s presence in Brazilian medical practice in the late 19th and early 20th centuries, officially recognized in pharmacopoeias and formularies with diverse therapeutic uses. Continued archival research will deepen understanding of how medical knowledge, cultural perceptions, and regulatory approaches shaped the trajectory of cannabis in Brazil.

Keywords: *Historical ethnobotany, Cannabis sativa, therapeutic uses, documentary research, knowledge recovery, medical history.*





CHEMICAL PROFILING OF *Inga laurina* EXTRACTS AND EVALUATION OF THEIR ANTIBACTERIAL AND ANTIBIOFILM ACTIVITIES AGAINST RESISTANT *Staphylococcus* spp. STRAINS ISOLATES FROM NEONATE

Stella Martins Castro^{1*}, Gabrielle Lavor de Queiroz¹, Marília dos Reis Nery Chen¹,
Fernanda Sampaio Cavalcante², Carla Monteiro Leal¹, Ivana Correa Ramos Leal¹.

stellapharma.sm@gmail.com

1- LAPRONEB, Laboratório de Produtos Naturais e Ensaio Biológicos. 2- LIH, Laboratório de Infecção Hospitalar, Instituto de Microbiologia Paulo de Góes, Centro de Ciências da Saúde, UFRJ, Av. Carlos Chagas Filho, 373, Cidade Universitária, Rio de Janeiro, RJ, Brazil.

Healthcare-associated infections (HAIs) are a major public health concern, with *Staphylococcus* species standing out among the main etiological agents. In this context, the leading Coagulase-Positive (CoPS) bacteria is *S. aureus*, whereas *S. haemolyticus* and *S. epidermidis* are the predominant Coagulase-Negative (CoNS) species, both able to induce sepsis in neonates, in addition to exhibit a strong ability to form biofilm. Furthermore, their ability to acquire antimicrobial resistance contributes significantly to increased morbidity and mortality. Therefore, it is necessary to investigate new therapeutic alternatives for the treatment of infections caused by these pathogens, such as from natural products sources. The genus *Inga*, as an example, is already recognized for their pharmacological activity. So, the present study aims to analyze the chemical profile of partitions (ethyl acetate (EtOAc), butanol and aqueous) obtained from *Inga laurina* (Fabaceae) crude extracts, derived from bark, pulp, seeds, and leaves. In addition, aim to investigate their antibacterial and antibiofilm potential against *Staphylococcus* spp. strains isolated from a neonatal Intensive Care Unit (ICU). For this purpose, *I. laurina* partitions were tested for antibacterial activity against 25 strains of *S. aureus*, *S. haemolyticus*, and *S. epidermidis*, using the macrodilution test at concentrations ranging from 128 to 512 µg/mL in order to establish their minimum inhibitory concentrations (MIC). Strains that demonstrated susceptibility were further evaluated for their biofilm formation in the presence of sub-MIC concentrations (<128 µg/mL) of the active partitions. The partitions were analyzed by HPLC-HRMS/MS and processed using MZmine 4.2. In parallel, feature-based molecular networking available on the GNPS2 platform and the software Sirius 5.8.6 were used to annotate substances present in the selected partitions. Among the evaluated, the leaf EtOAc partition (PAF) stood out, inhibiting approximately 88% of the tested *Staphylococcus* spp. Strains at xxx µg/mL. In the antibiofilm assay, the bark EtOAc partition (PAC) showed promising results against a *S. aureus* strain, with 95% inhibition at 128 µg/mL. From the HPLC-HRMS/MS analyses of the PAF, the following compounds were annotated: myricetin-3-*O*-hexoside, myricetin, myricetin-3-*O*-rhamnoside, myricetin-3-*O*-(2"-*O*-galloyl)-rhamnoside, quercetin-3-*O*-(2"-galloyl)-rhamnoside, and quercetin. *Inga laurina* demonstrated antibacterial and antibiofilm potential, particularly in the PAF. The chemical profile analysis enabled the annotation of flavonoids derivatives, which may be associated with this activity.

Keywords: Antibacterial activity; Antibiofilm; Metabolic profile; Fabaceae; *Inga laurina*.





***ANTINOCICEPTIVE AND ANTI-INFLAMMATORY ACTIVITY OF
COMPOUNDS ISOLATED FROM CHONDRODENDRON
MICROPHYLLUM (BUTE)***

Flávio Mendes de Souza^{1*}, Bruno Oliveira Moreira¹

flaviomendes@ufba.br

*1-IMS/CAT, Instituto Multidisciplinar de Saúde Anísio Teixeira, UFBA, Rua Hormindo Barros, 58,
45.029-094, Brazil*

Since ancient times plants have been used for treatment of various diseases, serving as the primary therapeutic option for early populations who ingested infusions of herbs, seeds, and leaves from different species in search of relief and cure for health problems. Brazil has the greatest plant genetic biodiversity in the world, yet it is estimated that only 8% of the species within the Brazilian flora have been studied for bioactive compounds, with approximately 1,100 evaluated for their medicinal properties. *Chondrodendron microphyllum*, commonly known as buti or bute, had its roots commercialized in the English market in the mid-20th century, with therapeutic indications for the treatment of kidney stones, bladder disorders, uterine cramps, abdominal pain, and as a diuretic. 6'-Hydroxy-6,12-dimethoxy-(+)-curine was one of the compounds isolated and identified in the chloroform fraction of *C. microphyllum* roots, as reported by Silva (2018). Animals used in the study were obtained from the Multidisciplinary Health Institute/ Campus Anísio Teixeira, following approval by the Animal Ethics Committee (process No. 108/2022). Male and female adult BALB/c mice, weighing 20-30g, were used in the tests. This study aimed to assess the antinociceptive activity of the isolated root compound. 6-hydroxy-6,12-dimethoxy-curine, at concentrations of 2,5, 5, and 10 mg/kg, through abdominal contortion tests, intraplantar formalin-induced tests, and Von Frey tests, as well as to evaluate the anti-inflammatory activity of the ethanolic extract (50, 100 and 200 mg/kg) and its hexane, dichloromethane, and ethyl acetate fractions (50mg/kg). Data analyzed by ANOVA demonstrated significant activity in *in vivo* tests, highlighting the importance of *C. microphyllum* in experimental studies.

Keywords: Medicinal plants, *Chondrodendron microphyllum* (bute), Antinociceptive activity, Anti-inflammatory activity, Bioactive compounds, *In vivo* assays.





CYTOTOXIC POTENTIAL OF INDOLE ALKALOIDS FROM *Tabernaemontana catharinensis* AGAINST COLORECTAL CARCINOMA CELLS

Ana Júlia Gomes Donada^{1*}, Rafael Freitas Corá¹, Sidnei Moura e Silva¹

ajgdonada@ucs.br

- LBIOP: Laboratório de Biotecnologia de Produtos Naturais e Sintéticos, Instituto de Biotecnologia, Universidade de Caxias do Sul, RS - Caxias do Sul 95070-560, Brazil.

Phytotherapy is estimated by the World Health Organization (WHO) to be used by almost 80% of the global population, mainly through plants rich in secondary metabolites with therapeutic potential. The genus *Tabernaemontana* (Apocynaceae) is notable for its indole alkaloids, associated with antimicrobial, anti-inflammatory, and antitumor activities. *Tabernaemontana catharinensis*, known as “jasmin-catavento”, is traditionally used in folk medicine, but systematic studies of its alkaloid profile and selective cytotoxicity remain scarce. This study investigated the extraction, chemical characterization, and cytotoxic activity of indole alkaloids from *T. catharinensis* leaves. Extraction was performed by ultrasound-assisted maceration in ethanol, followed by acid–base partitioning to obtain an alkaloid-rich fraction (AF). Chemical analysis by high-resolution mass spectrometry (HRMS) identified seven indole alkaloids, including ibogamine, affinisine, 16-epi-affinine, vobasine, voacangine, and coronaridine derivatives. Toxicity was assessed using the *Artemia salina* bioassay, while cytotoxicity was evaluated in vitro against HCT116 colorectal carcinoma cells and non-tumor MRC5 fibroblasts by MTT assays after 24 and 72 h. The extraction yielded 0.94% (m/m) of AF, consistent with literature values. The *A. salina* assay indicated moderate toxicity, with LD₅₀ 367.33 ± 2.45 µg mL⁻¹. In cell assays, AF significantly inhibited HCT116 viability, with IC₅₀ 28.49 ± 2.66 µg mL⁻¹ (24 h) and 20.86 ± 0.16 µg mL⁻¹ (72 h). MRC5 fibroblasts showed higher resistance (IC₅₀ 60.35 ± 3.25 µg mL⁻¹), demonstrating tumor selectivity. These findings highlight *T. catharinensis* as a promising source of indole alkaloids with selective cytotoxic effects against colorectal carcinoma cells. The alkaloid-enriched fraction demonstrated relevant antitumor activity, supporting its potential for drug discovery. Further mechanistic studies and *in vivo* models are needed to validate their pharmacological applications and therapeutic safety.

Keywords: *Tabernaemontana catharinensis*, indole alkaloids, colorectal cancer.





POSTER SESSION ABSTRACT

Session

Manufacturing and Quality Control of Herbal Drugs and Essential Oils



DEVELOPMENT AND VALIDATION OF A UV-VIS SPECTROPHOTOMETRIC METHOD FOR QUERCETIN QUANTIFICATION IN NANOSTRUCTURED SYSTEMS

Lara Beatriz de Andrade Silva^{1*}, Maria Alice Sousa Marinho¹, Jayne Ferreira da Silva Oliveira¹, Micaela Sousa Coutinho Silva¹, Isabela Dias dos Santos¹, Maria Poliana Leite Galantini¹, Gabriel Azevedo de Brito Damasceno¹, Robson Amaro Augusto da Silva¹, Juliano Geraldo Amaral¹.

lbeatriz@ufba.br

1-Instituto Multidisciplinar em Saúde – Campus Anísio Teixeira / Universidade Federal da Bahia, Rua Hormindo Barros, 58, Candeias, Vitória da Conquista, Bahia.

Quercetin, a flavonoid found in various foods, exhibits well-known antioxidant and anti-inflammatory properties. However, its therapeutic and cosmetic applications are limited by low solubility, instability, and low oral bioavailability. Nanostructured systems, such as microemulsions and lipid nanoparticles, have been explored to overcome these limitations. This study aimed to develop and validate a UV-Vis spectrophotometric method for the quantification of quercetin incorporated into nanostructured systems, optimizing sample preparation and evaluating essential analytical parameters. Different extraction solvents (methanol and methanol acidified with hydrochloric acid (HCl)) were tested in microemulsified quercetin samples (5 mg/mL), as well as various extraction techniques (centrifugation, ultrasound, and magnetic stirring). The optimized protocol consisted of ultrasonic bath (15 min) followed by centrifugation at 3200 rpm for 20 min. Spectrophotometric scanning (200–800 nm) identified maximum absorption at 370 nm, attributed to the molecule's conjugated electronic system. The calibration curve was prepared from a quercetin standard solution (100 mg/mL) diluted in methanol acidified with 0.01% HCl, at concentrations ranging from 3–7 µg/mL, showing excellent linearity ($R^2 = 0.999$) and reproducibility (standard deviation < 0.2). ANOVA indicated no significant differences ($p > 0.05$) between the solvents tested, allowing flexibility in solvent choice. Methanol acidified with 0.01% HCl was selected for the calibration curve due to its good compatibility with UV-Vis spectrophotometry. Preliminary results indicate the method's potential for reliable quercetin quantification in complex matrices, with full robustness, precision, and accuracy assessments currently in progress. The working range of 3–7 µg/mL was found to be optimal for ensuring sensitivity and reliability. In conclusion, the proposed protocol is simple, cost-effective, and suitable for quality control and pharmaceutical studies involving quercetin in nanostructured systems. Future work will include complete validation following official guidelines.

Keywords: quercetin, UV-Vis spectrophotometry, method validation, nanostructured systems, microemulsions.





DEVELOPMENT AND STABILITY EVALUATION OF LEMONGRASS ESSENTIAL OIL MICROEMULSIONS FOR POTENTIAL ANTIMICROBIAL USE

Isabela Dias dos Santos^{1*}, Yolanda Trindade de Oliveira², Maria Alice Sousa Marinho², Paulinne Moreira Lima², Catarina Silva Guimarães², Micaela Sousa Coutinho Silva¹, Jayne Ferreira da Silva Oliveira², Lara Beatriz de Andrade Silva¹, Caio Cezar dos Santos Pereira³, Robson Amaro Augusto da Silva¹⁻³, Gabriel Azevedo de Brito Damasceno¹⁻², Juliano Geraldo Amaral¹⁻².

mariaalice1000@live.com

1-Instituto Multidisciplinar em Saúde, Campus Anísio Teixeira, Universidade Federal da Bahia (UFBA), Vitória da Conquista, Bahia, Brazil. 2-Programa de Pós-Graduação em Biociências, Campus Anísio Teixeira, Universidade Federal da Bahia (UFBA), Vitória da Conquista, Bahia, Brazil. 3-Programa de Pós-Graduação em Ciências Fisiológicas, Campus Anísio Teixeira, Universidade Federal da Bahia (UFBA), Vitória da Conquista, Bahia, Brazil.

Microemulsions are promising systems for the encapsulation of essential oils, enhancing their stability, solubility, and potential pharmaceutical applications. This study aimed to develop microemulsions containing *Cymbopogon citratus* (lemongrass) essential oil, registered in SisGen (No. A389682), and to evaluate their physical stability and antimicrobial potential. Based on the construction of a pseudoternary phase diagram, different surfactant/oil ratios were tested to optimize the system. After evaluating the various ratios, the 7:3 (surfactant:oil) ratio was selected as the most suitable, consisting of Tween 80 and PEG-40. Two formulations were selected based on their macroscopic characteristics: ME10 and ME13. The emulsions were subjected to accelerated stability studies at different temperatures (25°C, 4°C, and 40°C) and times (T0, T5, T30, T60, and T90 days), with particle size, polydispersity index (PDI), and zeta potential evaluated by dynamic light scattering (DLS). The ME10 formulation maintained a particle size below 100 nm during the first 30 days, while ME13 exceeded this limit in the same period, reaching 161.15 nm, indicating loss of stability and loss of microemulsion characteristics. In the microbiological stage, antimicrobial activity was evaluated against *methicillin-resistant Staphylococcus aureus* (MRSA), ATCC 43300, using the spread plate technique. Samples were incubated with the microorganisms for 20 minutes prior to plating. Growth inhibition was observed for ME10 from the concentration of 20 µg/mL, while for ME13 inhibition occurred only from 30 µg/mL. The ME10 formulation promoted the greatest reduction in microbial load compared to ME13. These findings reinforce the feasibility of the developed microemulsions as pharmaceutical carriers with potential antimicrobial activity..

Keywords: Microemulsion, *Cymbopogon citratus*, *methicillin-resistant Staphylococcus aureus* (MRSA),





***QUALITY EVALUATION OF COMMERCIAL PEUMUS BOLDUS SAMPLES:
IMPLICATIONS FOR THE SAFETY AND EFFECTIVENESS OF HERBAL USE***

Laís Aparecida Moreira^{1*}, Luciana Moreira Chedier², Fabíola Dutra Rocha¹

laismoreira223@gmail.com

1- Departamento de Ciências Farmacêuticas, UFJF, Rua José Lourenço Kelmer, São Pedro, Juiz de Fora, MG, Brazil. 2- Instituto de Ciências Biológicas, UFJF, Rua José Lourenço Kelmer, São Pedro, Juiz de Fora, MG, Brazil.

Peumus boldus Molina is an endemic species of Chile, whose leaves are widely employed in traditional medicine due to their therapeutic properties¹. However, the scarcity of studies validating the quality of this herbal drug restricts its safe prescription by healthcare professionals. The aim of this study was to assess the quality of boldo do chile herbal drug acquired from three commercial sources in the city of Juiz de Fora and one via e-commerce. Packaging was evaluated in accordance with the Collegiate Board Resolution (RDC) 26/2014, and none of the samples fully complied with the established requirements. Botanical and chemical authenticity, as well as purity and chemical stability analyses, were performed based on the *Peumus boldus* monograph of the Brazilian Pharmacopoeia. Botanical and chemical authenticity was confirmed for all samples. Purity assessment revealed levels of foreign matter exceeding the specified limits (ranging from 5.46% to 6.11%; limit $\leq 2\%$), while moisture content varied between $5.66\% \pm 0.24$ and $14.83\% \pm 0.62$ (limit $\leq 10\%$). The content of inorganic substances complied with the regulatory threshold ($\leq 10\%$), ranging from $8.31\% \pm 0.31$ to $9.34\% \pm 0.08$. Acid-insoluble ash ranged from $4.55\% \pm 0.14$ to $6.98\% \pm 0.28$, exceeding the specified limit of $\leq 6\%$ in some samples. Chemical integrity was verified through the determination of total alkaloid content (minimum required $\geq 0.1\%$) by high-performance liquid chromatography (HPLC), as well as the quantification and composition of essential oil. Alkaloid levels ranged between 0.04% and 0.08%, while essential oil content varied from 0.55% to 0.83%. Overall, although all samples were authenticated, they exhibited inadequate packaging and failed to comply with the required quality standards regarding purity and chemical integrity.

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Keywords: *Peumus boldus* Molina, quality control, herbal drug.





VALIDATION OF *Maytenus ilicifolia* PHYTOTHERAPEUTIC PROFILES BY TLC-CD AND MACHINE LEARNING

Rodolfo S. Barboza^{1*}, Rodrigo C. Blanco¹, Thiago S. Dias¹, Matheus V. Curti¹, Maiara O. Salles¹, Priscila F. P. Santos², Daniella L. Vale¹

rodolfo-sb@hotmail.com

1- Instituto de Química, Centro de Ciências Matemáticas e da Natureza, Universidade Federal do Rio de Janeiro, 21941-909, Rio de Janeiro – RJ, Brasil.

2- Centro Federal de Educação Tecnológica Celso Suckow da Fonseca, Campus Angra dos Reis, 23953-030 Angra dos Reis – RJ, Brasil.

Brazil is recognized as one of the countries with the greatest biodiversity worldwide, harboring at least 20% of all known plant species¹ (Berlink 2012). The species *Maytenus ilicifolia* Mart. ex Reissek, commonly known as Espinheira Santa, is listed in the National List of Medicinal Plants of Interest to the Unified Health System (RENISUS, from Portuguese)². Due to its pharmacological properties and cost-effectiveness, herbal medicines derived from *M. ilicifolia* leaves are recommended by the Brazilian public health system and are widely used as complementary therapy for conditions such as gastritis and indigestion, among other gastrointestinal disorders. Within the scope of public health, there is an urgent need to develop quality control methods that ensure the integrity of *M. ilicifolia*-based phytotherapeutics. This study analyzed 25 samples of *M. ilicifolia* leaf-based medicinal products. The developed method using thin-layer chromatography combined with computational densitometry and machine learning enabled the classification of the samples into four distinct groups, underscoring the ineffective quality control of *M. ilicifolia* products marketed in Brazil and used as complementary treatments, revealing a pronounced lack of standardization in the plant material, with substances and/or their quantities varying significantly across the analyzed samples, raising serious public health concerns.

Keywords: *Maytenus ilicifolia*, Espinheira Santa, phytotherapeutics control, phenolic compounds.

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**CHEMICAL COMPOSITION AND BIOACTIVITY OF *PSIDIUM RUFUM*
ESSENTIAL OIL: CYTOTOXIC AND LEISHMANICIDAL EVALUATION**

Ana Beatriz Marques Soares^{1*}, Denise Crispim Tavares², Lizandra Guidi Magalhães Caldas², Rafael Ferreira da Silva³, Claudia de Moraes Rezende³, Virgínia Claudia Paulino Silva¹

anabeatrizms2002@gmail.com

1 – Universidade Federal de São Carlos, Centro de Ciências Agrárias, Araras, 13600-970, São Paulo, Brazil. 2 – Universidade de Franca, Centro de Pesquisa em Ciências Exatas e Tecnologia, Franca, 14404 600, São Paulo, Brazil. 3 – Universidade Federal do Rio de Janeiro, Instituto de Química, Rio de Janeiro, 21941-902, Rio de Janeiro, Brazil.

The essential oil (EO) from the leaves of *Psidium rufum* (Myrtaceae) was obtained by hydrodistillation using a Clevenger apparatus, with a modest yield of 0.5% (w/w). GC-MS and GC-FID analyses allowed the identification of 41 compounds, representing 98.6% of the total composition. The chemical profile was dominated by oxygenated sesquiterpenes (46.8%) and sesquiterpene hydrocarbons (29.5%), followed by oxygenated monoterpenes (12.5%) and monoterpene hydrocarbons (5.6%). The major constituents were 1,8-cineole (12.5%), spathulenol (10.3%), α -longipinene (9.8%), β -caryophyllene (7.5%), globulol (6.1%), and γ terpinene (4.2%). This prevalence of oxygenated terpenes is consistent with reported antimicrobial and cytotoxic properties in other Myrtaceae species. Cytotoxicity was assessed against human tumor cell lines (HeLa, MCF-7, and U-251MG) and non-tumor fibroblasts (GM07492A). The EO displayed IC₅₀ values of 21.9 ± 0.3 μ g/mL for HeLa, 25.7 ± 0.4 μ g/mL for MCF-7, and >100 μ g/mL for U-251MG. For non-tumor fibroblasts, the IC₅₀ was also >100 μ g/mL, resulting in selectivity indices of 3.86 (HeLa) and 3.04 (MCF-7), confirming selective cytotoxicity toward tumor cells while maintaining relative safety to normal cells. Leishmanicidal activity was evaluated against promastigotes of *Leishmania amazonensis*. At 24 h, the EO promoted moderate inhibition, with a maximum value of $50.18\% \pm 1.49$ at 50 μ g/mL and an IC₅₀ of 38.05 μ g/mL. However, at 48 h the activity decreased, reaching $28.71\% \pm 1.87$ at the same concentration, with IC₅₀ values above 50 μ g/mL. This reduction suggests a time-dependent decline, possibly associated with compound instability or parasite adaptation under prolonged exposure. In conclusion, this is one of the first reports on the biological activities of *P. rufum* essential oil, which combines a chemically rich composition dominated by oxygenated sesquiterpenes with selective cytotoxicity and moderate leishmanicidal effects. These findings highlight *P. rufum* EO as a promising natural source of bioactive molecules.

Keywords: *Psidium rufum*, essential oil, chemical composition, cytotoxicity, leishmanicidal activity





STEAM DISTILLATION AND SUPERCRITICAL CO₂ EXTRACTION OF OREGANO ESSENTIAL OIL FROM COLOMBIAN BIODIVERSITY: A COMPARATIVE STUDY ON YIELD, QUALITY, AND BIOACTIVITY

Yasmin Valero-Gutierrez^{1*}, Sara Ospina-Burbano¹, Camilo Pardo-Castaño¹, Mauricio Fortaleche-Caicedo¹, Alejandro Quintero-Velez¹, Ruben Camargo-Amado¹

yasminvalero.chemist@gmail.com

1-Escuela de Ingeniería Química, Universidad del Valle, Campus Meléndez Calle 13 #100-00, Cali, Valle del Cauca, Colombia.

Colombia, a megadiverse country, presents unique opportunities for the development of natural, biobased products. This study investigated *Origanum vulgare* cultivated in Tenerife, Valle del Cauca, Colombia, to obtain and characterize its essential oil using two extraction methods: steam distillation (SD) and supercritical CO₂ extraction (SFE). We applied a 2⁴⁺¹ fractional factorial design to optimize SFE conditions and maximize mass yield. The resulting extracts were characterized by GC-MS to compare volatile profiles between the two techniques. Additionally, a comprehensive quality and safety assessment was performed, including analyses for pesticide residues, heavy metals, and mycotoxins.

Bioactivity was assessed through antioxidant capacity (ORAC-L assay), total polyphenol content, and viability and cytotoxicity in HeLa cells. A prototype formulation incorporating the extracts was developed and subjected to a 4-month stability study, assessing physical, chemical, and microbiological parameters.

Results demonstrate that SFE under optimized conditions provided higher mass yields and superior safety profiles with reduced contamination risks, while both techniques yielded oils rich in carvacrol and other bioactive terpenes. The integrated comparative approach highlights the value of combining traditional and modern extraction techniques for developing safe, stable and functional products from Colombian biodiversity. The findings contribute to the manufacturing and quality control of essential oils and extracts, supporting local value chains and advancing the Colombian bioeconomy through science-based innovation. The authors are grateful for the support and funding of the research project with resources from the NATIONAL FUND FOR SCIENCE, TECHNOLOGY AND INNOVATION FRANCISCO JOSÉ DE CALDAS. Contract 112721-249-2024 / Project 109097.

Keywords: *Oregano essential oil, quality control, bioactivity, steam distillation, supercritical CO₂ extraction, factorial design, GC-MS, antioxidant activity, cytotoxicity, Colombian biodiversity.*





QUALITY BY DESIGN APPLIED TO THE PRODUCTION OF THE HERBAL MEDICINE FROM *Monteverdia ilicifolia* (Mart. ex Reiss.) Biral

Alberto Araujo de Caux^{1*}, Maria Isabel Rodrigues (2), Marcus Bruno S. Fortes (2), Rodney

Alexandre Ferreira Rodrigues¹ aaraujodecaux@gmail.com

1- Centro Pluridisciplinar de Pesquisas Químicas, Biológicas e Agrícolas - CPQBA UNICAMP.

2 - Faculdade de Engenharia de Alimentos - FEA - UNICAMP.

With the advancement of quality tools, new opportunities have emerged to study and optimize processes that were previously not systematically controlled. In this context, Quality by Design (QbD) stands out as a strategic approach to ensure the efficacy, safety, and quality of herbal medicines, such as those derived from *Monteverdia ilicifolia* (Mart. ex Reiss.) Biral, commonly known as "Espinheira Santa", which is recognized for its antidyspeptic, antacid, and gastric mucosa-protective properties ⁽¹⁾. This study aimed to evaluate the extraction and spray-drying processes for obtaining an Espinheira Santa herbal medicine using QbD principles. Through process mapping and risk assessment, potentially critical factors were identified and subsequently challenged by means of Design of Experiments (DoE). For the extraction step, a 12-run Plackett–Burman design (8 factors) was conducted; for scaling-up, a Central Composite Design (CCD) with 7 runs (2 factors) was applied; and for the spray-drying step, a Rotational Central Composite Design (RCCD) with 17 runs (3 factors) was carried out. The response variables studied in each design were those related to Critical Quality Attributes (CQAs), that is, attributes that impact efficacy and safety ⁽²⁾. The effects (linear, quadratic, and interaction) were estimated, and the models were evaluated by ANOVA using the statistical software RStudio Version 4.4.0. Factors showing significant effects (p-value < 0.1) were identified as critical ⁽³⁾. In the extraction step, the following factors were significant for at least one CQA: “extraction type” (decoction or infusion), “drug-to-extract ratio” (1% to 6%), “herbal drug form” (cut or powdered), “vessel type” (glass or metal), “water quality” (purified or distilled), “exposure” (open or closed), “boiling time” (2 or 5 min), “stirring” (0 to 600 rpm), and “extraction time” (10 to 30 min). In the spray-drying step, maltodextrin addition (0 to 60%), feed rate (3.5 to 7.5 mL/min), and inlet temperature (120 to 200 °C) were significant for at least one CQA. In conclusion, the QbD approach enabled the identification of critical factors associated with the extraction and spray-drying processes of Espinheira Santa, ensuring process capability.

Keywords: Espinheira Santa, Extraction, Design of Experiments, Scaling-up, Spray drying.

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Acknowledgments: CNPq, COCEN.





OPTIMIZATION OF AQUEOUS EXTRACTION OF MANGABA (*HANCORNIA SPECIOSA* GOMES) PULP FOR MAXIMIZED POLYPHENOL CONTENT AND ANTIOXIDANT ACTIVITY

Paula da Costa Garcia¹, Dâmaris Silveira¹, Pérola de O. Magalhães¹, **Yris Maria Fonseca-Bazzo^{1*}**

yrisfonseca@unb.br

1-Laboratory of Natural Products, Faculty of Health Sciences, University of Brasília (UnB), Asa Norte, Brasília, DF, Brazil. ZIP Code 70910-900.

This study aimed to optimize the aqueous extraction process of mangaba (*Hancornia speciosa* Gomes) pulp to maximize polyphenol content and antioxidant activity. Fruits were collected from Embrapa Cerrados (Planaltina, Brazil). Optimization was carried out using two Central Composite Rotational Designs (CCRD), analyzed by Response Surface Methodology (RSM). Independent variables were extraction time, pulp-to-solvent ratio, and temperature, while response variables included extraction efficiency (soluble solids), total polyphenol content and DPPH radical scavenging capacity. In the first experimental design (ED1), conducted at 30 °C, only the pulp-to-solvent ratio significantly influenced solids content and polyphenol concentration, with optimal results at ratios between 1:3 and 1:5 (m/v). Extraction time showed no significant effect, consistent with equilibrium diffusion described by Fick's second law. Extracts with higher pulp content presented greater polyphenol concentrations; however, antioxidant activity by the DPPH assay showed a negative correlation, likely due to fiber and latex interactions with phenolic compounds. The second experimental design (ED2) included temperature as an additional factor. Results confirmed the critical role of pulp-to-solvent ratio and highlighted the positive effect of elevated temperatures (up to 80 °C) on antioxidant activity, possibly due to enzyme inactivation and enhanced fiber solubilization. A strong positive correlation was observed between polyphenol content and extraction efficiency, while yield was negatively correlated, reflecting filtration challenges in concentrated extracts. To integrate multiple responses, a desirability function was applied, identifying optimal extraction conditions as 6 minutes, pulp-to-solvent ratio of 1:3.3 (m/m), and temperature of 80 °C. In conclusion, optimized dynamic maceration proved effective for producing aqueous extracts of mangaba pulp with high polyphenol content (284.8 µg /mL) and strong antioxidant activity (91.6 % inhibition). Acknowledgments: University of Brasília (UnB), National Council for Scientific and Technological Development (CNPq), Coordination for the Improvement of Higher Education Personnel (CAPES), and Federal District Research Support Foundation (FAPDF). Grant numbers: 00193 00001194/2021-47; 405961/2021-9.

Keywords: mangaba, nutraceuticals, polyphenol, antioxidant and extraction.





COMPARATIVE ANALYSIS OF LOW- AND HIGH-FIELD NMR FOR THE QUANTIFICATION OF CANNABINOIDS IN CANNABIS PRODUCTS

Lis Raquel Silva do Nascimento^{1*}, Anita Monteiro Meireles³, Adriano Otavio Maldaner²,
Renato Rosseto¹, Giuliana Muniz Vila Verde¹, Gilberto Lúcio Benedito de Aquino^{1,2}

lis@aluno.ueg.br

1-Research Laboratory on Bioproducts and Synthesis, State University of Goiás - CET, Anápolis, Goiás, Brazil. 2-National Institute of Criminalistics, DITEC/PF, Brasília, Brazil. 3-Department of Pharmacy - University of Brasília, Brasília, Federal District, Brazil.

Quantitative nuclear magnetic resonance spectroscopy (qNMR) is a robust and increasingly used technique for the analysis of products derived from *Cannabis sativa* L., offering a precise alternative to chromatographic methods. However, analytical precision critically depends on factors such as the equipment used (more accessible low-field spectrometers versus more precise high-field ones) and the choice of the internal quantification standard. Therefore, this work evaluated the impact of two internal standards, dimethyl sulfone (DMS) and 1,2,4,5-tetrachloro-3-nitrobenzene (TCNB), on cannabinoid quantification, with the goal of determining the optimal conditions for the use of low-field equipment. *Cannabis sativa* L. oil samples were prepared in deuterated chloroform (CDCl₃) and analyzed on 80 MHz and 600 MHz NMR spectrometers. Preparation conditions included the use of DMS and TCNB as standards, with the addition of deuterated water (D₂O) in some samples to evaluate the effect on signal suppression and solubility. The data were subjected to Student's t-tests to compare means and, crucially, to Bland-Altman plots to evaluate the individual concordance between measurements from the two instruments. The results showed that the use of the DMS standard resulted in significant differences ($p < 0.05$) between the 80 MHz and 600 MHz NMR, with the Bland-Altman plots revealing a bias and limited concordance. On the other hand, the TCNB standard with D₂O addition showed remarkable results. Under this condition, the differences in mean quantification were not statistically significant ($p > 0.1$), and the Bland-Altman plot confirmed a high concordance and a minimal bias between the two instruments, validating the interchangeability of the methods. We conclude that the choice of an internal standard is fundamental for the optimization of qNMR. The use of TCNB allows low-field NMR to be a viable and accessible alternative for quality control, offering precision and concordance comparable to high-field NMR for the quantification of cannabinoids in oil samples.

Keywords: *Cannabis sativa*, qNMR, CBD (Cannabidiol), Cannabinoids, Low-field NMR.





**MORPHOANATOMIC INVESTIGATION IN THE QUALITY CONTROL OF SPECIES
THAT COMPOSE AYAHUASCA GOIANA**

Warley Freitas Silva^{1*}, Maxwell Moreira Martins¹, Lis Raquel Silva do Nascimento¹,
Poliene Soares dos Santos Bicalho², Giuliana Muniz Vila Verde¹

warley2605@aluno.ueg.br

1-State University of Goiás, CCET, Anápolis, Goiás, Brazil; 2- State University of Goiás, CSEH,
Anápolis, Goiás, Brazil

Ayahuasca is an ethnobotanical beverage used in rituals, whose main constituents are the stem of the vine *Banisteriopsis caapi* and the leaves of *Psychotria viridis*¹. The correct botanical identification and verification of material purity are fundamental steps for the quality control and safety of plant-derived products². This work aimed to use a robust methodology of morphological and microscopic analysis, including scanning electron microscopy (SEM), for the authentication and differentiation of the powders of these two species. The material was collected in the region of Abadiânia, Goiás, and its *in situ* identification was performed by a responsible collector, based on distinctive morphological criteria such as the extrafloral nectaries in *B. caapi* and the domatia in *P. viridis*. The samples were subjected to controlled drying and pulverization. Analysis by light microscopy and histochemistry revealed details such as the arrangement of the parenchyma, stomata, and trichomes, highlighting the cellular differences between the species. The SEM of the powders complemented the observations, providing crucial ultrastructural data. The powder of *B. caapi* exhibited the morphology of woody fragments and calcium oxalate crystals, characteristic of the stem, in addition to allowing the observation of the conductive vessels in SEM. In contrast, the powder of *P. viridis* clearly revealed the cellular structure of the leaves and the morphology of the domatia trichomes, allowing a distinction between them. In conclusion, this study establishes pharmacognostic characterization parameters that contribute to the identification of *Banisteriopsis caapi* and *Psychotria viridis* powders. The microscopic and ultrastructural structures can be used as a morphological reference standard for quality control, preventing adulteration and contributing to the authenticity and safety of traditional ethnobotanical preparations.

Keywords: Ayahuasca, Quality Control, Scanning Electron Microscopy, *Banisteriopsis caapi*, *Psychotria viridis*.

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DEVELOPMENT OF AN ANTI-AGING SERUM CONTAINING *PASSIFLORA EDULIS* LEAF EXTRACT

Laura Aparecida Evangelista de Carvalho¹, João Paulo Dourado Abade^{1*}, Cláudio Moreira de Lima¹

llauracarvalho@academico.ufs.br

1-Departamento de Farmácia, Universidade Federal de Sergipe, Campus Lagarto, Lagarto, Sergipe, 49400-000, Brazil.

Aging is a natural and irreversible phenomenon that affects everyone, occurring mainly due to the accumulation of free radicals, unstable and highly reactive molecules, that cause damage to biomolecules. This damage, in addition to serious diseases such as cancer and atherosclerosis, can lead to aesthetic manifestations such as the appearance of wrinkles. In this scenario, the search for anti-aging cosmetics and drugs has grown exponentially, especially among middle-aged and elderly individuals, aiming to delay or prevent expression lines and skin changes. Naturally occurring compounds, such as those found in passion fruit (*Passiflora edulis*), have attracted great interest due to their high antioxidant content. The present study aims to develop anti-aging serum formulations containing *Passiflora edulis* extract. The leaf extract was obtained by ultrasound and maceration methods, followed by phytochemical screening of the crude ethanolic extract (EEB) and quantification of total flavonoids and phenolic compounds. Serum formulations containing 5, 10, and 20% EEB were produced and evaluated for physicochemical parameters (pH, density, spreadability, flavonoid and phenolic content) and antioxidant activity using the DPPH method. The extraction yield was 25.3% (ultrasound) and 26.15% (maceration). Phytochemical screening revealed the presence of flavonols, steroids, triterpenes, polyphenols, and saponins. Quantification showed phenolic compound content (75.6 ± 3.7 mg/g) and flavonoids (36.2 ± 1.4 mg/g) in the ultrasound-assisted extract, 75.9 ± 3.9 mg/g of phenolic compounds and 34.1 ± 2.9 mg/g of flavonoids in the extract obtained by maceration. The 20% serum and extract showed high antioxidant activity, as well as adequate pH and spreadability. The serum containing *Passiflora edulis* shows potential as a promising alternative for preventing signs of skin aging.

Keywords: Antioxidant; Anti-aging; Cosmetics; Phytochemical screening





Quantification of caffeine in different plant matrices and by different techniques

João Victor da Silva Santana Santos^{1*}, Cassandra Mendonça de Oliveira¹, Alexia Sabrina Lisboa Costa¹, Beatriz Araujo Lima de Oliveira¹, Yan Gustavo Mota Santos¹, Mariana Cruz Passos², Felipe Gabriel Henrique Julião³, Natalia Nogueira Saraiva¹, James Almada da Silva¹

jvictor09.jvs@gmail.com

1-Departamento de Farmácia Lagarto, Universidade Federal de Sergipe Campus Professor Antônio Garcia Filho, Lagarto-SE, 49400-000, Brazil. 2-Programa de pós-graduação em ciências aplicadas a saúde, Universidade Federal de Sergipe Campus Professor Antônio Garcia Filho, Lagarto-SE, 49400-000, Brazil. 3- Programa de pós-graduação em Química, Universidade Federal de Sergipe, São Cristovão-SE, 49100-000, Brazil.

The consumption of plant-based beverages is an ancient practice, associated with both cultural aspects and the physiological effects of their bioactive constituents. In Brazil, coffee, yerba mate, and green tea are among the most popular beverages, with caffeine being the main compound of interest. This xanthine alkaloid exerts a stimulating effect on the central nervous system by inhibiting adenosine receptors, resulting in increased alertness and reduced fatigue. In addition to its pharmacological effect, quantifying caffeine in different matrices is important for quality control, product standardization, and comparative evaluation of the efficiency of extraction methods. This study aimed to determine the caffeine levels in coffee beans (*Coffea arabica*), yerba mate leaves (*Ilex paraguariensis*), and green tea (*Camellia sinensis*), as well as to compare different extraction processes. Initially, aqueous extracts were obtained by infusion (10 min) using 5 g of plant drug. They were then subjected to high-performance liquid chromatography (HPLC) analysis using a calibration curve with a caffeine standard ($R^2 = 0.99$). The average concentrations obtained were 76.7, 18.5, and 14.1 $\mu\text{g/mL}$ in coffee, yerba mate, and green tea, respectively. Based on these results, coffee was selected for comparative evaluation of extraction methods, employing infusion, decoction, and pressurization. Starting from 8.8 g of plant drug and each extraction lasting 2 min, the aqueous extract was obtained. The concentrations obtained were similar: 26.5, 26.7, and 25.5 $\mu\text{g/mL}$, respectively. This suggests that the methods present equivalent efficiencies for caffeine extraction. It is concluded that coffee stands out as the matrix with the highest caffeine content among those analyzed and that, regardless of the method employed, the extraction of the alkaloid presents consistent results. These findings reinforce the importance of choosing the plant matrix for caffeine intake and demonstrate the viability of simple methods, such as infusion, for efficiently obtaining the compound.

Keywords: *Coffea arabica*, *Ilex paraguariensis*, *Camellia sinensis*, HPLC-DAD, Caffeine





***in vitro* AND *in silico* ANTI-INFLAMMATORY POTENTIAL OF A
COUMAROYL OLEANOLIC ACID DERIVATIVE FROM *Miconia
albicans*: VIA NF-KB PATHWAY MODULATION**

Annabel Azevedo da Silva^{1,2*}, Dhara Leite Lopes¹, Isabella Mary Alves Reis², Humberto
Fonseca Freitas³, Manoelito Coelho dos Santos Junior³, Cristiane Flora Villarreal¹ e
Alexsandro Branco^{1,2}

branco@uefs.br

1- PPGFar, Faculdade de farmácia, UFBA, rua Barão de Jeremoabo s/n, Salvador, BA, 40170.115,
Brazil. 2- LabFito, DSAU, UEFS, Av. Transnordestina, s/n, Feira de Santana, BA, 44036-900, Brazil.
3- LLM, DSAU, UEFS, Av. Transnordestina, s/n, Feira de Santana, BA, 44036-900, Brazil.

Miconia albicans (“canela-de-velho”) is widely used in traditional medicine to alleviate inflammation and joint pain, particularly in osteoarthritis, a chronic inflammatory condition in which mediators such as IL-1 β induce mitochondrial dysfunction and nitric oxide (NO) production, promoting cartilage degradation and disease progression. The study describes the isolation of an acylated triterpene from *M. albicans* and the evaluation of its anti-inflammatory activity to better understand its ethnopharmacological relevance. The hydroalcoholic crude extract underwent successive fractionation by flash open-column chromatography, followed by semipreparative HPLC purification, which led to the isolation of a coumaroyl triterpene ester (1). Its structure was elucidated using 1D and 2D NMR spectroscopy in combination with tandem mass spectrometry (MS/MS). The **1** was evaluated *in vitro* for cytotoxicity in J774 macrophages, and its anti-inflammatory potential was assessed via inhibition of NO production in LPS/IFN- γ -stimulated J774 macrophages. Subsequently, the structure was evaluated for its interaction with the NF- κ B pathway through molecular docking. The isolated compound was analyzed by MS/MS in positive mode showed a molecular ion peak [M+H]⁺ at *m/z* 619.38, with fragment ion at *m/z* 455.05 corresponding to the loss of coumaric acid. The structural elucidation using 1D and 2D NMR, combined with comparison to literature data, allowed the identification of 23-hydroxy-27-p-coumaroyloxy-olean-12-en-28-oic acid (**1**). The **1** significantly inhibited NO production at non-cytotoxic concentrations. A concentration-dependent reduction was observed at 100 and 200 μ g/mL ($p < 0.0001$), with the 200 μ g/mL dose exceeding the inhibitory effect of dexamethasone (40 μ M; $p < 0.0001$), emphasizing the potential of compound **1** as a modulator of the inflammatory response.

Keywords: *Miconia albicans*, coumaroyl triterpene ester, anti-inflammatory activity, osteoarthritis.





MAPPING THE METABOLIC DIVERSITY IN SIX BIGNONIACEAE PLANT SPECIES

Marcelino Santos do Rosário^{1*}, João Luiz Bronzel Junior¹, Juliana Rodrigues¹, Helena Mannocho-Russo², Lúcia Garcez Lohmann³; Vanderlan da Silva Bolzani¹

marcelino.santos@unesp.br

¹NuBBE, Universidade Estadual Paulista “Júlio de Mesquita Filho”, Araraquara, SP

² University of California San Diego, CA, US

³ University of California, Berkeley, CA US

Introduction: Considering the magnitude of Brazilian biodiversity, there are still few studies on the natural products biosynthesized by plant species found in six distinct biomes, a valuable body of scientific and applied research that remains understudied and economically exploited. The Bignoniaceae family, composed of approximately 800 species, is widely distributed throughout the country and is an example of a taxon that has been little investigated regarding natural products, their biological functions, and pharmacological properties. This project aims to develop an approach based on the state-of-the-art metabolomics of species in this Angiosperm family, which is also the objective of this project. **Material and Methods:** Six Bignoniaceae plant species were used in this study, each one representing a specific clade in the family. Individual plant extracts were analyzed via UHPLC-QTOF-MS. The data obtained were converted to “.mzML” format and preprocessed using MZmine 4 software. The “.csv” and “.mgf” files were used for statistical analysis using MetaboAnalyst and for metabolite annotation using GNPS and SIRIUS. For molecular networks, the Feature-based Molecular Networking analysis mode was used. **Results and discussion:** PCA analysis of the metabolic profiles of Bignoniaceae species demonstrated chemical differentiation among plant species. This is the first evidence that each species has its own chemical identity within the Bignoniaceae family, potentially linked to different classes of secondary metabolites. Through molecular networks, it was possible to identify different classes of natural products in the six plants studied, including flavones, cinnamic acids and derivatives, iridoids, phenylethanoids, flavonols, flavanones, xanthones, chalcones, lignans, and secoiridoids. Flavonoids were the most predominant class in the samples, being reported in all six plant species studied. The authors would like to thank INCT/CNPq Proc. No. 465637/2014-0; FAPESP Thematic No. 2014/50926-0 and fellowship 2024/02602-2).

Keywords: Bignoniaceae; Secondary metabolite; Molecular networking; FBMN.





POSTER SESSION ABSTRACT

Session
Metabolomics and RESEM



SEASONAL EVALUATION OF THE CHEMICAL COMPOSITION OF *Piper Fuligineum* AND *Piper Macedoi* ESSENTIAL OILS

João Pedro Doelo Pereira Leite^{1*}; Raquel Maria Ferreira de Sousa¹

jpdoelo123@gmail.com

I-NuPPeN, Instituto de Química, UFU, Av. João Naves de Ávila, 2121, Bloco 1D, Uberlândia, Minas Gerais, 38400-902, Brazil.

Natural products from plants continue to be a key resource for the discovery of bioactive compounds with pharmaceutical, agricultural, and ecological relevance. The genus *Piper* is especially rich in secondary metabolites, many of which show insecticidal, ovicidal, and larvicidal potential. This study focuses on the metabolomic characterization of two morphologically similar species, *Piper macedoi* and *Piper fuligineum*, both known for their bioactivity and native to southeastern Brazil. Both species are shrubby, found near water sources, sometimes with their roots submerged. The fruits appear in spike-like structures, which is characteristic of the genus as a whole. The leaves are similar in shape; however, the main morphological difference lies in their texture and size: *P. fuligineum* has smaller and rougher leaves compared to the smoother and larger leaves of *P. macedoi*. The plants were collected in close proximity, less than 100 meters apart, at the “Fazenda Experimental do Glória” (UFU, Uberlândia, MG), minimizing environmental variability. Leaf samples (Herbarium code at the University of Brasília: 311774 for *P. fuligineum* and 311780 for *P. macedoi*) were collected every two months over the course of one year (September 2024, November 2024, January 2025, March 2025, and May 2025). Essential oils were obtained by hydrodistillation (yields – *P. macedoi*: 0.206 ± 0.029 %; *P. fuligineum*: 0.201 ± 0.029 %) and analyzed using GC-MS and GC-FID. The aim is to investigate differences in the chemical profiles of the two species throughout seasonal changes, in order to understand how environmental variation affects the metabolic responses of each species. Although morphologically similar, *P. macedoi* and *P. fuligineum* may exhibit distinct chemical adaptation strategies, which can aid in species differentiation and provide insights into their ecological roles and biotechnological potential. Acknowledgments: FAPEMIG, CAPES and CNPq.

Keywords: *Piper macedoi*, *Piper fuligineum*, metabolomics, GC-MS, GC-FID, seasonal variation, natural products





GENUS-SPECIFIC METABOLIC SIGNATURES IN ORCHIDACEAE REVEALED BY LC-HRMS/MS AND MULTIVARIATE STATISTICAL ANALYSIS

Milbya Lima Costa^{1*}, Gesiane da Silva Lima², Gabriel Franco dos Santos², Naará da Silva Balbino², Salva Asghar¹, Danielle Ferreira Dias¹, Marisi Gomes Soares¹, Nerilson Marques Lima¹

milbya.costa@sou.unifal-mg.edu.br

1- Institute of Chemistry, Federal University of Alfenas, Alfenas, MG 37130-001, Brazil. 2- Chemistry Institute, Federal University of Goiás, 74690-900 Goiania (GO), Brazil

Untargeted metabolomics based on HPLC-HRMS/MS was applied to discriminate species from three Orchidaceae genera (*Vanda*, *Laelia*, and *Cymbidium*) and to identify genus-specific metabolic markers. A total of 28 samples were analyzed using a methanol-based extraction followed by SPE cleanup and LC-HRMS/MS analysis. Data processing and metabolite annotation were performed using molecular networking workflows (GNPS) and multivariate statistical analysis. From the dereplication of molecular features, 61 secondary metabolites were putatively annotated, encompassing flavonoids, terpenes, alkaloids, phenolic acids, lignans, stilbenes, and quinones, alongside a wide range of primary metabolites such as amino acids and sugars. Among secondary metabolites, flavonoids emerged as the most abundant and taxonomically informative class, with 19 structurally characterized compounds. Distinct distribution patterns were observed: *Laelia* exhibited the highest flavonoid diversity, including isovitexin and apigenin 6,8-digalactoside as dominant compounds. *Cymbidium* showed high levels of rutin and phenolic acids such as 3-(2-hydroxyphenyl)propionic acid, while *Vanda* displayed the lowest flavonoid abundance but a higher content of quinones and phenolic acids, suggesting a different metabolic specialization. Terpenoids were the most abundant class overall, particularly enriched in *Cymbidium* and *Laelia*, consistent with their biosynthetic versatility. Chromenones such as 7-hydroxy-4,8-dimethylchromen-2-one and anthraquinones like alizarin were also identified, with structural validation based on MS/MS fragmentation and GNPS spectral matches. Lignans and glycosylated derivatives, including (+)-syringaresinol β -D-glucoside, were preferentially found in *Laelia*, indicating potential chemophenetic significance. Multivariate analysis (PCA and PLS-DA) revealed clear clustering of samples according to genus, with specific metabolites driving the separation. Chemometric loading plots identified isovitexin, rutin, syringic acid, sinapic acid, and alizarin as major discriminators. These compounds may serve as putative chemotaxonomic markers for genus-level identification within Orchidaceae. Furthermore, observed metabolite patterns suggest that shikimate and phenylpropanoid pathways are central to the secondary metabolism of these genera, supporting the use of metabolomics in understanding orchid chemodiversity and taxonomy.

Keywords: HRMS-based untargeted metabolomics, chemodiversity, terpenoids, flavonoids, chemometric

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DECIPHERING THE PHYTOCHEMICAL LANDSCAPE OF PURPLE ELEPHANT GRASS GENOTYPES THROUGH INTEGRATED HRMS AND NMR DATA: IMPLICATIONS FOR ANIMAL NUTRITION AND HEALTH

Salva Asghar^{1*}, Erica A. Batista², Elgia Procopio Diniz², Eric de Souza Gil², Gesiane da Silva Lima², Danielle Ferreira Dias¹, Marisi Gomes Soares¹, Nerilson Marques Lima¹

salva.asghar@sou.unifal-mg.edu.br

1- Institute of Chemistry, Federal University of Alfenas, Alfenas, MG 37130-001, Brazil. 2- Federal University of Goias, 74690-900 Goiania (GO), Brazil

Elephant grass (*Cenchrus purpureus*) is a strategic forage crop cultivated across tropical regions due to its high biomass yield, nutritional value, and adaptability. This study aimed to compare two Embrapa genotypes (S1 and S2) through untargeted metabolomic profiling and assessment of their antioxidant and anti-inflammatory properties. Hydroalcoholic extracts were analyzed using HRMS Orbitrap ESI (+), ¹H-NMR, and voltammetric techniques. Spectrophotometric assays revealed that S1 exhibited the highest antioxidant potential (DPPH IC₅₀: 2.5 µg/mL) and total phenolic content (39.8 mg GAE/100 g), indicating a strong correlation between phenolic abundance and antioxidant capacity. Voltammetric analysis showed anodic peaks at E_{pa} ≈ 0.2 V or lower, characteristic of polyphenolic compounds, with peak intensities suggesting higher concentrations of electroactive species in S1. Metabolomic analysis revealed 142 putatively identified metabolites, including flavonoids, anthocyanins, tannins, phenolic acids, phenylpropanoids, and terpenes, supported by molecular networking and *in silico* fragmentation tools. Pathway enrichment analysis indicated strong activity in the shikimate and phenylpropanoid biosynthetic routes, with high abundance of flavonoid subclasses such as flavones (tricin, luteolin glucosides, apigenin derivatives) and flavonols (kaempferide). Anthocyanins such as delphinidin-3-O-galactoside and cyanidin-3-O-pentoside were confirmed via ¹H-NMR chemical shifts (δ 9–10 ppm for H-4 and δ 3–4 ppm for glycosidic linkages). S2 showed higher anthocyanin content but lower antioxidant activity, likely due to lower levels of redox-active aglycones. Cytokine quantification revealed that both genotypes reduced pro-inflammatory mediators, indicating immunomodulatory potential. These effects are attributed to phenolic acids, flavonoids, and tannins, known to engage in redox cycling and inflammation regulation. Overall, the S1 genotype demonstrated greater metabolic diversity, stronger antioxidant response, and superior bioactivity, highlighting its potential as a multifunctional forage crop with therapeutic and nutritional benefits. Notably, untargeted metabolomics revealed significant qualitative and quantitative differences in the secondary metabolite profiles of the two genotypes. While S2 was richer in anthocyanin glycosides and conjugated polyphenols, S1 exhibited a broader distribution of free phenolics, aglycones, and phenylpropanoids, which correlated more directly with redox activity and anti-inflammatory effects. These findings underscore the application of metabolomic fingerprinting not only in identifying bioactive constituents but also in guiding genotype selection for functional and nutraceutical applications in tropical forage systems.

Keywords: Untargeted metabolomic, Polyphenols, Anti-inflammatory activity, nutraceutical applications





BIOACTIVITY SCREENING OF BRAZILIAN AND AMERICAN CULTIVARS OF HOPS (*Humulus lupulus* L.): COMPARATIVE ANALYSIS OF ANTI-INFLAMMATORY, NEUROPROTECTIVE, ANTIBIOFILM, AND ANTIBIOTIC PROFILES

Miller Santos Ferreira^{1*}, Renato Almeida Oliveira¹, Albert Katchborian-Neto¹, Daniela Chagas-Paula¹, Danielle Ferreira Dias¹, Marisi Gomes Soares¹

millersantosferreira@gmail.com

1-UNIFAL Federal University of Alfenas, Gabriel Monteiro da Silva, 700, Alfenas, Minas Gerais, 37130-001, Brazil.

Hops (*Humulus lupulus* L.) are well known for their role in the brewing industry but have gained increasing attention due to their pharmacological potential, driven by various bioactive compounds¹. This study aims to systematically screen the biological activities of extracts from different American hop cultivars grown in Brazil, comparing them to the same cultivars grown in their original regions in the United States.

Four primary biological activities were evaluated: anti-inflammatory activity via PGE₂ inhibition, neuroprotective effects, antibiofilm action, and antibiotic activity. Preliminary analyses showed that extracts BR5, BR6, US2, and US5 significantly inhibited PGE₂ production, suggesting their potential as anti-inflammatory candidates.

In parallel with the biological assays, a metabolomics approach using LC-MS/MS will be conducted to identify potential chemical biomarkers associated with each biological activity. Statistical analysis will be performed using multivariate techniques and machine learning methods, enabling robust correlations between chemical profiles and observed bioactivities.

This study not only contributes to the discovery of pharmacologically relevant bioactive compounds but also provides a comparative insight into the chemical and biological differences between cultivars grown under different environmental conditions. The integrated approach strengthens strategies for selecting and valorizing the most promising genotypes for pharmaceutical and functional ingredient applications.

Keywords: *Humulus Lupulus*, chemometrics approach, LC-MS-based metabolomics,

I.Silva, E., Oliveira, L. M., Andrade, B. N., Ribeiro, L. C., Lima, S. D., & Santos, C. A. (2023). Evolving biofilm inhibition and eradication in clinical settings through plant-based antibiofilm agents. Phytomedicine, 115, 154797. <https://doi.org/10.1016/j.phymed.2023.154797>

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FROM FORAGE TO FUNCTION: CHEMICAL PROFILE AND REDOX AND ANTI-INFLAMMATORY EVALUATION OF ELEPHANT GRASS EXTRACTS

Nerilson Marques Lima^{1*}, Salva Asghar¹, Matheus P. G. Carmo¹, Renato A. Oliveira¹, Erica A. Batista², Eric de S. Gil², Gracimério José Guarneire³, Sandra B. R. de Castro³, Alessandra de Paula Carli³, Caio César de S. Alves³, Danielle Ferreira Dias¹, Marisi Gomes Soares¹

nerilson.lima@unifal-mg.edu.br

1- Federal University of Alfenas, Alfenas, MG 37130-001, Brazil. 2-

Federal University of Goiás, Goiania, GO 74690-900, Brazil. 3 - Universidade Federal dos Vales do Jequitinhonha e Mucuri, Teófilo Otoni, MG 39803-371, Brazil

Elephant grass (*Cenchrus purpureus*) is a highly valuable forage species, widely cultivated for its exceptional dry matter yield, nutritional quality, palatability, vigor, persistence, and versatile applications in animal feeding systems. This study aimed to investigate the anti-inflammatory potential of elephant grass extracts and correlate it with their free radical scavenging capacity through electrochemical and chemical profile analyses. The chemical profile of the extracts was obtained using LC-HRMS/MS with a Q-Exactive Orbitrap mass spectrometer operating in positive ESI mode. Data were processed using GNPS tools with integrated annotation strategies. Antioxidant activity was evaluated by voltammetry in triplicate, while anti-inflammatory effects were assessed through MTT-based cell viability and NO production in J774A.1 macrophages. Only the highest concentration (1:10 dilution) showed cytotoxicity, while all other tested concentrations maintained >70% viability. Extracts PCEC, T41.2, and T47.1 significantly reduced nitric oxide (NO) production at all tested dilutions (1:10–1:1000), whereas BRS, T12.9, T23.1, and THE10 were effective at 1:100 and 1:1000. CPU and T25.11 extracts inhibited NO only at 1:100. The voltammetric analysis revealed distinct antioxidant profiles among the elephant grass genotypes. Anodic peaks with Epa1 values ≤ 0.2 V, consistent with phenolic compounds, indicated high radical scavenging potential. Higher anodic peak intensities were observed for the PCEC and T231 samples, indicating a greater electron-donating capacity and, consequently, stronger antioxidant activity. The classical molecular networking analysis of the seven elephant grass genotypes revealed a total of 306 unique metabolites. The natural product pathways, 73 metabolites were associated with the shikimate and phenylpropanoid pathways, 40 with the fatty acid pathway, and 154 with the terpenoid pathway. Among the annotated compounds, 27 flavonoids were annotated, with 20 belonging to the flavone subclass. Additionally, chalcones and flavanones were detected. Of the total flavonoids, 25% were identified as aglycones and 75% as glycosides, primarily conjugated with glucose or rhamnose. Notable flavonoids included luteolin, swertisin, isovitexin, homoorientin, vitexin-2"-O-rhamnoside, chrysoeriol, tricetin, isoschaftoside, and hesperidin. Other polyphenols that may contribute to the observed antioxidant activity were also annotated, including cinnamic acid derivatives such as *p*-coumaric acid, ferulic acid, and sinapic acid. The results highlight the promising antioxidant and anti-inflammatory properties of elephant grass, supported by electrochemical behavior and chemical composition.

Keywords: Forage crops, Polyphenols, Anti-inflammatory activity, Functional plants, Free radical scavenging

Acknowledgment: FAPEMIG, CAPES, CNPq





NEW TRITERPENE SAPONIN, METABOLOMIC PROFILE, CYTOTOXICITY AND ANTIPLASMODIAL ACTIVITIES OF *Combretum mellifluum*

Francisco Othoniel de Araújo Ribeiro^{1*}, Herbert Gonzaga Sousa¹, Teresinha de J. Aguiar dos Santos Andrade², Amanda Luisa da Fonseca³, Ana Claudia Souza Pinto³, Fernanda Alice de Oliveira³, Kézia Katiani Gorza Scopel⁴, Fernando de Pilla Varotti³, Bruno Antônio Marinho Sanchez⁵, Ana Jérsia Araújo⁶, José Delano Barreto Marinho Filho⁶, Rafaela Maria da Silva Ribeiro⁶, Mariana Helena Chaves¹, Gerardo Magela Vieira Júnior¹

othoniel4037@gmail.com

1- Department of Chemistry, UFPI, Teresina, PI 64049-550, Brazil. 2- Nucleus of Applied Research to Sciences, IFMA, Timon, MA 65630-000, Brazil. 3- Laboratório de Bioquímica Medicinal, UFSJ, Divinópolis, MG, 35501-296, Brazil. 4- Núcleo de Pesquisa em Parasitologia, UFJF, Juiz de Fora, MG 36036900, Brazil. 5- Laboratório de Imunopatologia e Doenças Tropicais, UFMT, Sinop, MT 78550-728, Brazil. 6- Laboratório de Cultura de Células do Delta, UFDFPar,

Numerous species from *Combretum* (Combretaceae) genus are used in folk medicine, including for malaria treatment. *Combretum mellifluum* Eichler (“mofumbo-da-chapada”), found in various regions of Brazil, contains steroids, triterpenes, lignans, flavonoids, and other phenolics, with reported antioxidant and cytotoxic activities. This study reports the isolation of a mixture of two triterpene saponins (**1+2**) and their cytotoxic potential. The metabolomic profile of the leaves and stem bark from *C. mellifluum* as well as its antiplasmodial activity were analyzed. The mixture was isolated by column chromatography, NMR, and MS identified a new saponin 28-*O*- α -rhamnopyranosyl 3-*O*- α -rhamnopyranoside-16-*O*- α -arabinopyranoside-3 β ,16 α -dihydroxy-24-methylenecycloartan-28-oate (**1**) and amphipaniculoside C (**2**) (Fig.1A). The mixture showed cytotoxicity against SW-480 and MDA-MB-231 cancer cell lines (IC₅₀ = 14.83 and 15.06 μ g/mL) but no effect on L929 non-tumoral cells (>25 μ g/mL). LC-MS profiling of hexane, ether, ethyl acetate, and hydromethanol fractions (from ethanolic extracts) was obtained via MZmine 3.9 and GNPS molecular networking, being annotated 28 metabolites distributed in nine classes, including *O*- and *C*-glycosylated flavonoids (Fig. 1B), proanthocyanidins, *O*-methylated flavonoids, flavan-3-ols, triterpene saponins, an ellagic acid derivative, a flavonol, and a chlorophyll derivative. Antiplasmodial tests against *Plasmodium falciparum* (W2 strain) showed activity for the hexane (9.8 $\pm$ 2.02 μ g/mL) and ether (8.91 $\pm$ 1.75 μ g/mL) leaf fractions, and the ethyl acetate bark fraction (13.44 $\pm$ 2.35 μ g/mL). The findings advance knowledge on the chemical composition and antimalarial potential of *C. mellifluum*.

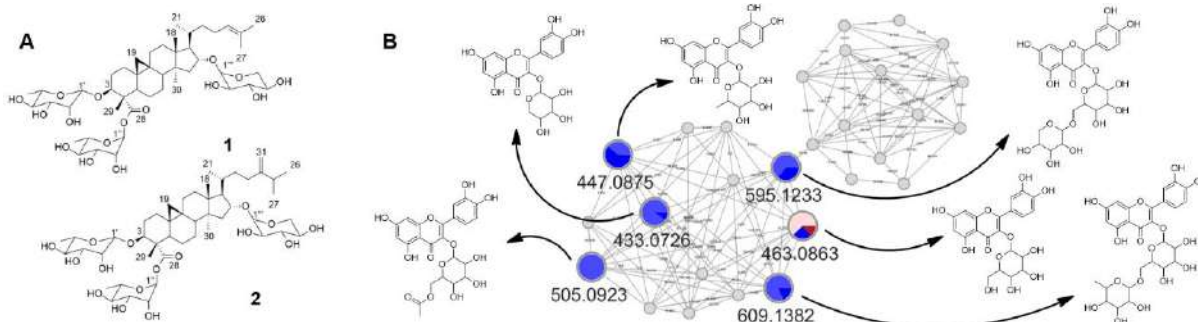


Figure 1: Mixture of saponins (**1+2**) isolated from the ethanolic extract from *C. mellifluum* leaves (A). Flavonoid glycoside cluster in negative ionization mode (B).

Keywords: *Combretum mellifluum*; Triterpene saponin; Molecular Networking; Cytotoxicity; Antiplasmodial activity

¹Silva, J. S. et al. *Toxicol. Environ. Health, Part A* **2021**, 85(9), 364.

²Mirowski, P. S. et al. *Nat. Prod. Res.* **2022**, 36(24), 6224.



**METABOLOMIC ANALYSIS AND ANTIMICROBIAL ACTIVITY OF FRACTIONS
FROM THE ETHYL ACETATE PHASE OF CASEARIA SYLVESTRIS**

Maiara Silva Miranda Andrade^{1*}, Beatriz Isabel Mota do Carmo¹, Ana Clara Lima Nunes Silva¹, Francisco Ozório Bessa Neto¹, Rodrigo Cayô da Silva¹, Augusto Leonardo dos Santos¹, Patricia Sartorelli¹

Contact: maiara.andrade@unifesp.br

1-Universidade Federal de São Paulo, Diadema/SP - Brazil.

Phytochemical studies on *Casearia sylvestris* Sw. (Salicaceae), popularly known as “guaçatonga”, have revealed a predominance of clerodane diterpenes. These metabolites are taxonomic markers for the genus *Casearia* and are associated with diverse biological activities, including anti-inflammatory, antitumor, and antiulcerogenic effects¹. The chemical profile of CSA fractions, obtained from chromatographic separation of the ethyl acetate phase, was characterized by UHPLC-HR-ESI-MS/MS. Fragmentation data were processed using the *Global Natural Products Social Molecular Networking* (GNPS2) platform, enabling molecular networking and putative metabolite annotation. The analysis revealed clusters consistent with clerodane diterpene spectra, showing characteristic neutral losses of butanoic acid (88 Da) and acetaldehyde (44 Da). The antimicrobial activity of CSA fractions was assessed by the agar diffusion method against clinically relevant strains: *Acinetobacter baumannii* ATCC 19606, *Escherichia coli* ATCC 25922, *Enterobacter cloacae* clinical isolate 79101, *Klebsiella pneumoniae* ATCC 700603, *Pseudomonas aeruginosa* ATCC 27853, *Enterococcus faecalis* ATCC 29212, methicillin-resistant *Staphylococcus aureus* (MRSA) 29213, and *S. aureus* ATCC 43300. Notably, zones of inhibition were observed for *P. aeruginosa*, a pathogen classified by the World Health Organization (WHO) as a critical-priority target for new antimicrobial development due to high resistance rates and limited therapeutic options². Samples CSA-16B-1, CSA-16B-2, and CSA-21-5, derived from chromatographic fractionation of the ethyl acetate fraction, exhibited inhibition zones of 12.9 mm, 16.1 mm, and 8.0 mm, respectively, indicating a potential inhibitory effect against this difficult-to-treat microorganism. According to the WHO, multidrug-resistant *P. aeruginosa* is a major cause of severe hospital-acquired infections, associated with high morbidity and mortality, particularly in immunocompromised patients. The detection of inhibitory activity against this species in the ethyl acetate fractions of *C. sylvestris* highlights the relevance of further studies aimed at isolating and characterizing active compounds for the development of novel antimicrobial agents. The authors acknowledge the support of the participating institutions and the financial assistance of CEPID-ARIES, FAPESP, CAPES, CNPq, and CEMUD-UNIFESP.

Keywords: *Casearia sylvestris*, clerodane diterpene, GNPS2, antimicrobial activity

¹XIA, L. et al. The genus *Casearia*: a phytochemical and pharmacological overview. *Phytochemistry Reviews*, v. 14, p. 99-135, 2015.

²WHO Bacterial Priority Pathogens List, 2024: bacterial pathogens of public health importance to guide research, development and strategies to prevent and control antimicrobial resistance. Geneva: World Health Organization; 2024.





QUANTITATIVE LIPIDOMICS AND METABOLOMICS IN FERMENTED RAW CONILON COFFEE BEANS FROM ESPÍRITO SANTO

Ana Laura Macedo Brand^{1,3*}, Ana Carolina Rosa da Silva¹, Lucas Louzada Pereira², Rafael Garret¹, Claudia Moraes de Rezende³

alaurambrand@gmail.com

1-Laboratório de Metabolômica, Instituto de Química, Universidade Federal do Rio de Janeiro, Avenida Horácio Macedo, 1281, Rio de Janeiro, RJ, Brazil. 2-Laboratório de Análise e Pesquisa em Café, Instituto Federal de Educação, Ciência e Tecnologia do Espírito Santo, Rua Elizabeth Minete Perim, Venda Nova do Imigrante, ES, Brazil. 3-Laboratório de Análise de Aromas, Instituto de Química, Universidade Federal do Rio de Janeiro, Avenida Athos da Silveira Ramos, 149, Rio de Janeiro, RJ, Brazil.

Brazil is the second largest producer of *Coffea canephora* Pierre, with cultivation concentrated in Espírito Santo and Rondônia. Espírito Santo alone accounts for about 30% of global conilon coffee production, employing more than 250,000 people. Coffee beans contain around 10% oil, mainly triacylglycerols (TGs), and a notable unsaponifiable fraction rich in kaurane-type diterpenes such as cafestol, kahweol, and 16-*O*-methylcafestol. Minor constituents include phospholipids, sterols, tocopherols, and ^β*N*-alkanoyl-5-hydroxytryptamides (C_n-5HTs). While cafestol and C_n-5HTs show biological activities, they are also linked to hypercholesterolemia and gastric discomfort. Post-harvest processing reduces bean moisture, removes pulp and mucilage, and stabilizes beans for storage and roasting. Because cherries are rich in sugar and water, fermentation occurs naturally; however, induced fermentation provides controlled conditions that promote biochemical reactions and microbial development, generating aroma and flavor precursors that may migrate into the seed. Considering the role of lipids in seed development and bean quality, this study aimed to characterize the lipid fraction of conilon coffee beans from Espírito Santo processed by different post-harvest methods. This study applied quantitative lipidomics by liquid chromatography–high-resolution mass spectrometry (LC-HRMS) to profile lipid classes and developed a validated high-performance liquid chromatography–diode array detector (HPLC-DAD) method to quantify diterpenes. Coffees were processed by the dry method (control) and four fermentation protocols. Fermented coffees exhibited significantly lower TGs, cafestol, and C_n-5HTs contents compared to control beans. PLS-DA analysis confirmed a clear separation between fermented and dry-processed samples, mainly influenced by TGs and C_n-5HTs. These results demonstrate that lipidomics is an effective tool to evaluate processing, and controlled fermentation modifies the lipid profile of conilon beans, potentially reducing compounds linked to negative health effects while preserving or enhancing sensory properties.

Keywords: Lipidomics; Robusta coffee; Fermentation, Quantification; LC-MS

References: (1)Brand, et al., *Food Biosci.*, 2024, 57, 103472. (2)Tinoco et al., *Food Res. Int.*, 2019, 115, 487–492.





VARIATION IN METABOLOME AND GENE EXPRESSION OF *Citrus sinensis* x *Citrus limonia* IN RESPONSE TO HUANGLONGBING

Jessica Cristina Amaral^{1*}, Danielle Fernandes da Silva², Chrystiaine Helena Campos de Matos², Maria Fatima das Graças Fernandes da Silva², Luciano Silva Pinto³, Sergio Florentino Pascholati¹.

jcamaral@usp.br

1- Department of Plant Pathology and Nematology, University of São Paulo (USP)/Luiz de Queiroz College of Agriculture (ESALQ), Piracicaba-SP, Brazil. 2- Department of Chemistry, Federal University of São Carlos (UFSCar), São Carlos-SP, Brazil. 3- Food Research Center, Department of Food and Experimental Nutrition, University of São Paulo (USP), São Paulo-SP, Brazil.

Huanglongbing (HLB), also known as citrus greening disease, is the most destructive disease affecting citrus crops. It is caused by the phloem-restricted bacteria *Candidatus Liberibacter asiaticus* (CLas), *C. Liberibacter africanus*, and *C. Liberibacter americanus*, and is transmitted by the insect vector *Diaphorina citri*. Currently, there are no commercially available rootstocks or scion varieties resistant to the disease, and infected plants cannot be cured. Despite extensive research efforts, the molecular mechanisms underlying CLas infection and colonization in citrus remain poorly understood. In this study, the interaction between citrus and CLas was investigated using LC-HRMS/qTOF in both positive and negative ionization modes. Samples of central and lateral roots from healthy and CLas-infected *C. sinensis* x *C. limonia* plants grown in a greenhouse were subjected to metabolomic analysis. Feature-Based Molecular Networking (FBMN) on the GNPS platform enabled the annotation of metabolites that were significantly altered in response to CLas infection. Significant differences, determined using the paired t-test, were observed in the concentrations of demethylsuberosin, ostenol, 5-methoxyseselin, xanthyletin, seselin, and limonin. These compounds contributed to the classification of samples into four distinct groups in the PCA: central roots, lateral roots, lateral roots of healthy plants and lateral roots of infected plants. In addition, gene expression analysis of candidate key enzymes in the prenylated coumarin biosynthetic pathway DXR, DXS2, PT1, and PT2, was performed by qPCR in *C. sinensis* x *C. limonia* lateral roots. CLas infected plants exhibited downregulation of DXR (2-fold), DXS2 (5.7-fold), and PT1 (3.6-fold), whereas PT2 expression was upregulated 2.6-fold compared to healthy controls. Overall, our findings demonstrate that CLas infection induces metabolic changes and modulates the expression of genes involved in prenylated coumarins biosynthesis. The results indicate that the plant mounts a biochemical response to bacterial infection by suppressing the biosynthesis of linear pyranocoumarins and favoring the production of angular pyranocoumarins, which are prenylated at C-8.

Keywords: metabolomics, gene expression, Citrus, Huanglongbing





**VARIABILITY IN RUTIN CONCENTRATIONS IN LEAVES OF FOUR VARIETIES
OF *Hancornia speciosa* (APOCYNACEAE)**

Marco Aurélio Batista^{1*}, Monatha Nayara Guimarães Teófilo¹, Leonardo Gomes Costa¹,
Danielle Gonçalves Teixeira dos Santos¹, Lázaro José Chaves², Andreia Juliana Rodrigues
Caldeira¹, Joelma Abadia Marciano de Paula¹

* m_batista@outlook.com.br

¹PD&IBio, Laboratório de Pesquisa, Desenvolvimento e Inovação de Produtos da Biodiversidade,
Universidade Estadual de Goiás, UEG, BR 153, n 3105, Anápolis, GO, Brazil. ²Setor de
Melhoramento Vegetal, Universidade Federal de Goiás, UFG, Av. Esperança, s/n, Goiânia, GO,
Brazil.

Hancornia speciosa Gomes (Apocynaceae), known as “mangabeira”, is studied for its pharmacological properties, such as antioxidant and anti-inflammatory effects, due to the presence of flavonoids like rutin in its leaves. However, the studies do not specify the botanical varieties used, which could affect the levels of bioactive compounds and have implications for the quality control of these plant materials. The objective of this study was to analyze the rutin concentrations in the leaves of four *H. speciosa* varieties cultivated at the Federal University of Goiás germplasm bank. The study was registered in SisGen (A2F6935). Leaf samples of the varieties *H. speciosa* var. *speciosa*, *H. speciosa* var. *cuyabensis*, *H. speciosa* var. *gardneri*, and *H. speciosa* var. *pubescens* were collected from three individuals of each variety and then desiccated. The extracts were prepared in a 1:10 ratio (g/mL) using ethanol P.A. 95% and analyzed by high-performance liquid chromatography (HPLC-DAD) to quantify rutin, which was used as a reference standard to build the analytical curve. Rutin concentrations varied among the varieties. *H. speciosa* var. *speciosa* showed the highest levels, ranging from 227.11 ± 7.90 µg/mL to 1271.93 ± 4.63 µg/mL. *H. speciosa* var. *cuyabensis* ranged from 355.21 ± 22.83 µg/mL to 1169.51 ± 45.79 µg/mL. *H. speciosa* var. *gardneri* had concentrations between 180.19 ± 21.12 µg/mL and 620.95 ± 58.15 µg/mL, while *H. speciosa* var. *pubescens* exhibited the lowest values, from 170.34 ± 61.29 µg/mL to 243.14 ± 11.19 µg/mL. These chemical variations directly affect the quality of herbal raw materials. *H. speciosa* var. *speciosa* and *H. speciosa* var. *cuyabensis* appear to be the most promising for pharmacological uses because they have the highest levels of rutin. The observed chemical variability emphasizes the importance of specifying the botanical variety used when obtaining the plant material.

Keywords: Apocynaceae, HPLC-DAD, quality control, rutin, chemical variability.





**OPTIMIZATION OF AN ECOLOGICAL ANALYTICAL PROCEDURE FOR
METABOLIC PROFILING *Theobroma grandiflorum* AND *Theobroma cacao***

Maria Gabriela de Albuquerque Santiago^{1*}, Danili Teixeira Piedade de Oliveira, Lucas Gomes de Brito¹, Leonardo de Oliveira Sartori¹, Martin Kássio Leme da Silva¹, Cristiano Soleo de Funari¹

m.santiago@unesp.br

1-GreenBiotech Network, DBB, UNESP, Av. Universitária, 3780, Botucatu, SP, Brazil.

The *Theobroma* spp. is composed of a group of fruit trees native to the Amazon with great economic and cultural relevance. *T. cacao* L. (cocoa) stands out as it is widely cultivated in Brazil and used in the food, cosmetic, and pharmaceutical industries, followed by *T. grandiflorum* (cupuaçu)^[1]. This work aimed to develop a highly efficient and green analytical procedure for analyzing parts of these species from a multivariate approach. The separation by UHPLC-DAD/UV-MS was optimized from a four-factor Doehlert design, while the extraction was from a two-factor central rotational compound design from a mixture of cupuaçu parts (leaf, husk, seed, and pulp). An optimal separation ($R^2 = 0.85$) was achieved with 5% of 50% MeOH in 20 min, using 0.2% HCOOH in the mobile phase, which resulted in 80.5 ± 2.4 peaks at $\lambda = 280$ nm. Then, an optimal extraction ($R^2 = 0.80$) was achieved using dynamic maceration with 30% ethanol for 60 min, resulting in 88.8 ± 2.8 peaks at $\lambda = 280$ nm. The full optimized condition, from sample preparation to separation, was applied to each part of the cupuaçu separately. Leaves had the highest number of peaks (85.0 ± 0.0), followed by husks (80.5 ± 0.7), seeds (65.5 ± 2.1) and pulp (42.0 ± 2.8). For comparison, the developed method was also satisfactorily applied to different parts of cocoa, resulting in 83.0 ± 2.8 , 59.5 ± 2.1 and 70.0 ± 1.4 in leaves, husks and seeds, respectively. The adopted multivariate approach led to a high level of chemical information for individual parts of both cupuaçu and cocoa, while employing only recommended solvents^[2]. This globally optimized analytical procedure will be applied for compound annotation using UHPLC-QtoF-MS/MS. The authors would like to thank CNPq (131186/2024-8 and 03675/2021-7) and CAPES (88887.172509/2025-00).

Keywords: Green natural products chemistry, design of experiments, metabolomics, green analytical chemistry

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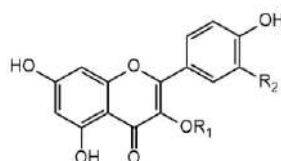
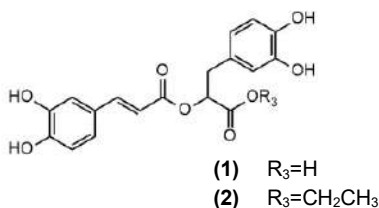


Chemical Profile of *Cyanocephalus rugosus* and Inhibitory Evaluation Against Neglected Tropical Diseases

Emiret Otoni de Faria^{1,5*}, Tanja Schirmeister², Lorena Ramos Freitas De Sousa³, Sergio Tadeu Sibov⁴, Lucilia Kato¹.
emiret.faria@ifg.edu.br

1- Institute of Chemistry, UFG, Brazil. 2- Institute of Pharmaceutical and Biomedical Sciences (IPBW), UniMainz, Mainz, Germany. 3- Institute of Chemistry of UFCAT, Catalao. 4- Plant Tissue Culture Laboratory, UFG, Brazil. 5- Federal Institute of Goias, Brazil.

Cyanocephalus rugosus (Lamiaceae) is a species little explored in terms of its chemical profile and pharmacological potential. This herb found in the Cerrado of Goiás was domesticated and introduced into an agroforestry system (SAF). SAF provides agricultural productivity with ecological principles, being a sustainable approach to conventional agriculture through land use over time. This work proposed to study the chemical profile of an aromatic plant grown in an agroforestry system and how these environmental conditions influence the production of secondary metabolites in *C. rugosus*. The ethanolic extracts of the species were evaluated for inhibitory activity against dengue virus type 2 (DENV-2) serine proteases and the enzyme rhodesaina (*Trypanosoma brucei*). Identification was performed by LC-MS and spectral libraries. Rosmarinic acid (**1**), ethyl rosmarinate (**2**) and another 41 compounds were identified for the first time in the species. The promising results of enzyme inhibition led us to bioguided fractionation and identification of the active compound. The active fraction was identified as quercitrin (**3**), originating from the extract of aerial parts showed 69% inhibition (1mg.mL⁻¹) against DENV-2. The global metabolite profile is being analyzed by PCA and PLS-DA to compare the chemical profile of the species after introduction into the SAF. The results reinforce the potential of *C. rugosus* as a source of bioactive compounds for the development of a new therapy against neglected tropical diseases (Dengue and Human African trypanosomiasis) and present the cultivation of this in a sustainable agriculture system as a viable way to obtain compounds of technological interest.



(3) R₁= rhamnoside R₂=OH

Kaempferol R₁=H R₂=H
Quercetin R₁=H R₂=OH

Keywords: *Cyanocephalus rugosus*, bioactive, proteases, DENV-2, *Trypanosoma brucei*, metabolomics, sustainable agriculture.

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METABOLOMIC PROFILING OF GREEN AND MATURE BEANS OF COFFEA ARABICA GENOTYPES BY GC-MS: INSIGHTS INTO QUALITY MARKERS

Ana Carla Rangel Rosa^{1*}, Vinícius Guimarães Nasser², Adésio Ferreira¹, Marcia Flores da Silva Ferreira¹, Geraldo Humberto Silva², Murilo de Oliveira Souza³, Mário Ferreira Conceição Santos¹

anacarlarangelrosa@yahoo.com

1 - Graduate Program in Genetics and Plant Breeding, UFES, Alegre - ES, Brazil 29500-000. 2 - Institute of Exact and Technological Sciences, UFV, Rio Paranaíba - MG, Brazil 38810-000. 3 - Federal Institute of Espírito Santo, IFES, Alegre - ES, Brazil 29500-000.

The metabolomic profiling of coffee beans provides valuable insights into the biochemical factors that determine beverage quality, particularly for *Coffea arabica*, the most widely cultivated species for specialty coffees. In this study, green and mature beans from three *C. arabica* genotypes (Arara, Catucaí 785-15, and Catucaí 62), collected in experimental fields located in Brejetuba, Espírito Santo, Brazil, were subjected to gas chromatography coupled to mass spectrometry (GC-MS) to characterize their chemical composition, followed by multivariate statistical analysis. A total of 28 metabolites were identified, comprising sugars, organic acids, phenolic compounds, and alkaloids. Clear biochemical shifts were observed during ripening, with mature beans enriched in sucrose, fructose, and chlorogenic acids, while green beans exhibited higher levels of trigonelline, caffeine, and certain amino acids. Principal Component Analysis (PCA) revealed a distinct separation between green and mature beans and a partial exploration among genotypes. Arara was characterized by higher accumulation of reducing sugars and a sweeter chemical profile, Catucaí 785-15 by balanced levels of phenolics contributing to acidity and aromatic complexity, and Catucaí 62 by elevated caffeine and chlorogenic acid levels, associated with stronger body and bitterness. Hierarchical clustering and heatmap analyses confirmed that maturation stage was the primary discriminant factor, although genotypic differences remained evident, suggesting a strong genetic control of metabolite accumulation. These findings highlight key metabolic markers for maturation and genotype, providing valuable tools for selecting superior *C. arabica* cultivars with enhanced sensory quality. This work reinforces metabolomics as a powerful strategy for the research and valorization of Brazilian specialty coffee.

Keywords: PCA, Multivariate analysis, Specialty coffee, Espírito Santo, Chlorogenic acid, Maturation stage.





COMPARATIVE ANALYSIS OF THE CHROMATOGRAPHIC PROFILE OF A RUBIACEAE SPECIES CULTIVATED *IN VITRO* UNDER DIFFERENT WAVELENGTHS BY HPLC-DAD

Emilly de Jesus Franco Silva^{1*}, Milton Nascimento da Silva¹, Sônia das G. S. R. Pamplona², Osmar Lameira Alves³, Thalia da Silva Oliveira⁴, Thainara da Silva Oliveira⁴

Emillyjfrancosilva@gmail.com

1- Biotechnology College, Federal University of Pará, R. Augusto Corrêa, 127-483, Belém, Brazil.

1,2- Amazon Integrated Metabolomics Center, Institute of Exact and Natural Sciences, Federal University of Pará, Belém 66075-110, Brazil; 3- EMBRAPA Eastern Amazon, Belém 66095-903, Brazil, 4- Biotechnology College, Federal University of Pará, R. Augusto Corrêa, 127-483, Belém, Brazil.

Species of the Rubiaceae family are recognized for producing alkaloids of pharmacological interest. The naturally low yield of these secondary metabolites represents a challenge for their large-scale application. *In vitro* cultivation, including manipulation of light conditions, culture medium, and temperature, offers a promising alternative for optimizing metabolite production. This study aimed to compare the chromatographic profile of the species cultivated *in vitro* under different light wavelengths (green, yellow, and white treatments) with leaves collected under natural conditions (control treatment) using HPLC. Sample preparation was carried out with 100 mg of dried leaves and plantlets, extracted with 2.0 mL of ethanol by ultrasonic bath for 30 minutes (2x). The resulting solution was filtered through an SPE cartridge for HPLC-DAD analysis. Chromatographic analysis was performed on a C-18 column (150 × 4.60 mm); room temperature; mobile phase: A (water, 0.1% formic acid) and B (acetonitrile, 0.1% formic acid); gradient elution (10–100% ACN); flow rate: 1.0 mL/min; injection volume: 30 µL; analysis time: 30 min; detection: 200–400 nm. Comparative analysis of the chromatograms revealed no significant qualitative differences among the treatments. However, variations in signal intensity were observed in the retention time range of 1.90–10.0 min. The white-light treatment exhibited more intense peaks compared to the others, suggesting a higher concentration of certain compounds. In the retention time range of 9.7–10.2 min, no peaks were detected under yellow light treatment, while signals were present under both white and green light.

Keywords: *In vitro*; light; HPLC; chromatographic profiles; secondary metabolites.





SPME Fiber and Twister in a Closed System for Volatile Organic Compound Analysis in *Lissotriton vulgaris*.

Fabiola Almeida Garcia 1, Rayko Halitschke 2, Martin Kaltenpoth 3, Norberto Pepporine Lopes¹, Nicole van Dam 4, Monica Barman 4, Andres Brunetti 3, 5

1- NPPNS, Department of Biomolecular Sciences, Faculty of Pharmaceutical Sciences of Ribeirão Preto, Department of Physics and Chemistry, University of São Paulo

2 Mass Spectrometry and Metabolomics, Max Planck Institute for Chemical Ecology, Jena, Germany.

3- Department of Insect Symbiosis, Max Planck Institute for Chemical Ecology, Jena, Germany

4- Science Support Platform / Plant Biotic Interactions, Leibniz Institute of Vegetable and Ornamental Crops (IGZ) e.V

5-Institute of Subtropical Biology (CONICET-UNAM), National University of Misiones, Posadas, Argentina

Volatile organic compounds (VOCs) are hypothesized to play a critical role in amphibian ecology, potentially contributing to communication, defense, and attraction. However, their study is constrained by technical challenges, such as animal manipulation and low concentrations. We developed a novel *in vivo* methodological approach to analyze VOCs in three populations of the common newt (*Lissotriton vulgaris*) in Germany. The system consisted of a closed glass cylinder allowing the simultaneous sampling with SPME fibers and Twisters. To our knowledge, this is the first reported method for field-based volatile collection in amphibians, particularly caudates (newts and salamanders), where knowledge of VOC production is almost completely lacking. Two adult specimens were sampled in the glass cylinder (n=6 per population, 3 females, 3 males, 2 individuals per cylinder), and extracts were analyzed by GC-MS. Data were processed in LabSolutions, analyzed in MZmine, and manually annotated using NIST 23 databases for fragment comparison, with retention indices calculated for compound confirmation. SPME provided the higher number of annotated compounds with monoterpenes and sesquiterpenes as the main chemical classes. In turn, Twister, applied for the first time in live animals, identified alcohols, ketones, and alkanes, offering a complementary profile. SPME exhibited greater sensitivity for trace compounds but had fragile fibers and higher noise, whereas Twister offered robust adsorption and field versatility. This study demonstrates the feasibility of the closed system sampling approach and the complementarity of SPME and Twister, providing an innovative tool for ecological research.

Keywords: SPME Fiber, Twister, Volatile Organic Compounds, Closed System





ANOTATION OF IRIDOIDS AND SECO IRIDOIDS IN KUTCHUBAEA INSIGNIS AND FERDINANDUSA HIRSUTA (RUBIACEAE)

Gabriel Santana Crispim^{1,2*}, Luana da Conceição Moreira^{1,2}, Cecilia Veronica Nunez^{1,2}

gabrielsantana852@gmail.com

1- Laboratório de Bioprospecção e Biotecnologia – LABB, Coordenação de Tecnologia e Inovação – COTEL, Instituto de Pesquisas da Amazônia – INPA, Av. André Araújo, 2936, Manaus, AM, 69067 - 375, Brazil. 2- Programa de Pós-Graduação em Biotecnologia – PPGBIOTEC, Universidade Federal do Amazonas – UFAM, Av. General Rodrigo Octavio Jordão Ramos, 1200, Manaus, AM, 69067-005, Brazil.

Iridoids are a class of secondary metabolites with biological potential that are reported in several plants. In the Rubiaceae species, they are mainly reported in the Ixoroideae subfamily, which includes plants of the *Kutchubaea* and *Ferdinandusa* genera, for which there are very few reports of phytochemical studies. Considering this gap, the objective of this study was to investigate the chemical constituents of these species. Initially, we performed a clean-up step using a Sep-Pak C18 (2 g/12 mL) on methanolic extracts from leaves, branches, and fruits that were analyzed by liquid chromatography coupled to mass spectrometry (LC-MS), with fragmentation (MS2) spectra converted to mzML format for molecular network analysis on the GNPS2 platform. To create the network and library match, it was set a minimum 0.50 cosine between the spectral library and the ions, a tolerance of 0.02 was used between the fragment ions and the precursor ions because the experiments were acquired on a high-resolution spectrometer. To verify the annotations, the fragmentation patterns were checked manually. Of the metabolites annotated in these species, eight iridoids were putatively identified: genipin, monotropein methyl ester (galioside), geniposide, sweroside, epivogeloside, secologanin, swertiamarin, and secologanin 7-methyl ester. Furthermore, molecular network analysis revealed that each species had unique biosynthesis for each subclass of these iridoids, since iridoids were annotated in *Kutchubaea insignis* and seco iridoids in *Ferdinandusa hirsuta*. These results demonstrated the potential for isolating these iridoids in these species. The authors would like to thank the funding agencies FAPEAM, CAPES, CNPq, and FINEP for their financial support, and CA-LTQPN/INPA for the mass spectrometry analyses.

Keywords: LC-MS based molecular network, phytochemistry, chemosystematics, iridoids annotation, chemometrics.





**BIOCHEMICAL AND MOLECULAR CHARACTERIZATION OF
ANTIBACTERIAL PEPTIDES OBTAINED FROM BASIDIOMYCETE
MUSHROOMS ISOLATED FROM THE BOTANICAL GARDEN OF THE
UNIVERSIDAD TECNOLÓGICA DE PEREIRA**

Luz Stella Ramírez Aristizabal¹, Ángela María Arango Londoño^{1*}, Adalucy Álvarez Aldana²

luramire@utp.edu.co

1-Universidad Tecnológica de Pereira, Faculty of Technology, School of Chemical Technology, Laboratory of Microbiology and Biological Activity, Pereira, Colombia. 2- Universidad Libre, Pereira Section, Faculty of Health Sciences, Microbiology Program, Pereira, Colombia.

Keywords: Antimicrobial resistance, antibacterial peptides, basidiomycete, natural products

The escalating global health crisis of antimicrobial resistance needs the urgent discovery of novel therapeutic agents from underexplored natural sources. Our region, and particularly the Botanical Garden of the Universidad Tecnológica de Pereira (JBUTP), is a biodiversity hotspot, home to a vast and largely unexplored array of fungal species with significant biotechnological potential. This research addresses this critical challenge by investigating the rich fungal biodiversity of the JBUTP as a promising reservoir for antibacterial compounds. The primary objective of this initial phase was the isolation, cultivation, and comprehensive identification of basidiomycete fungal specimens exhibiting potential for producing bioactive substances. Fungal specimens (coded JAD01, JAD02, JAD03) were collected from various decaying substrates within the JBUTP, adhering to established collection protocols and permits. Laboratory cultivation was initiated using diverse media (PDA, Sabouraud, Rose Bengal Agar) to assess optimal growth patterns. Identification employed a multi-faceted approach, combining detailed macroscopic (e.g., pore structures, fruiting body characteristics) and microscopic analyses (e.g., hyphae, spores, clamp connections from mycelia and carpophore sections). Molecular identification was performed via ITS ribosomal DNA region sequencing, and preliminary findings confirmed that the collected fungi belong to the Phylum Basidiomycota, specifically within the order Polyporales, aligning with previous regional biodiversity reports. Macroscopic and microscopic observations consistently revealed morphological features typical of these groups. Molecular identification successfully confirmed isolate JAD 01 as *Cubamyces menziesii*, JAD 02 as *Coprinellus disseminatus* and JAD 03 as *Rigidoporus microporus*. These verified identifications establish a robust foundation for subsequent stages of the research, which will focus on the extraction, purification, and characterization of antibacterial peptides from these specific fungal species.





CHEMICAL PROFILING OF *Picramnia sellowii* (PICRAMNIACEAE): UHPLC-QToF-MS/MS EVIDENCE FOR QUASSINOIDS

Alicia Ludymilla Cardoso de Souza^{1*}, Jéssica Cristina Amaral², João Batista Fernandes¹,
Maria Fátima das Graças Fernandes da Silva¹

alicia.ludymilla@gmail.com

1- Laboratory of Natural Products, Department of Chemistry, Federal University of São Carlos (UFSCar), Rod. Washington Luis s/n km 235, São Carlos, SP, 13565-905, Brazil. 2- Department of Plant Pathology and Nematology, Luiz de Queiroz College of Agriculture (ESALQ), University of São Paulo (USP), Av. Pádua Dias, 11, Piracicaba, SP, 13418-900, Brazil.

The family Picramniaceae currently comprises the genera *Picramnia*, *Alvaradoa*, *Nothotalisia*, and the recently described genus *Aenigmanu*, which has not yet been included in the family clade recognized by the Angiosperm Phylogeny Group (APG) (THOMAS et al., 2021). Picramniaceae was segregated from Simaroubaceae, where it was previously classified as the subfamily Picramnioideae. Simaroubaceae is characterized by the presence of quassinoids, which led to the exclusion of the genera belonging to Picramniaceae, as species of this family contain anthraquinones that have not yet been reported in any other group of Simaroubaceae. Until recently, there was no chemical evidence to support the classification of Picramniaceae within Simaroubaceae or in close relationship to taxa associated with Rutaceae and Meliaceae. However, recent investigations have revealed several nortriterpenes with limonoid-like skeletons, as well as the annotation of quassinoids in the genus *Picramnia* (GIMENES et al., 2020; SILVA et al., 2022). Considering the morphological relationship of *Picramnia* with Simaroubaceae, the present study also aimed to explore the chemical diversity of *Picramnia sellowii* and evaluate whether quassinoids were produced in low concentrations. Ethanolic extracts of *P. sellowii* leaves and fractions obtained by SPE column purification (fractions F1–F4) were analyzed by untargeted UHPLC-QToF-MS/MS. The resulting data were processed, deconvoluted, and compared with spectral libraries such as METLIN, GNPS, Fiehn/Vaniya Natural Products Library, and BMDMS-NP for quassinoid annotation. In fraction F2, five quassinoids were annotated in *P. sellowii*, including quassin (C₂₂H₂₈O₆; *m/z* [M+H]⁺ 389.1953, *m/z* [M+Na]⁺ 411.1776). Efforts are currently being directed toward the isolation of these compounds. This study revealed that the chemical evidence is consistent with the traditional classification of *Picramnia* within Simaroubaceae. The authors thank their institutions for support and CAPES and INCT-CBIP for financial assistance.

Keywords: Quassinoids, Picramniaceae, *Picramnia sellowii*, chemosystematic, mass spectrometry, metabolomics

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From Chemophenetics to Cytotoxicity: mapping the chemical landscape of Conchocarpus J.C. Mikan and Dryades Groppo, Kallunki & Pirani species

Julia Nascimento Caldas¹, Victor Menezes Sipoloni (PG)¹, Maria Vitória de Oliveira (IC)², Julia de Franca Macedo (IC)², Elthon G. Ferreira (PQ)³, Carla Poleselli Bruniera (PQ)², Paula Christine Jimenez (PQ)³, Livia Soman de Medeiros (PQ)⁴, Thiago André Moura Veiga (PQ)⁴

jncaldas@unifesp.br

1-Programa de Pós-Graduação em Biologia Química; Instituto de Ciências Ambientais, Químicas e Farmacêuticas, Universidade Federal de São Paulo, Diadema, Brasil. 2-Instituto de Ciências Ambientais, Químicas e Farmacêuticas, Universidade Federal de São Paulo, Diadema, Brasil. 3-Instituto de Ciências do Mar, Universidade Federal de São Paulo, Santos, Brasil. 4- Departamento de Química, Instituto de Ciências Ambientais, Químicas e Farmacêuticas, Universidade Federal de São Paulo, Diadema, Brasil

Recently, the genus *Dryades* was segregated from *Conchocarpus* based on robust morphological and molecular evidence¹; however, its chemical markers and biological potential remain largely unexplored. To address this gap, we are applying an integrative strategy that combines advanced metabolomic approaches, high-resolution mass spectrometry (HRMS), nonconventional extraction procedures, and cytotoxicity assays to elucidate the key chemical distinctions between these genera. Thus far, we have examined eight *Conchocarpus* species and three *Dryades* species. Alkaloid-enriched fractions were prepared via ethanol extraction followed by acid-base partitioning and subsequently tested against the colorectal carcinoma cell line HCT-116. Remarkably, seven species exhibited significant cytotoxic activity. In parallel, LC-MS/MS data were used to construct a Feature-Based Molecular Network (FBMN) on the GNPS² platform, enabling the annotation of major compound families, particularly amides and alkaloids. Altogether, this study provides unprecedented chemophenetic insights into the segregation of *Conchocarpus* and *Dryades*, while also underscoring their potential as reservoirs of cytotoxic metabolites. Ongoing investigations are expected to refine these findings and foster the discovery of novel chemical markers with both chemotaxonomic and pharmacological relevance. This research was supported by CAPES (88887.951003/2024-00) and FAPESP (2024/03978-6).

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Keywords: Chemophenetic, *Conchocarpus*, *Dryades*, Cytotoxicity, Alkaloids





PRELIMINARY CHARACTERIZATION OF FLAVONOIDS FROM *OURATEA CASTANEIFOLIA* AND *OURATEA SEMISERRATA*

Vinícius Costa Cruz^{1*}, Nayara Yanne Cardoso Pereira¹, Priscilla Rodrigues Valadares
Campana¹, Fernão Castro Braga¹

vinii.cruz@gmail.com

*1-Laboratório de Fitoquímica, Departamento de Ciências Farmacêutica, Faculdade de Farmácia,
UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil*

The genus *Ouratea* is characterized by the presence of biflavonoids, which are considered its chemotaxonomic markers. The species *Ouratea castaneifolia* and *Ouratea semiserrata* are native from Brazil and their phytochemical composition have not yet been fully explored. The aim of this study is to perform a putative identification of flavonoids and biflavonoids in the ethanolic extracts from fruits of the specie *O. castaneifolia* and leaves of *O. semiserrata*. Sequential flash fractionation of the extracts was performed on silica gel using n-hexane, dichloromethane, ethyl acetate, and methanol. Subsequently, the ethyl acetate fraction of *O. semiserrata* and methanolic fraction of *O. castaneifolia* were subjected to open column of Sephadex LH-20. Chromatographic analyses were performed by UPLC-DAD-ESI-MS/MS. A C18 column was used, mobile phase: water (A) and acetonitrile (B) acidified with 0.1% formic acid, gradient of 5-95% B, detection in UV (200-500 nm). The ESI-MS analyses were performed in exploratory negative ionization mode (m/z 100 to 1500 Da). For ESI-MS/MS, a collision energy ramp from 20 to 70 eV and 5 to 30 eV with a fixed cone voltage of 62 eV and 30 eV were used for biflavonoids and flavonoids, respectively. The methanolic subfraction A of *O. castaneifolia* shown flavonoids identified as quercetin, kaempferol, apigenin and luteolin diglycosides, respectively (m/z 609 Da, rutin; m/z 593 D; m/z 577 and m/z 607 Da) and triglycosides of quercetin and kaempferol (m/z 755 Da and m/z 739 Da). The subfraction B shown biflavonoids as apigenin dimers (m/z 537 and monomethoxylated at m/z 551 Da). From *O. semiserrata*, a subfraction with two phenolic acids derived from benzoic acid were identified (m/z 391 Da, lanceoloside A; m/z 419 Da, diestherglycoside) along with fully hidroxilated and monomethoxylated biflavonoids (m/z 537 and 551 Da, respectively), as well as apigenin (m/z 269 Da). Therefore, these results contribute to expanding the knowledge on the chemical constitution of the *Ouratea* genus, reinforcing the importance of phytochemical prospecting of native plant species, and the importance of biflavonoids as chemical markers of this genus. Future investigations aimed at structural elucidation by NMR and evaluation of biological activity will be conducted. Acknowledgments: FAPEMIG, CNPq and PRPq.

Keywords: *Ouratea*, phytochemistry, chemosystematics, flavonoids, medicinal plants.





BIOACTIVE POTENTIAL OF *Psidium guineense* ESSENTIAL OILS AND EXTRACTS FOR ANTI-AGING COSMETIC APPLICATIONS

Tamires Cordeiro^{1*}, Ana Carolina Haag Bochnie², Ana Paula Costa Rodrigues¹, Ana Camila Micheletti,¹ Danielle Bogo², Nídia Cristiane Yoshida¹
tamires.cordeiro@ufms.br

1-Laboratory of Research on Bioactive Natural Products (PRONABio), Institute of Chemistry, Federal University of Mato Grosso do Sul (UFMS), Campo Grande-MS, Brazil. 2-Graduate Program in Health and Development in the Central-West Region, Faculty of Medicine, UFMS, Brazil.

Brazil, recognized for its remarkable biodiversity, hosts a vast array of plant species with dermocosmetic potential, especially within the Cerrado and Pantanal biomes. The pursuit of innovative materials and sustainable technologies in cosmetic formulations has been increasingly driven by organic cosmetology, which prioritizes plant-derived ingredients such as oils, waxes, and extracts. Globally, the cosmetics industry reached an estimated value of €240 billion in 2022, with the European Union (€88 billion), the United States, China, Brazil, and Japan leading the market. In this context, the present research investigates the native Myrtaceae species *Psidium guineense*, popularly known as “araçá-do-campo”, which produces edible fruits traditionally valued for their flavor and ethnopharmacological applications. Despite this cultural relevance, its chemical composition and potential technological applications remain poorly characterized. To address this knowledge gap, essential oils and ethanolic extracts were obtained from the leaves and fruits of *P. guineense*, and subsequently evaluated for antibacterial, antioxidant, and enzyme-inhibitory activities (elastase and hyaluronidase). In vitro cytotoxicity was assessed against normal murine fibroblast (NIH-3T3) cell lines using the Sulforhodamine B (SRB) assay, with all samples showing GI₅₀ values above 250 µg·mL⁻¹, indicating their non-cytotoxic profile toward normal cells. The samples exhibited no antimicrobial activity against the reference strains of *Staphylococcus aureus* and *Escherichia coli* (MIC ≥ 1000 µg/mL). However, in combination with ampicillin, the fruit essential oil showed an additive effect against a clinical multidrug-resistant *S. aureus* strain, in the checkerboard assay. Antioxidant activity, determined by the DPPH radical assay, revealed marked differences between plant parts: fruit extract and essential oil exhibited approximately 90% inhibition, whereas leaf extracts showed around 10%, highlighting the high radical-scavenging potential of the fruit. In enzymatic inhibition assays, essential oils derived from both leaves and fruit demonstrated elastase inhibition levels of approximately 90%, and inhibition of hyaluronidase by c. 45%. The pronounced antioxidant and enzyme-inhibitory activities of *P. guineensis* essential oils, particularly from the fruit, demonstrate their strong potential as bioactive agents. By effectively inhibiting elastase and hyaluronidase—enzymes directly linked to extracellular matrix degradation and skin aging—these oils emerge as promising candidates for the development of anti-aging formulations.

Keywords: aracá-do-campo, antioxidant, enzyme-inhibiting, hyaluronidase, elastase, cosmeceutical products





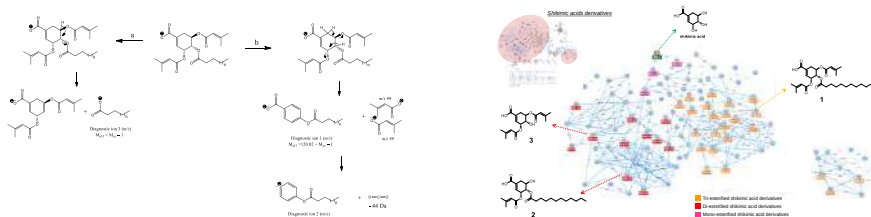
**CHARACTERIZATION OF BIOACTIVE SHIKIMIC ACID DERIVATIVES FROM
SENECIO OLEOSUS GUIDED BY DIAGNOSTIC IONS AND MOLECULAR
NETWORKING**

Nathália da Silva Malaco¹, **Thaíma Oliveira Souza e Silva^{1*}**, Anderson Valdiney Gomes Ramos¹, Bianca Del Bianco Sahn², Marta Regina Barroto do Carmo³, Leticia Costa Lotufo², Maria Helena Sarragiotto¹, Debora Cristina Baldoqui¹

ra141046@uem.br

1-Departamento de Química, Universidade Estadual de Maringá, Av. Colombo 5790, Maringá, PR, Brazil, 2-Departamento de Farmacologia, Instituto de Ciências Biomédicas, Universidade de São Paulo, Av. Prof. Lineu Prestes, 1524, São Paulo, SP, Brazil, 3-Departamento de Biologia Geral, Universidade Estadual de Ponta Grossa, Av. Carlos Cavalcanti, 4748, Ponta Grossa, PR, Brazil

Senecio is a large and chemically diverse genus comprising over 1,200 species. In Brazil, approximately 68 species are found, predominantly in rural and mountainous areas. This study aimed to investigate specialized metabolites of *Senecio oleosus* through isolation and dereplication strategies, and to evaluate the antiproliferative activity against tumor cell lines. Three new compounds were isolated: 3 α ,5 β -disenecioyloxy-4 α -dodecanoyloxy-shikimic acid (**1**), 3 α -senecioyloxy-4 α -dodecanoyloxy-shikimic acid (**2**) and 3 α ,5 β -disenecioyloxy shikimic acid (**3**). The fragmentation patterns and diagnostic ions were established based on MS/MS spectra of these isolated compounds. The cleavage of ester linkages at positions C-3 and C-5 produced a fragment ion at m/z $M_{di1} = 120.02 + M_{ac} - 1$, corresponding to a shikimate core retaining the ester moiety at C-4. Subsequent loss of CO₂ yielded a fragment at m/z $M_{di2} = M_{di1} - 44$. The base peak at m/z $M_{di3} = M_{ac} - 1$ resulted from the loss of the fatty acid linked to C-4. Using these fragmentation patterns as a guide, and GNPS2 MS2 m/z highlight tool to emphasize fragment ions at m/z M_{di1} , M_{di2} and M_{di3} , fifteen tri-substituted shikimic acid derivatives were putatively identified. A similar strategy enabled the detection and partial structural elucidation of shikimic acid derivatives analogous to compounds **2** and **3**. Compound **1** exhibited promising results against the HCT116 cancer cell line, with an IC₅₀ of 10.5 μ g mL⁻¹ (20.2 μ M). Esterified shikimic acid derivatives were the predominant specialized metabolites in *S. oleosus*. In total, 35 derivatives were putatively identified, and triesterified analogues demonstrated promising anticancer potential.



Keywords: Metabolome, structural elucidation, diagnostic ions, GNPS2, Asteraceae, antiproliferative activity



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Section: 05

METABOLOMICS FOR AGRICULTURE APPLICATIONS AND DRUG DISCOVERY

Ana Cláudia Chagas de Paula Ladvoat¹, Paula Carolina Pires Bueno², Danielle Ferreira Dias³, Marisi Gomes Soares³, **Daniela Aparecida Chagas-Paula**^{3*}

daniapchpa@gmail.com

1- Faculty of Pharmacy, Federal University of Juiz de Fora, Rua José Lourenço Kelmer, Juiz de Fora, Minas Gerais, 36036-900, Brazil. 2- Leibniz Institute of Vegetable and Ornamental Crops, IGZ. Theodor-Echtermeyer-Weg 1, Großbeeren, 14979, Germany. 3- Institute of Chemistry, Federal University of Alfenas, Alfenas, Minas Gerais, 37130-001, Brazil.

LC-MS-based untargeted metabolomics is a powerful strategy used to evaluate a broad range of metabolites from different biological sources. In this sense, our research group has been applying metabolomics to address challenges in several areas of science, including chemical ecology, agriculture, human health and drug discovery. In one of our current projects, we are using untargeted metabolomics to understand how different *Coffea arabica* varieties cope with *Hemileia vastatrix*, one of the most dangerous pathogens affecting coffee plantations, causing coffee leaf rust (CLR). In that project, we aim to find the possible metabolites correlating with CLR resistance, as well as to understand how it reflects in the final beverage quality. So far, our preliminary results on the leaves and beans, CLR-resistant and -susceptible cultivars, have pointed out distinct compounds correlating with the resistant profile and others with their beverage quality. In the area of drug discovery, we are addressing Parkinson's disease (PD), a neurodegenerative disease with an increasing rate of incidence. The pathophysiology of PD is complex and includes neurodegeneration, inflammation and others. The available treatments cannot disrupt the disease progression and present significant side effects. Thus, we have been investigating natural products with dual anti-inflammatory and neuroprotective activities, which could treat and prevent PD progression. Some of the metabolites detected in *Ocotea spp.*, *Banisteriopsis caapi* and *Psychotria viridis* extracts showed significant anti-inflammatory and neuroprotective activities. Some of these metabolites, i.e. the alkaloid harmine, were isolated and further evaluated regarding their respective mechanisms of action, using different cell models. The promising anti-inflammatory and neuroprotective results highlight their relevance for further studies. Therefore, those findings corroborate the potential of metabolomics to contribute to different scientific challenges. Acknowledgments: CAPES, FAPEMIG APQ02882-24, APQ05607-24, CNPq 304916/2025-0, 408115/2023-8, all farms i.e. Santa Helena, PROCAFE, EMATER, EPAMIG, IFSULDEMINAS.

Keywords: *Coffea arabica*, *Hemileia vastatrix*, natural products, Parkinson's disease, neuroprotection.



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CBD-RICH Cannabis sativa var. LIFTER: CHEMICAL COMPOSITION AND EDAPHOCLIMATIC ADAPTATION TO CERRADO CONDITIONS FOR MEDICAL APPLICATIONS

Jéssica de Souza de Paula^{1*}, Joice Aguiar Teixeira Carvalho¹, Talita Vilalva Freire², Karen Midori Takahashi³, Guilherme Fiorese da Silva Moraes¹, João Batista de Souza¹, Felipe Garcia do Nascimento Nechar², Nídia Cristiane Yoshida^{1*}

depaula.biobach@gmail.com; nidia.yoshida@ufms.br

1- Laboratory of Research on Bioactive Natural Products (PRONABio), Instituto de Química, Universidade Federal de Mato Grosso do Sul (UFMS), Campo Grande-MS, Brazil. 2-Associação Divina Flor, Campo Grande-MS, Brazil. 3-FAENG, UFMS, Campo Grande-MS, Brazil.

The medicinal use of *Cannabis sativa* has been expanding due to its broad spectrum of pharmacological properties, primarily attributed to phytocannabinoids such as Δ^9 -tetrahydrocannabinol (THC) and cannabidiol (CBD). In Brazil, patient access remains limited by dependence on imported products, a gap that patient associations, supported by academia, are striving to mitigate through local cultivation initiatives. This study investigated the chemical composition and adaptation of *Cannabis sativa* var. Lifter (LF), a high-CBD chemotype (Oregon CBD Company, USA), cultivated under organic management in the Brazilian Cerrado, for medicinal purposes. The study was conducted under a collaboration agreement established between Associação Divina Flor—the first patient association dedicated to medicinal *Cannabis* production in Mato Grosso do Sul—and the Federal University of Mato Grosso do Sul (UFMS) [Partnership Term N° 05/2023, Process N° 23104.015596/2023-84]. Dried inflorescences of *C. sativa* plants were individually extracted using an ultrasound-assisted method with methanol and analyzed by high-performance liquid chromatography with diode array detector (HPLC-DAD), employing cannabinoid standards and optimized mobile phases to ensure reliable separation and quantification. The 134 analyzed LF plants exhibited consistently high CBD levels and a homogeneous chemical profile. Cannabidiol content ranged from 201.672 to 495.407 $\mu\text{g/mL}$, while mean THC content remained around 10 $\mu\text{g/mL}$, confirming its CBD-rich profile. This chemical uniformity suggests strong edaphoclimatic adaptation to Cerrado-specific abiotic factors, such as high solar incidence, elevated temperatures, and seasonal water fluctuations. These findings demonstrate the potential of locally cultivated LF for producing standardized, CBD-rich oils and underscore the importance of systematic chemical monitoring. This work provides scientific evidence supporting controlled *Cannabis* cultivation in Mato Grosso do Sul and contributes to advancing agricultural and analytical practices for cannabis-derived phytotherapeutics.

Keywords: cannabidiol, tetrahydrocannabinol, phytocannabinoids, phytochemical profile, HPLC.





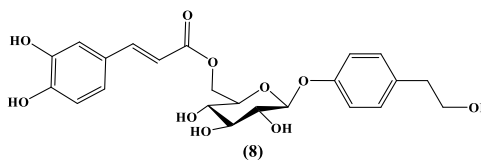
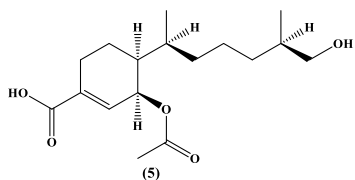
**PHYTOCHEMISTRY OF *MOQUINIASTRUM SORDIDUM*: GNPS-GUIDED
DEREPLICATION, TWO NEW METABOLITES, AND STEREOCHEMICAL
ELUCIDATION USING IPAP/PIP-HSQMBC**

Tamires Cordeiro^{1*}, **Francielli Alana Pereira Valeze¹**, Bianca D. B. Sahm², Fernanda F. Dourado¹, Marta R. B. do Carmo³, Letícia Costa Lotufo², Ernani A. Basso¹, Maria Helena Sarragiotto², Debora Cristina Baldoqui¹

alanafranhp@gmail.com

1- Departamento de Química, Universidade Estadual de Maringá, Av. Colombo, 5790, Maringá, PR, Brazil. 2-Instituto de Ciências Biomédicas, Universidade de São Paulo, Av. Prof. Lineu Prestes, 1524, São Paulo, SP, Brazil. 3- Departamento de Biologia Geral, Universidade Estadual de Ponta Grossa, Av. Carlos Cavalcanti, 4748, Ponta Grossa, PR, Brazil.

Recent taxonomic revisions based on molecular phylogenetics transferred species from *Gochnatia* to *Moquiniastrium*, which now includes 22 species, 19 in Brazil's Cerrado and Atlantic Forest. Here, we report a phytochemical study of *Moquiniastrium sordidum*. The plant was extracted with ethanol, yielding a crude extract partitioned into hexane, dichloromethane, ethyl acetate, and hydromethanolic fractions. Dereplication was performed using UHPLC-HRMS with molecular networking. Chromatographic separation afforded nine compounds, including two new metabolites: a sesquiterpene (**5**) and a phenolic glycoside (**8**). Known compounds identified were simiarenol (**1**), oleanolic acid (**2**), hispidulin (**3**), tyrosol (**4**), genkwanin (**6**), and apigenin (**7**). The relative configuration of compound **5** was established using *pip*-HSQMBC-IPAP NMR, which afforded accurate long-range ^{2,3}*J*_{CH} coupling constants. With four stereogenic centers, conformational searches (CREST) followed by DFT calculations (ORCA) were performed. Comparison between Boltzmann weighted theoretical parameters and experimental data enabled assignment of the absolute configuration as 1*R*, 6*S*, 7*S*, 11*R*. Dereplication enabled the putative identification of 45 metabolites: 12 flavonoids, 10 chlorogenic acid derivatives, 5 hydroxycinnamic acid derivatives, 9 terpenes, and 9 others. Manual inspection of fragmentation patterns, supported by GNPS2 tools, facilitated recognition of structural families within the molecular network. Preliminary cytotoxic screening against HCT-116 cells showed that the dichloromethane fraction inhibited proliferation by 92% at 50 µg/mL, while activity dropped below 50% at 5 µg/mL.



Keywords: *Moquiniastrium sordidum*, *Gochnatia sordida*, dereplication, diagnostic fragment ions.





LUPULIN GLANDS MICROSAMPLING: NEW APPROACH FOR HOPS METABOLOMIC FINGERPRINT EXPLORATION

Ana Fernanda Guimarães Trindade^{1*}, Marília Elias Gallon², Fernando Batista da Costa¹

ana.fernanda.trindade@alumni.usp.br

1-Asterbiochem, Laboratório de Farmacognosia, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, FCFRP, USP, Avenida Professor Doutor Zeferino Vaz,s/n, Ribeirão Preto, SP, Brasil 2-Núcleo de Pesquisa em Produtos Naturais e Sintéticos, NPPNS, Faculdade de Ciências Farmacêuticas de Ribeirão Preto, FRCRP, USP, Avenida Professor Doutor Zeferino Vaz,s/n, Ribeirão Preto, SP, Brasil.

Hops (*Humulus lupulus* L.) have been used for centuries in beer production, primarily due to lupulin, a resin with a complex chemical composition found in the lupulin glands in the inflorescences. Lupulin glands are glandular trichomes responsible for biosynthesizing secondary metabolites that confer the plant's characteristic properties, whereas the surrounding plant tissue, supposedly, contributes minimally to hop chemical traits. Several studies on the plant species have predominately focused on analyzing the inflorescence as a whole, since in beer production entire inflorescences are used (i.e., they are not separate into different types of plant tissue). Consequently, studies that investigate the chemical composition of trichomes are rare. Even more scarce are studies of trichomes originated from tropically grown hops. This study aimed to analyze the metabolic fingerprint of glandular trichomes from hops cultivated in tropical regions using microsampling as a sampling technique. The plants were grown in six regions in the states of São Paulo and Minas Gerais and analyzed using liquid chromatography coupled to mass spectrometry followed by unsupervised and supervised multivariate statistical analysis (Principal Component Analysis - PCA and Partial Least Squares Discriminant Analysis - PLS-DA). Samples from two commercial hop cultivars (Cascade and Comet) were evaluated. The samples included isolated trichomes, inflorescence extracts, and imported pellets (Germany). Chromatograms obtained from the trichomes revealed the methodology suitable for metabolic studies, presenting clear, well-defined picks, and similar pattern to previous studies utilizing hops extracts from the whole inflorescence. PCA (R^2X 0,872 e Q^2 0,825) displayed the data for all samples in two non-overlapping clusters. One containing trichomes and one containing inflorescences and pellets. Once this behavior was evident, PLS-DA was applied in order to reveal metabolites responsible for the segregation between different types of samples. Based on VIPs (Variable Importance Projection) obtained in the PLS-DA analyses, secondary metabolites were annotated (verified in house library and literature). Flavonoids and α - and β -acids were amongst the chemical classes annotated. These results revealed significant chemical distinctions between the samples, providing valuable insights into the composition of hops cultivated under tropical climate and chemical contribution of each structure analyzed, and further suggesting the method as a simple but robust strategy for hop chemical analysis.

Keywords: Brazilian hops; glandular trichomes; metabolomics; LC-MS/MS.





DETECTION OF NAPHTHOQUINONES IN DIFERENT BULB EXTRACT OF *Eleutherine bulbosa*

Mylena Costa Lucachinski^{1*}, Igor Ramón de Sousa Graça², Waldireny Rocha Gomes³

*mcl.mbt25@uea.edu.br

1- Programa de Pós-Graduação Biotecnologia e Recursos Naturais-MBT, Universidade do Estado do Amazonas-UEA. 2- Programa de Pós-Graduação de Química- PPGQ, Universidade Federal do Amazonas-UFAM. 3- Química de Produtos Naturais e Biotecnologia da Amazônia (QPNBA), Programa de Pós-Graduação de Ciências Farmacêuticas, Universidade Federal do Amazonas-UFAM

Eleutherine bulbosa, popularly known as marupazinho, is a native species of the Amazon region, traditionally used in teas prepared from its bulbs to treat gastrointestinal disorders, amebiasis, irregular menstruation, hemorrhoids, strokes, and gastric ulcers. Scientific interest in this species has focused mainly on the presence of eleutherol, a naphthoquinone metabolite associated with potential biological activities. However, little is known about how different extraction conditions influence the detection of this bioactive compound. This work aimed to investigate the presence of eleutherol in *E. bulbosa* bulb extracts obtained with solvents of different polarities, in order to understand how extraction affects its chemical availability. Bulbs were collected from the experimental area of the Federal University of Amazonas (UFAM), cut into 2 × 2 mm pieces, and subjected to ultrasound-assisted maceration for 20 minutes, using a proportion of 1 g of fresh bulb per 1 mL of solvent. A total of 27 extracts were prepared, filtered, and analyzed by tandem mass spectrometry (MS/MS). Mass spectrometry proved to be an efficient and accessible tool for eleutherol detection, allowing not only the identification of its presence in different extracts but also the assessment of variations in intensity according to solvent polarity. The compound was detected in almost all extracts, except in methanol/water (8:2), being the major component in TBME and n-butanol extracts, and the second major component in solvents such as hexane, acetonitrile, ethanol/water (7:3), and ethanol/water (1:1). In contrast, methanol-based solvents showed only low levels of eleutherol. The results demonstrate that solvents of intermediate polarity favored eleutherol extraction, highlighting the importance of methodological choices in phytochemical studies. Moreover, the direct application of mass spectrometry, due to its speed and sensitivity, proved to be a promising strategy for the prospection of bioactive metabolites in medicinal plants, providing new insights into the actual chemical composition of traditional *E. bulbosa* preparations. The authors acknowledge the support of CAPES, the Graduate Program in Biotechnology and Natural Resources of the Amazon (UFAM), and FAPEAM for funding.

Keywords: Eleuterol, MS/MS Solvent polarity, *Eleutherine Bulbosa*.





POSTER SESSION ABSTRACT

Session

Recent Advances on Isolation and Structure Elucidation of Secondary Metabolites



STEREOCHEMISTRY OF FUROFURAN LIGNANS BY OPTICAL ROTATORY DISPERSION: INTERPLAY BETWEEN THEORY AND EXPERIMENT

Eric Yoshitaka Lee^{1*}, Eloá Rodrigues Mestriner², Camila Luiza Cunha², Victor de Moraes Santos Sousa¹, Isabele Rodrigues Nascimento², João Marcos Batista Junior¹

eric.lee@unifesp.br

1-Instituto de Ciência e Tecnologia, Universidade Federal de São Paulo, R. Talim 330, Vila Nair,, São José do Campos, SP, 12231-280 Brazil. 2- Instituto de Química, Universidade Estadual Paulista, Av. Prof. Francisco Degni 55, Jardim Quitandinha, Araraquara, SP, 14800-900, Brazil.

Furofuran lignans are important bioactive secondary metabolites widely distributed in the plant kingdom. Even though their biosynthesis is described from the enantioselective dimerization of two phenylpropanoid units, varying enantiomeric compositions have been reported in different plant species. Additionally, their absolute configuration assignments are mostly based on empirical comparisons of optical rotation values and electronic circular dichroism spectra obtained for structurally related molecules. Since the main structural differences among furofuran lignans reside on the substitution patterns of the aromatic moieties, as well as their relative orientations, this approach is risky and prone to error propagation. Currently, the most reliable procedure to use chiroptical spectroscopy involves the comparison of experimental data with those obtained by quantum chemical calculations. Thus, in the present work, we describe the use of optical rotatory dispersion (ORD) at 589, 578, 546, 436, 405 and 365 nm, associated with density functional theory (DFT) calculations, for the stereochemical analysis of the furofuran lignans sesamin, episesamin, eudesmin, epieudesmin, kobusin and phillygenin isolated from Aristolochiaceae species. The chiroptical properties of the target compounds were evaluated in methanol, acetonitrile and chloroform solutions. The results obtained allowed for an independent verification of the absolute configurations reported in the literature, besides providing information about the influence of different structural features and solvent effects for the specific rotation of this class of secondary metabolites.

Keywords: ORD, DFT, natural products, absolute configuration, conformational analysis, chiroptical methods

Acknowledgments: FAPESP





NEW ALKENE-ALKYNE- γ -LACTONES ISOLATED BY HPCCC AND CYTOTOXIC POTENTIAL FROM *Sextonia rubra*

Sarah Larissa Gomes Flores^{1*}, Isadora Moita de Araújo¹, João Vitor de Melo Pereira⁴,
Celina de Jesus Guimarães^{2,4}, Colin Bright³, Claudia Pessoa⁴, Gilda Guimarães Leitão⁵,
Anderson Cavalcante Guimarães⁶

[*sarah.flores@ufam.edu.br](mailto:sarah.flores@ufam.edu.br)

1-Departamento de Química, Instituto de Ciências Exatas-UFAM, 69077-00, Manaus, AM, Brazil. 2-Fundação Centro de Oncologia do Estado do Amazonas, 69040-040, Manaus, AM, Brazil. 3-Dynamic Extractions Ltd, Mamhilad House, Rowan Suite, Mamhilad Park Estate, Mamhilad, UK NP4 0HZ., UK. 4-Núcleo de Pesquisa e Desenvolvimento de Medicamentos-UFC, 60020-181, Fortaleza, CE, Brazil. 5- Instituto de Pesquisa de Produtos Naturais-UFRJ, 21941-630, Rio de Janeiro, RJ, Brazil.

Sextonia rubra (Lauraceae) is known as raw material for the timber industry and is the only member of its genus found in northern Brazil. Research indicates that *S. rubra* has larvicidal, antioxidant, termiticidal, and fungicidal properties, mainly due to the biomarker compounds rubrenolide and rubrynlide. This study reports the isolation of two novel γ -lactones from the hexane extract of *S. rubra* bark by high-performance counter-current chromatography (HPCCC) and evaluates their cytotoxic properties. HPCCC is a reproducible method that avoids loss of samples by adsorption or denaturation and uses analytical-grade solvents. The fractions were analyzed using thin-layer chromatography and nuclear magnetic resonance. The hexane extract (600 mg) was fractionated by HPCCC, using the preparative column in a step-gradient normal phase elution mode. The solvent systems consisted of eight ratios about hexane-ethyl acetate-methanol-water (HEMWat, v/v/v/v) S28 (1:0:1:0), S26 (9/1/9/1), S24 (5/1/5/1), S22 (3/1/3/1), S20 (2/1/2/1), S18 (6/5/6/5), S16 (5/6/5/6) and S14 (1/2/1/2)¹. The lower phase was employed as the stationary phase, while the upper phases served as mobile phases. The stationary phase retention (*S_f*) at the first step of the gradient was 86%. Fractions F76 (35.4 mg) and F77 (36.0 mg), rich in γ -lactones were purified by analytical column in a step-gradient, normal elution mode (HEMWat) S21 (5/2/5/2), S20, S19 (3/2/3/2) and S18, for both samples the *S_f* was 75%. This procedure yielded two main samples: **F76-16** (2.5 mg) and **F77-66** (3.8 mg). The NMR data analysis proposed two new lactones 9-acetyl-5-dec-18-ynyl-3-(7-hydroxybutyl)oxolan-2-one (**1**) and 9-acetyl-5-dec-18-enyl-3-(7-hydroxybutyl)oxolan-2-one (**2**). The compound (**1**) presented cytotoxic activity against prostate cancer, inhibiting 63 % of the cells with IC₅₀ of 4.70 μ g/mL and against promyelocytic leukemia cells a IC₅₀ of 6.80 μ g/mL. The isolation was performed in two steps, without the use of any adsorption chromatography procedure. Furthermore, **1** should be subject to further investigation into the mechanism of action.

¹ N. Sumner. Developing counter-current chromatography to meet the needs of pharmaceutical discovery. Journal of Chromatography v. 1218, n. 36, p. 6107-6113, 2011

Keywords: Louro Gamela, Counter-current Chromatography, Prostate cancer, NMR.





**ISOLATION OF CANNABINOIDS BY PREPARATIVE
HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY:
TETRAHYDROCANNABINOL AND CANNABIDIOLIC ACID**

Victória Andrade Peluso Perêllo da Costa^{1*}, Prof. Dr. Daniel Pecoraro Demarque¹

victoriaperello@usp.br

1- Laboratório de Farmacognosia, Departamento de Farmácia, Faculdade de Ciências Farmacêuticas, Bloco 15, Universidade de São Paulo, Av. Prof. Lineu Prestes, 580, São Paulo, SP, 05508-000, Brazil.

Cannabis sativa L. (Cannabaceae) is a plant of growing pharmacological interest due to its wide range of bioactive compounds, with emphasis on its phytocannabinoids.¹ This study aimed to isolate cannabinoids from resin samples extracted from *C. sativa* inflorescences using preparative high-performance liquid chromatography (preparative HPLC), followed by structural identification. 2,4-dihydroxy-3-[(1*R*,6*R*)-3-methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-6-pentylbenzoic acid (cannabidiolic acid or CBDA) was isolated from the non-decarboxylated resin of the Feno Swiss variety, while (–)-*trans*- Δ^9 -tetrahydrocannabinol (tetrahydrocannabinol or THC) was obtained from the decarboxylated resin of the Northern Lights variety. Initial analyses were performed separately by analytical HPLC for each resin. To improve separation efficiency, fractionation with Sephadex LH-20 using methanol as eluent was carried out individually. The resulting eluates were pooled into three fractions based on chemical similarity, assessed by thin-layer chromatography (ethyl acetate:hexane 1:1). These fractions were further analyzed by analytical HPLC, and fraction 2, the most abundant in both cases, was selected for preparative HPLC using a 71-minute method. The samples were prepared by dissolving in 10 mL of acetonitrile and 5 mL of water, both containing 0.1% formic acid, with acetonitrile as solvent B and water as solvent A. A small sample of the collected peaks were reanalyzed by analytical HPLC, and those with sufficient purity and content were dried and dissolved in deuterated chloroform for ¹H and ¹³C NMR analysis. Identification, based on comparison with spectral data reported by Brenneisen *et al.* (2004)², confirmed the successful isolation of CBDA and THC from their respective resin samples. This work contributes to the development of strategies for cannabinoid isolation, especially when commercial standards are not available. The authors thank their institution for support and CAPES for financial assistance.

Keywords: *Cannabis sativa*, cannabidiolic acid, tetrahydrocannabinol, preparative HPLC, ¹H NMR, ¹³C NMR.

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2. HOURFANE, Sohaib et al. A comprehensive review on *Cannabis sativa* ethnobotany, phytochemistry, molecular docking and biological activities. *Plants*, v. 12, n. 6, p. 1245, 2023.





UNCOVERING BIOACTIVE AGENTS FROM AMAZONIAN MYRTACEAE WITH ANTIDIABETIC AND ANTIVIRAL ACTIONS: A 15-YEAR RESEARCH OVERVIEW

Marcos B. Machado^{1*}, Andrezza S. Ramos¹, Kidney O.G. Neves¹, Edinilze S. C. Oliveira¹, Leonard D.R. Aço², Natasha M. Cassani³, Flávia L. D. Pontes⁴, Emerson S. Lima², Francinete R. Campos⁴, Francisco Celio M. Chaves⁵, Edgar A. Sanches⁶, Jaqueline de A. Bezerra⁷, Ana Carolina G. Jardim³, Renner A. Costa⁸, Kelson M. T. Oliveria⁸, Alan D. C. Santos^{1,9}

marcosmachado@ufam.edu.br

1-NEQUIMA, Departamento de Química, ICE, UFAM, 69067-005, Manaus, AM, Brazil. 2- FCF, UFAM, 69067-005, Manaus, AM, Brazil. 3-Laboratório de Pesquisa Antiviral, UFU, 38405-302, Uberlândia MG, Brazil, 4- Departamento de Farmácia, UFPR, 80210-170, Curitiba, PR, Brazil, 5- Embrapa Amazônia Ocidental, 69010-970, Manaus-AM, Brazil, 6-Laboratorio de Polimeros Nanoestruturados, ICE, UFAM, 69067-005, Manaus, AM, Brazil, 7- IFAM, 69020-120, Manaus, AM, Brazil, 8- Departamento de Química, ICE, UFAM, 69067-005 9- Núcleo de Pesquisa de Produtos Naturais, UFSM, 97105-900, Santa Maria, RS, Brazil

The Amazon biome, which covers nearly half of Brazil's territory and represents 25 % of the world's remaining forests, has long been the focus of multidisciplinary research. Biologists, pharmacologists, chemists, and other specialists have identified metabolites with significant potential for the pharmaceutical, agrochemical, cosmetic, and food industries. However, achieving the sustainable use of this biodiversity has posed a challenge for Brazilian governments over the last 60 years. Production, quality control, and logistics involving natural resources have been the main bottlenecks hindering the region's sustainable development. In this context, the NEQUIMA (Núcleo de Estudos Químicos de Micromoléculas da Amazônia) research group, in partnership with the UFAM NMR Laboratory and partner institutions, is dedicated to identifying compounds with antiglycation, antiviral, and nutraceutical potential in Amazonian matrices, employing NMR and MS as its principal analytical tools, assisted by ECD and computational methods for the unequivocal determination of organic molecules of interest. Furthermore, NEQUIMA develops encapsulated bioproducts and NMR-based analytical methods to quantify active ingredients, while also contributing to the discovery of new antiglycation and antiviral compounds. Through these activities, NEQUIMA contributes to the training of human resources (undergraduate, master's, and doctoral students in Chemistry), to the publication of scientific articles, and to the valorization and sustainable development of the Amazon biome.

Keywords: Amazon, ¹H NMR-based metabolomics, qNMR, antiglycan, antiviral, chemometrics

Acknowledgements: FAPEAM, CNPq, CAPES, and FINEP agencies.





CHEMICAL CHARACTERIZATION OF LYCHNOPHORA PIRANIANA: A NEW SPECIES NAMED IN HONOR OF PROFESSOR JOSÉ RUBENS PIRANI

Manuela Pezzato Toledo Prado^{1*}, Marília Ellias Galon¹, Marcelo Monge^{1,2}, Norberto Peporine Lopes¹.

manuela.pezzato@usp.br

1-Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Núcleo de Pesquisa em Produtos Naturais e Sintéticos - Universidade de São Paulo (USP), Avenida do Café, s/n, CEP 14040-903, Ribeirão Preto, SP, Brasil. 2-Plant Biology Graduate Program, Institute of Biology, Federal University of Uberlândia, Av. Ceará, 1188 - Umuarama, CEP 38405-240, Uberlândia, MG, Brasil.

The genus *Lychnophora* (Asteraceae) comprises approximately 30 species endemic to Brazil, primarily distributed in the rupestrian fields of the *Cerrado* and *Serra do Espinhaço*. Popularly known as 'arnicas', these plants are traditionally used in folk medicine for their anti-inflammatory and analgesic properties in the alternative treatment of muscle pain, contusions, and inflammations. Studies have demonstrated that *Lychnophora* species are rich in specialized metabolites such as flavonoids, diterpenes, and sesquiterpene lactones, which are frequently associated with various pharmacological activities, including anti-inflammatory and antioxidant effects. Beyond their ethnobotanical significance, *Lychnophora* species also hold economic relevance, particularly in the production of cosmetics and phytotherapeutics like anti-inflammatory creams and essential oils. Recently, novel species have been described to the genus, enriching taxonomic knowledge and expanding the possibilities for discovering bioactive compounds with the potential for developing new therapies.

This project aimed to perform the chemical characterization of *Lychnophora piraniana*, a new *Lychnophora* species named in honor of botanist José Rubens Pirani, whose contributions to the Brazilian flora are significant to the genus. Using liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) followed by data mining techniques, 230 metabolites were detected. Among these, several phenolic compounds, including flavonoids and hydrocinnamic acid derivatives, and sesquiterpene lactones were annotated. The detailed characterization of these compounds can reveal novel substances, contributing to the development of innovative therapeutic products and highlighting Brazilian biodiversity.

Keywords: *Lychnophora piraniana*, Metabolomics, Mass Spectrometry (LC-MS/MS), Natural Products and Asteraceae





***ADDITIONAL QUINONES ISOLATED FROM THE BULBS OF
Eleutherine bulbosa (Miller) Urban (IRIDACEAE)***

Igor Ramón de Sousa Graça^{1*}, Matheus Vinicius Natividade Belém¹, Felipe Moura Araújo Da Silva², Hector Henrique Ferreira Koolen³, Waldireny Rocha Gomes⁴

ramonigor555@gmail.com

1-Departamento de Química, Universidade Federal do Amazonas, UFAM, Av. General Rodrigo Octávio, 6200, Manaus, AM, 69067-005, Brazil. 2-Coordenação de Tecnologia e Inovação, COTEL, Instituto Nacional de Pesquisas da Amazônia, INPA, Av. General Otávio, 6200, Manaus, AM, 69067-005, Brazil. 3-Escola Superior de Ciências da Saúde, Universidade do Estado do Amazonas, UEA, Av. Carvalho Leal, 1777, Manaus, AM, 69065-001, Brazil. 4-Faculdade de Ciências Farmacêuticas, Universidade Federal do Amazonas, UFAM, Av. General Rodrigo Octávio, 6200, Manaus, AM, 69067-005, Brazil.

Eleutherine bulbosa (Mill.) Urb. is an herbaceous plant of the family Iridaceae, popularly known as “marupari” and “marupazinho.” It is native to tropical countries of South America and also occurs in Africa and Asia. In Brazil, it is distributed across the Amazon, Cerrado, Atlantic Forest, Pantanal, and Caatinga biomes. Several classes of compounds have already been described for this species, with emphasis on the identification and isolation of quinones, particularly naphthoquinones and anthraquinones, both in *E. bulbosa* and its synonyms. This chemical diversity has motivated the continuation of phytochemical studies, with a focus on the isolation and structural elucidation of metabolites. In this context, the aim of the present study was to investigate the chemical composition of the bulb of *E. bulbosa* using both classical and modern phytochemical approaches. The dichloromethane extract, obtained by maceration at room temperature (24 g after drying), was subjected to chromatographic analyses using open column chromatography (CC), thin-layer chromatography (TLC), and preparative thin-layer chromatography (PTLC). Structural elucidation of the isolated compounds was carried out mainly by Nuclear Magnetic Resonance (NMR) spectroscopy, including one-dimensional (¹H, ¹³C, and DEPT-135) and two-dimensional (COSY, HSQC, and HMBC) experiments, complemented by Mass Spectrometry (MS). Two compounds were isolated: the anthraquinone methyl ester of 8-hydroxy-3,4-dimethoxy-1-methylanthracene-9,10-dione-2-carboxylic acid and the naphthoquinone 3-[2-(acetoxyp)propyl]-2-hydroxy-8-methoxy-1,4-naphthoquinone. The results obtained are relevant to the chemotaxonomy of the genus *Eleutherine*, particularly for the species under study.

Keywords: *Marupazinho*, chromatographic analyses, NMR, quinones, chemotaxonomy.





***ISOLATION AND CHARACTERIZATION OF A NEW BOSTRYCIN ANALOGUE
PRODUCED BY A NOVEL ENDOPHYTIC FUNGUS OF THE GENUS DIAPORTHE***

Eldrinei Gomes Peres^{1*}, Carlos Vinícius Azevedo da Silva¹, Greguy Looban Cavalcante de Lima², Edvan Alves Chagas², Gleucinei da Silva Castro³, Gilvan Ferreira da Silva³, Thalisson Amorin de Souza⁴, Jociano da Silva Lins⁴, Josean Fechine Tavares⁴, Hector Henrique Ferreira Koolen⁵

eldrineibk96@gmail.com

1-Universidade Federal do Amazonas, UFAM, Av. General Rodrigo Octávio, 6200, Manaus, AM, 69067-005, Brazil. 2-Embrapa, Av. Brasil, 3911, Boa Vista, RR, 69315-292, Brazil. 3-Embrapa, Rodovia AM-010, Km 29, s/n, Zona Rural - Manaus, AM, 69010-970, Brazil. 4-Laboratório Multiusuário de Caracterização e Análises, Universidade Federal da Paraíba, CAMPUS I - Castelo Branco III, João Pessoa - PB, 58051-900, Brazil. 5-Universidade do Estado do Amazonas, Av. Carvalho Leal, 1777, Manaus, AM, 69065-001, Brazil.

The search for bioactive natural products as a basis for developing new drugs to treat existing and emerging diseases has driven numerous studies, primarily involving plants and microorganisms. Microorganisms are among the main producers of bioactive substances, and fungi have attracted great interest due to their high biosynthetic capacity. Species of the genus *Diaporthe*, especially those that are endophytic, are widely recognised for their ability to produce a diverse array of metabolites with various biological activities. In this context, this study aimed to isolate and characterise the compounds produced by a new species of *Diaporthe* (MMSRG-125), isolated from stem explants of the Amazonian plant camu-camu (*Myrciaria dubia* (Kunth) McVaugh). Initially, the fungal strain was cultivated in potato-dextrose medium for 50 days at 28 °C. After the incubation period, the aqueous phase and the mycelium were separated by filtration, resulting in two extracts: the broth extract and the mycelial extract. The methanolic extract of the mycelium was subjected to fractionation by vacuum liquid chromatography (VLC) and compound isolation using HPLC. Structural characterisation was performed by NMR and mass spectrometry (MS). As a result, two anthraquinone derivatives, analogues of bostrycin, were isolated and characterised: 4-hydroxybostrycin and a novel analogue, 4-hydroxy-6-ethoxybostrycin. These findings highlight the potential of this new *Diaporthe* species as a promising source for the production of bioactive compounds and novel structural analogues with possible biological applications.

Keywords: *Diaporthe* sp., endophytic fungus, anthraquinone, bostrycin, isolation and structural characterisation





ALKAMIDES FROM *Zanthoxylum rhoifolium* ROOT

Matheus Vinicius Natividade Belém^{1*}, Igor Ramón de Sousa Graça¹, Felipe Moura Araújo Da Silva², Thalisson Amorin de Souza³, Josean Fechine Tavares³, Hector Henrique Ferreira Koolen⁴, Waldireny Rocha Gomes⁵

matheusbelem248@gmail.com

1-Departamento de Química, Universidade Federal do Amazonas, UFAM, Av. General Rodrigo Octávio, 6200, Manaus, AM, 69067-005, Brazil. 2-Coordenação de Tecnologia e Inovação, COTEL, Instituto Nacional de Pesquisas da Amazônia, INPA, Av. General Otávio, 6200, Manaus, AM, 69067-005, Brazil. 3-Programa de Produtos Bioativos Naturais e Sintéticos, PGPNSB/UFPB, João Pessoa, PB, Brazil. 4-Escola Superior de Ciências da Saúde-UEA, Manaus, AM, Brasil, 5-Faculdade de Ciências Farmacêuticas, UFAM, Manaus, AM, Brazil.

Zanthoxylum rhoifolium Lam. (Rutaceae), commonly known as "mamica-de-cadela", "limãozinho", or "tinguaciba", is a species widely distributed across South America, predominantly occurring in the Brazilian biomes of the Cerrado, Atlantic Forest, and Amazon. Species of the genus *Zanthoxylum* are recognized for their phytochemical diversity, containing alkaloids, phenolic compounds (such as lignans, coumarins, and flavonoids), as well as steroids and terpenes, located in various parts of the plant, including roots, stems, branches, and leaves. Given this context, phytochemical investigations focused on the isolation of metabolites. Metabolites are of great relevance, especially considering the chemical and pharmacological potential of this species. In this study, we aimed to isolate and identify compounds present in *Z. rhoifolium*. The hexane extract of the roots (11.5 g), obtained by cold maceration, was subjected to fractionation procedures using Column Chromatography (CC), Preparative Thin-Layer Chromatography (PTLC), and High-Performance Liquid Chromatography (HPLC). The structural characterization of the isolated compounds was performed using Nuclear Magnetic Resonance spectroscopy (1D and 2D ¹H and ¹³C NMR) and Mass Spectrometry (MS). As a result, four alkamides were isolated: γ -sanshool, hazaleamide, (2E,4E,8Z,11E)-N-isobutyltetradeca-2,4,8,11-tetraenamide, and (2E,4E,8Z)-N-isobutyltetradeca-2,4,8-trienamide. Although these substances have previously been reported in other species of the genus, their isolation reinforces the chemical potential of *Z. rhoifolium*. Numerous studies have highlighted promising pharmacological activities of alkamides—analgesic, anti-inflammatory, antimicrobial, and antiparasitic—justifying further research to evaluate their biological properties and therapeutic potential.

Keywords: Mamica-de-Cadela, compounds, amides, phytochemistry, isolation, HPLC





**OBTAINING A GLYCOSYLATED FLAVONOID-ENRICHED FRACTION FROM
Agave sisalana RESIDUE VIA MACROPOROUS ADSORPTION RESIN
PURIFICATION AND FLASH CHROMATOGRAPHY**

Annabel Azevedo da Silva^{1,2*}, Gedson Sampaio Gomes², Louise Souza Santos², Isabella Mary Alves Reis², Alessandro Branco^{1,2}

annabelfarma@gmail.com

1-PPGFar, Faculdade de farmácia, UFBA, rua Barão de Jeremoabo s/n, Salvador, BA, 40170.115, Brazil. 2-Laboratório de fitoquímica, DSAU, UEFS, Av. Transnordestina, s/n, Feira de Santana, BA, 44036-900, Brazil.

Agave sisalana is extensively cultivated in Bahia for fiber production, generating large amounts of waste. About 95% of the plant material is discarded. Previous studies describe that the residual biomass is rich in flavonoids and glycosides due to the higher expression of biosynthetic genes in processed leaves. Glycosylated flavonoids were obtained from the liquid residue of *A. sisalana*, a by-product of the defibration process. In this study, a two-step purification process was developed, initially involving enrichment on a macroporous adsorption resins, followed by purification via silica gel flash chromatography. The static adsorption step was conducted under constant agitation in a shaker (172 rpm) at 25 °C. A total of 200 mL of sisal liquid residue was contacted with 86 g of PuroSorb PAD950 resin, corresponding to a bed volume of 118 mL. Following adsorption, the resin was transferred and packed into a chromatographic column (36 mm diameter × 115 mm length) for the desorption stage. Dynamic desorption was performed according to the methodology adapted from Freitas *et al.*, 2026. Elution with a 40% (v/v) ethanol–water solution produced a flavonoid-rich fraction. Next, the enriched fraction (2.56 g) was subjected to flash chromatography on a silica gel column (pore size: 60 Å; particle size: 220–440 mesh), eluted in three eluents of increasing polarity in ethanol and water, resulting in six fractions monitored by HPLC-DAD. The fraction 6 (0.0532mg) presented characteristic profiles of glycosylated flavonoids, and tandem mass spectrometry (MS/MS) analysis allowed the characterization of two major glycosylated flavonoids: kaempferol 3-rutinoside-4'-glucoside and kaempferol 3-(2"-rhamnosylrutinoside). The proposed method demonstrates potential for preparative-scale application in the separation and purification of glycosylated flavonoids, providing a sustainable approach for the valorization of agro-industrial residues and expanding the use of bioactive compounds.

Keywords: *Agave sisalana*, glycosylated flavonoids, purification, macroporous resin, residue.

Reference: FREITAS, Esther Emily Silva et al. Adsorption and nanoencapsulation: Innovative strategies for recovery and protection of flavonoids from *Malpighia emarginata* DC (acerola) pomace extract. **Food Chemistry**, p. 145121, 2026.





Myricitrin isolated by countercurrent chromatography from the leaves of Myrcia sylvatica (Myrtaceae)

Bruno Ricardo Oliveira Reis^{1*}, Sarah Larissa Gomes Flores¹, Gilda Guimarães Leitão²,
Anderson Cavalcante Guimarães¹, Marcos Batista Machado.¹

[*bruno.reis@ufam.edu.br](mailto:bruno.reis@ufam.edu.br)

1-Departamento de Química, Instituto de Ciências Exatas-UFAM, 69077-00, Manaus, AM, Brazil. 2-
Instituto de Pesquisa de Produtos Naturais-UFRJ, 21941-630, Rio de Janeiro, RJ, Brazil.

Myrcia Sylvatica (Myrtaceae), known in folk medicine as "pedra-ume-caá," is found from eastern South America to eastern Brazil. It is widely used in the Amazon as a tea made from its dried leaves to treat conditions such as diabetes, diarrhea, mouth ulcers, intestinal inflammation, and hemorrhages. Research indicates that *M. sylvatica* has antidiabetic properties. This study's main objective is to isolate and characterize the organic compound myricitrin, a flavonoid, obtained from the dry extract of *M. sylvatica* leaves using high-performance countercurrent chromatography (HPCCC), as well as to evaluate its antiglycation activity. High-performance chromatography (HPCCC) is a reproducible method that avoids sample loss due to adsorption or denaturation and uses analytical-grade solvents. Fractions were analyzed by thin-layer chromatography and nuclear magnetic resonance. The ethyl acetate extract (400 mg) was fractionated by HPCCC, using the preparative column in normal mode and nonlinear gradient elution. The solvent systems consisted of five ethyl acetate-butanol-water ratios (v/v/v): S6 (1/0/1), S5 (4/1/5), S4 (3/2/5), S3 (2/3/5) and S2 (1/4/5). The lower phase was used as the stationary phase, while the upper phases served as mobile phases. The retention of the stationary phase (Sf) in the first gradient step was 74.3% and in the second step 72.2%. The flavonoid-rich fractions are 1F10 (9.10 mg) and 2F10 (15.5 mg), with Myricitrin being the major component. The organic structure was characterized using NMR and MS data. Therefore, this study establishes a method for isolating and characterizing flavonoids with antiglycation potential, contributing to the development of future studies on pedra-ume-caá species.

Keywords: *Myrcia Sylvatica*, HPCCC, antidiabetic and NMR.

Reference:

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ANALYSIS OF HIGH VALUE-ADDED POLYPHENOLS SUBSTANCES PRESENT IN BANANA BIOMASS RESIDUES USING DESIGN OF EXPERIMENTS (DoE) ALLY WITH MACROPOROUS POLYMERIC RESINS (MPR)

Ian Gardel Carvalho Barcellos-Silva¹, Ananda da Silva Antonio², Monica Costa Padilha³, Valdir Florencio da Veiga-Junior^{1*}.

iangardel123@gmail.com

1- Chemical Engineering Section, Military Institute of Engineering, Praça General Tibúrcio, 80, Praia Vermelha, Urca, 22., 290-270 Rio de Janeiro, RJ, Brazil; 2- Federal University of Rio de Janeiro, Forensic Analysis Center (NAF-LADETEC / IQ-UFRJ), Rio de Janeiro, RJ 21941- 909, Brazil; 3- Federal University of Rio de Janeiro, Chemistry Institute, Brazilian Doping Control Laboratory, Rio de Janeiro 21941-909, Brazil (LBCD / UFRJ-IQ), Rio de Janeiro, RJ 21941- 909, Brazil.

The valorization of residual biomass into high-value products represents a sustainable approach to improving the manufacturing process of agricultural systems. Banana peels are rich in flavonoids and phenolics with recognized anti-inflammatory and antioxidant activities, which are increasingly being explored for applications in food supplements, pharmaceuticals, and cosmetics. Epigallocatechin gallate (EGCG) is a bioactive flavonoid that holds substantial market value in these applications. The application of macroporous polymeric resins (MPR) and Design of Experiments (DoE) are methods utilized as a substitute for purification and recovery procedures of bioactive chemicals, mostly for the extraction of compounds like polyphenols. Obtaining concentrated extracts with flavonoids and phenolics from large-scale biomass waste is a sustainable and viable approach. The purpose of this work is to extract high added-value flavonoids, such as epigallocatechin gallate, from banana peels selectively using macroporous polymeric resins. Four different resin types were tested: XAD-2, XAD-4, XAD-7, and XAD-16. To perform the extractions, *Chemoface* software was used to organize experimental designs. Initially, a 2² full factorial design was applied to select the best macroporous polymeric resin. Subsequently, a 2³ design with two central points was used to optimize the extraction of epigallocatechin gallate using the previously selected resin. The particle size was fixed at 1.20 cm in both experiments (> 1/2 mesh). In the 2² design, the studied variables were: crude extract/dry resin ratio (1:2; 1:4; 1:10) and agitation speed in the shaker (100–200 rpm). In planning 2³, the following parameters were investigated: extraction temperature (30–50 °C), extraction time (1–3 h) and ethanol concentration in the desorption solvent (60–80%). The use of full factorial design combined with resins Amberlite XAD-7 line allows the optimization extraction of high-value flavonoids, such as epigallocatechin gallate, from banana peels.

Keywords: sustainable extraction, design of experiments, epigallocatechin gallate, enzymatic tests





ISOLATION AND STRUCTURAL ELUCIDATION OF THE FLAVONOIDS QUERCITRIN AND AFZELIN FROM THE LEAVES OF *COPAIFERA OBLONGIFOLIA*

Cecília Fernandes Patta Muller Marques^{1*} Ana Carla Rangel Rosa², Rafael Corrêa Ramos³, Lizandra G. Magalhães³, Renato Luis Tame Parreira³, Mario Ferreira Conceição Santos¹, Wilson R. Cunha³

ceciliafernandespmm@gmail.com

1- Center for Exact, Natural and Health Sciences, Federal University of Espírito Santo, Alegre - ES, Brazil 29500-000. 2 - Program in Genetics and Plant Breeding, Federal University of Espírito Santo, Alegre - ES, Brazil 29500-000. 3 - Center for Exact and Technological Sciences, University of Franca, Franca - SP, Brazil 14404-600.

The *Copaifera* genus is a prominent source of secondary metabolites with pharmacological relevance, motivating the development of efficient phytochemical strategies for the isolation of its constituents. This study aimed to develop a comprehensive chromatographic protocol to isolate and identify the major flavonoids present in the leaves of *Copaifera oblongifolia*, a species that remains chemically underexplored. The process began with the obtention of a crude hydroalcoholic extract (64.84 g) from dried and powdered plant material (913.7 g) through five successive extractions. The extract was then subjected to liquid-liquid partitioning, yielding an enriched dichloromethane fraction (FD) of 8.9 g. This fraction was submitted to fractionation over a silica gel 60 column, using a solvent gradient of increasing polarity, which generated 110 fractions of 45 mL each. Thin-layer chromatography analysis revealed that fractions 8 to 11 showed similar chromatographic profiles and were subsequently pooled. The final purification of this group was achieved by preparative High-Performance Liquid Chromatography (HPLC) on a Gemini C-18 column, using an isocratic mobile phase of methanol and acidified water (57:43 v/v) at a flow rate of 10.0 mL/min. This procedure successfully yielded 70 mg of compound 1 and 30 mg of compound 2 in high purity. Structural elucidation, based on extensive analysis of mass spectrometry (ESI-MS) and nuclear magnetic resonance (¹H and ¹³C NMR) data, and by comparison with literature values, unambiguously identified the compounds as the flavonoids quercitrin (1) and afzelin (2). The developed multi-step chromatographic methodology proved to be robust and effective for the targeted isolation of flavonoids from *C. oblongifolia*, providing pure substances in sufficient quantities for subsequent studies, such as biological activity assays.

Keywords: Phytochemistry, Secondary Metabolites, Chromatography, Fabaceae, Spectroscopic Analysis.





PHYTOCHEMICAL STUDY OF THE METHANOL EXTRACT FROM THE LEAVES OF REMIJIA AMAZONICA (RUBIACEAE)

Fábio Geraldo de Souza^{1*}, David Ribeiro da Silva², Luana da Conceição Moreira³, Gabriel Santana Crispim³, Cecilia Veronica Nunez^{1,2,3}

fgeraldodesouza@gmail.com

1-Programa de Pós-Graduação em Ciências Biológicas (Botânica), Instituto Nacional de Pesquisas da Amazônia - INPA, Av. André Araújo, 2936, Manaus, AM, Brazil. 2- Coordenação de Tecnologia e Inovação, COTEL-INPA, Av. André Araújo, 2936, Manaus, AM, Brazil. 3- Programa de Pós-Graduação em Biotecnologia, Universidade Federal do Amazonas, UFAM, Av. Rodrigo Otávio, 1200, Manaus, AM, Brazil.

Remijia amazonica (Rubiaceae) is a species known as Amazonian cinchona, found in the North and Central-West regions of Brazil. Studies conducted with the genus *Remijia* have shown significant phytochemical potential, with the isolation of alkaloids, flavonoids, phenolic acids, steroids, and triterpenes. In this context, the present study aimed to evaluate the phytochemical profile of the methanolic extract of *R. amazonica* leaves. The botanical material was collected from the Adolpho Ducke Forest Reserve in Manaus, Amazonas, Brazil, dried in a forced circulation oven (<50°C), ground, and subsequently extracted in an ultrasonic bath with solvents in increasing order of polarity: hexane and methanol (MeOH). Subsequently, a liquid-liquid partition of the MeOH extract was performed, yielding three phases: dichloromethane (FDCM), ethyl acetate (FEtOAc), and hydromethanolic (FH₂O/MeOH). The following methodologies were used to isolate and identify the substances: comparative thin layer chromatography (TLC), open column chromatography (CCA), analysis of one- and two-dimensional ¹H and ¹³C NMR (nuclear magnetic resonance) data (HSQC, HSQCedit, HMBC, DEPT, and COSY), combined with mass spectrometry and comparisons with the literature. Phytochemical analysis of the FDCM phase indicated the presence of alkaloids when revealed with Dragendorff's reagent in CCDC and terpenes when revealed with anisaldehyde and Ce(SO₄)₂. The EtOAc and H₂O/MeOH phases, when stained with anisaldehyde, presented a reddish coloration, and after staining with FeCl₃ and NP/PEG, they showed evidence of substances with aromatic rings. Through FDCM fractionation, two *Corynanthe*-type indole alkaloids with a molecular mass of 383 u were isolated and identified, designated 11-methoxy-3-isorauniticine and 9-methoxy-3-*iso*-19-epiajmalicine. This corroborates the genus, since indole alkaloids are considered chemosystematic markers of the genus *Remijia*, in addition to a coumarin (scopoletin). All three substances were described for the first time in the species and in the genus *Remijia*. Therefore, these results highlight the great chemical potential of the species and reinforce the need for further research to contribute to the genus and the Rubiaceae family. The authors would like to thank PPGBOT-INPA, PPGBIOTEC-UFAM, CNPq, CAPES, FAPEM, FINEP and LTQPN-INPA.

Keywords: *Indole alkaloids, coumarin, phytochemistry, chemosystematic markers.*





**ISOLATION OF AN INDOLIC ALKALOID AND IRIDOID FROM
BRANCHES OF
KERIANTHERA PRECLARA**

Luana da Conceição Moreira^{1,2*}, David Ribeiro da Silva¹, Fábio Geraldo de Souza¹,
Gabriel Santana Crispim^{1,2}, Cecilia Veronica Nunez^{1,2}

luannamoreira38@gmail.com

1- Laboratório de Bioprospecção e Biotecnologia – LABB, Coordenação de Tecnologia e Inovação – COTEI, Instituto de Pesquisas da Amazônia – INPA, Av. André Araújo, 2936, Manaus, AM, 69067-375, Brazil. 2- Programa de Pós-Graduação em Biotecnologia – PPGBiotec, Universidade Federal do Amazonas – UFAM, Av. General Rodrigo Octavio Jordão Ramos, 1200, Manaus, AM, 69067-005, Brazil.

Species of the Rubiaceae family are known for producing pharmacologically relevant alkaloids such as quinine and emetine, as well as other substances such as anthraquinones, saponins, iridoids, and flavonoids. *Kerianthera preclara* J.H.Kirkbr. is a native species from the Amazon region, with records of collections reported only for the state of Amazonas and no previous chemical studies. The objective of this work was to carry out a phytochemical investigation of the *K. preclara* branches methanolic extract, which was analyzed by comparative thin layer chromatography (TLC) and ¹H nuclear magnetic resonance (NMR). This extract, when revealed with Dragendorff's reagent, showed orange spots, indicating the presence of nitrogenous substances. Therefore, it was subjected to liquid-liquid partition and further chromatographic fractionations allowing the isolation the indole alkaloid cinchonamine from the dichloromethane phase and the iridoid kingside from the ethyl acetate phase. Structural identification was performed by one- and two-dimensional ¹H, ¹³C NMR, combined with data from the scientific literature. The ¹H NMR spectrum of cinchonamine showed signals in δ 11.16 (1H, s, NH), δ 7.48 (1H, d, J = 7.8 Hz, H-9), δ 7.40 (1H, d, J = 8.0 Hz, H-12) δ 7.09 (1H, ddd, J = 8.0; 6.9; 0.9 Hz, H-11), δ 6.98 (1H, ddd, J = 7.8; 6.9; 0.8, H-10), δ 6.10 (1H, ddd, J = 17.3; 10.3, 7.5 Hz, H-19), δ 5.13 (1H, d, J = 10.3 Hz, H-18a), δ 5.22 (1H, d, J = 17.3 Hz, H-18b), δ 4.51 (1H, t, J = 9 Hz, H-3), δ 3.50 (1H, m, H-5a), δ 3.65 (1H, m, H-5b), δ 3.13 (1H, m, H-21a), δ 3.25 (1H, m, H-21b), δ 2.86 (1H, dd, J = 8.8; 5.7 Hz, H-6a), δ 2.99 (1H, dt, J = 14.3, 4.7 Hz, H-6b), δ 2.54 (m, H-20), δ 2.73 (m, H-17), δ 2.14 (m, H-14), δ 1.99 (m, H-15), δ 1.67 (m, H-16a), 2.06 (m, H-16b). In the ¹H NMR spectrum of kingside, a signal was observed in δ 7.50 (1H, s, H-3), δ 1.36 (3H, d, J = 6.6 Hz, H-10), δ 3.63 (3H, s, OMe), δ 5.55 (1H, d, J = 5.5, H-1), δ 4.72 (1H, dq, J = 4.5; 6.4 Hz), an anomeric hydrogen in δ 4.50 (1H, d, J = 7.8 Hz, H-1') and several signals compatible with the glucosyl unit in the region δ 2.80-3.20. The results of this research deepen the chemical knowledge about *K. preclara* and reinforce its potential for future chemical and biological investigations. The authors would like to thank CAPES, CNPq, FAPEAM, FINEP and LTQPN-INPA.

Keywords: Phytochemistry, cinchonamine, kingside, ¹H-NMR





***ISOLATION AND MOLECULAR CHARACTERIZATION OF A NEW
XANTHONE FROM THE BRANCHES OF VISMIA SANDWITHII EWAN
(HYPERICACEAE)***

Maria Izabel Correia Osorio¹, Gabriel Santana Crispim¹, Fábio Geraldo de Souza¹, Luana da Conceição Moreira¹, Cecilia Veronica Nunez^{1*}

cvnunez@gmail.com

1-Instituto Nacional de Pesquisas da Amazônia, Laboratório de Bioprospecção e Biotecnologia (LABB/INPA). Av. André Araújo, 2936, Petrópolis, Manaus - AM, 69067-375, Brazil.

Species of the genus *Vismia* present anthraquinones, xanthenes, benzophenones, flavonoids, triterpenes, and other classes of metabolites. Despite their pantropical distribution, many species found in the Amazon rainforest region have a gap in phytochemical studies, such as *Vismia sandwithii* Ewan. Anthraquinones and triterpenes have been isolated from this species, but only the hexane extracts have been evaluated. Therefore, the objective of this study was to conduct a phytochemical study of methanolic extracts. To explore the potential of this species, the methanolic extracts of the branches were fractionated. Initially, this extract's dichloromethane phase showed signs of phenolic substances. After chromatographic fractionation, a xanthone was isolated. The isolated substance was analyzed by nuclear magnetic resonance (NMR), and the spectroscopic data were compared with the literature. The analysis of the ¹H spectra revealed a potential quinone in which one of the rings had only a single hydrogen and would be substituted at C-6, C-7, and C-8, and only one chelated hydroxyl. Among the correlations observed from the two-dimensional experiments, it was possible to determine the position of this hydrogen at H-5, which correlated with two carbons bonded to phenolic hydroxyls (C-6 and C-7) and the carbonyl at C-9. These correlations were key to determining the substitution of the second ring. After the analysis was complete, the structural information, including the molecule's design in SMILES code, was search on the SciFinder (Chemical Abstracts Service) and PubChem (National Center for Biotechnology Information, NCBI) databases. It was observed that this substance was not found in these databases, only those xanthenes with substituents in different positions. Based on this, the isolated substance's structure was elucidated as 1,7,6-trihydroxy-8-methoxy-9H-xanthen-9-one, a new xanthone from *Vismia sandwithii*. The authors would like to thank CAPES, CNPq, FAPEAM, FINEP and LTQPN-INPA.

Keywords: 1,7,6-trihydroxy-8-methoxy-9H-xanthen-9-one, quinones, NMR, structure elucidation, xanthenes





CHEMICAL STUDY OF PARKIA DECUSSATA DUCKE (FABACEAE)

Maria Gabriela Da Cas Rachid Pietro^{1,2}, Gabriel Santana Crispim^{2,3}, David Ribeiro da Silva²,
Luana da Conceição Moreira^{2,3}, Fábio Geraldo de Souza^{1,2}, **Cecilia Veronica Nunez**^{1,2,3*}

cecilia@inpa.gov.br

1-Programa de Pós-Graduação em Ciências Biológicas (Botânica), Instituto Nacional de Pesquisas da Amazônia – INPA, Av. André Araújo, 2936, Manaus, AM, Brasil. 2-Coordenação de Tecnologia e Inovação, COTEI – INPA, Av. André Araújo, 2936, Manaus, AM, Brasil. 3-Programa de Pós-Graduação em Biotecnologia, Universidade Federal do Amazonas – UFAM, Av. Rodrigo Otávio, 1200, Manaus, AM, Brasil.

Species of the Fabaceae family are rich producers of secondary metabolites, mainly flavonoids, terpenes, alkaloids, and other bioactive metabolites. The genus *Parkia* (Fabaceae) also expresses the family's chemosystematics, however, some species within the genus, such as *Parkia decussata* Ducke, lack phytochemical studies. Considering this gap, this study aimed to conduct a chemical study of the species. To this end, branches and leaves (rachis and leaflets) were collected, dried in a forced circulation oven (<50 °C), grounded and extracted with solvents in increasing order of polarity: hexane and methanol, using an ultrasonic bath. For phytochemical analysis of the extracts, comparative thin layer chromatography (TLC) was used. Subsequently, a liquid-liquid partition of the MeOH extract of the leaves was performed, obtaining four phases: hexane (P_{Hex}), dichloromethane (P_{DCM}), ethyl acetate (P_{EtOAc}) and hydromethanolic (P_{H₂O/MeOH}). For the isolation of the substances open column chromatography (CCA) were used. Nuclear magnetic resonance (NMR) of ¹H and ¹³C, one and two dimensions (COSY, HSQC, HMBC and DEPT 135°) were used for identification of the substances. The extracts selected for fractionation were the hexane phase, which, upon revealing the chromatographic plate with the Anisaldehyde reagent, revealed signs of terpenes. Fractionation allowed the isolation and identification of one terpene (lupeol) and two steroids (stigmasterol and β-sitosterol). The EtOAc phase, revealed signs of phenolic substances upon revealing with FeCl₃ reagent, and through fractionation, a flavonoid (quercetin) was isolated and identified. Therefore, the present study corroborated the chemotaxonomy of the genus (terpenes, phenolic acids, and flavonoids). The authors thanks to CNPq, CAPES, FAPEAM, FINEP and LTQPN-INPA.

Keywords: *Parkia decussata*, flavonoid, terpene, steroids, biological activity, phytochemistry





**DETECTION OF β -CARBOLINE ALKALOIDS IN BANISTERIOPSIS
CAAPI (MALPIGHIACEAE) LEAVES BY LEAF SPRAY MASS
SPECTROMETRY (LS-MS)**

Fernanda Dias Viana^{1*}, Felipe Moura Araujo da Silva², Waldireny Rocha Gomes¹

nandafediasviana@gmail.com

1-Laboratório de Química Orgânica e Cromatografia, PPGCF, UFAM, Av. Rodrigo Octavio, 1200, Manaus, AM, 69067-005, Brazil. 2-Coordenação de Tecnologia e Inovação (COTEI), Instituto Nacional de Pesquisas da Amazônia, Manaus, AM, 69067-375, Brazil.

Leaf Spray Mass Spectrometry (LS-MS) is a rapid and cost-effective analytical technique that requires minimal sample preparation and allows the direct analysis of plant materials such as leaves, bark, roots, and fruits. This method provides preliminary access to chemical profile of different samples, enabling the detection of a wide range of chemical classes in intact plant tissues while minimizing sample handling. In addition to generating chemical profiles, the technique also enables the acquisition of tandem fragmentation spectra, facilitating the annotation of natural products from various classes. *Banisteriopsis caapi*, popularly known as mariri, is native to the Amazon region, belongs to the Malpighiaceae family, and exhibits insecticidal, bactericidal, and fungicidal activities. It is widely recognized as one of the main ingredients of the ayahuasca beverage, traditionally employed in shamanic rituals. The pharmacological interest in this species is largely attributed to the presence of β -carboline alkaloids such as harmine, harmaline, and tetrahydroharmine, which act as monoamine oxidase inhibitors (MAOIs), thereby preventing the degradation of dimethyltryptamine (DMT), a psychoactive alkaloid found in ayahuasca. In this context, the aim of this study was to detect and annotate β -carboline alkaloids in *B. caapi* leaves through straightforward LS-MS approach. The mass spectrum obtained in positive mode showed a base peak at m/z 213 $[M + H]^+$, identified as the alkaloid harmine based on MS/MS spectral analysis. The application of LS-MS proved effective for the direct detection of β -carboline alkaloids in *B. caapi* leaves without the need for prior extract preparation. By combining speed, simplicity, and sensitivity, this methodology represents a promising tool for the rapid prospecting of natural products in plant samples, supporting preliminary chemical studies of medicinal species and those of ethnopharmacological relevance.

Keywords: Harmine, harmaline, secondary metabolites, mass spectrometry.





LACTONES ISOLATED BY HPCCC FROM CITOTOXIC EXTRACT OF *Sextonia rubra* WASTEWOOD

***Karen Floriza Costa Mota*^{1*}**, Sarah Larissa Gomes Flores¹, Celina de Jesus Guimarães²⁻³, João Vitor de Melo Pereira³, Cláudia do Ó Pessoa³, Gilda Guimarães Leitão⁴, Anderson Cavalcante Guimarães¹.

[*karenn2017.costa@gmail.com](mailto:karenn2017.costa@gmail.com)

1-Departamento de Química, Instituto de Ciências Exatas-UFAM, 69077-00, Manaus, AM, Brazil. 2-Fundação Centro de Oncologia do Estado do Amazonas, 69040-040, Manaus, AM, Brazil. 3-Núcleo de Pesquisa e Desenvolvimento de Medicamentos-UFC, 60020-181, Fortaleza, CE, Brazil. 4- Instituto de Pesquisa de Produtos Naturais-UFRJ, 21941-630, Rio de Janeiro, RJ, Brazil.

Sextonia rubra (Lauraceae) is a significant Amazonian timber species and the sole representative of its genus in Brazil. Despite industrial value, its wood processing generates large amounts of underutilized residues. Phytochemical investigations revealed the presence of γ -lactones, rubrenolide, and rubrynnolide, as biomarkers and are responsible for biological activities. In this work, the hexane extract of *S. rubra* bark was analyzed against tumor cells and fractionated by high-performance countercurrent chromatography (HPCCC). The hexane extract was subjected to cytotoxic assays, and 600 mg of sample was processed using HPCCC with a semi-preparative column 136mL in step-gradient normal-phase elution. The solvent systems used were hexane–ethyl acetate–methanol–water (HEMWat, v/v/v/v) 1/0/1/0, 9/1/9/1, 5/1/5/1, 3/1/3/1, 2/1/2/1, 6/5/6/5, 5/6/5/6, and 1/2/1/2¹. The lower phase of 1/0/1/0 was employed as the stationary phase and the upper phases of the systems as mobile phases, with stationary phase retention (*Sf*) = 86%. Fraction F77 (36.0 mg) was further purified in the analytical 26mL column in a step-gradient, normal elution mode (HEMWat) 5/2/5/2, 2/1/2/1, 3/2/3/2, and 6/5/6/5¹, *Sf* = 75%. The compounds were determined by mass spectrometry (MS) and nuclear magnetic resonance (NMR). Hexane extract demonstrated inhibition of growth by 60–92%. The IC₅₀ values (μ g/mL) were: 8.11 for prostate carcinoma (PC3), 20.45 for astrocytoma (SNB-19), 20.47 for human colon carcinoma (HCT-116), and 9.12 for promyelocytic leukemia (HL-60). The procedure in one step generated 01-F35 (3.9 mg) (1) and 01-F69 (1.6 mg) (2), while the isolation in the analytical column yielded 01-F77-64 (4.2 mg) (3). The MS and NMR analyses suggested the presence of γ -lactones majoranolide (1), majorenolide (2) and majorynnolide (3)². The results show that *S. rubra* wastewoods are a valuable source of bioactive compounds with potential for the development of new anti-tumor agents. The HPCCC was efficient in isolating minority lactones without the use of any adsorption chromatography procedure.

¹ N. Sumner. Developing counter-current chromatography to meet the needs of pharmaceutical discovery. Journal of Chromatography v. 1218, n. 36, p. 6107-6113, 2011

² FRAGA, Braulio M.; DÍAZ, Carmen E.; BOLAÑOS, Patricia; BAILÉN, María; ANDRÉS, María Fe; GONZÁLEZ-COLOMA, Azucena. Alkane-, alkene-, alkyne- γ -lactones and ryanodane diterpenes from aeroponically grown *Persea indica* roots. Phytochemistry, v. 176, p. 112398, 2020.

Keywords: Countercurrent chromatography, Cytotoxic activity, *Louro Gamela*.





PHENOLIC COMPOUNDS ISOLATED BY HPCCC FROM *Sextonia rubra* BARKS

Bruna Amazonas Pinho^{1*}, Sarah Larissa Gomes Flores¹, Gilda Guimarães Leitão²,
Anderson Cavalcante Guimarães¹
[*brunaamazonasufam@gmail.com](mailto:brunaamazonasufam@gmail.com)

1-Departamento de Química, Instituto de Ciências Exatas-UFAM, 69077-00, Manaus, AM, Brazil. 2-
Instituto de Pesquisa de Produtos Naturais-UFRJ, 21941-630, Rio de Janeiro, RJ, Brazil.

S. rubra (Lauraceae) is one of the most investigated species in the timber trade of Amazonas and is the only representative of its genus in Brazil. Phytochemical studies with crude extracts of the barks and branches have indicated larvicidal, termiticidal, fungicidal and antioxidant activities. In this study we describe the isolation and purification of phenolics compounds by high-performance countercurrent chromatography (HPCCC) from the ethyl acetate (EAE) and butanol (BE) extracts of the bark of *S. rubra* as well as the evaluation of their antioxidant potential. The fractions were analyzed using thin layer chromatography (TLC), MS and NMR. The EAE (3.3 g) and BE (5.1 g) were fractionated by HPCCC, using the semi-preparative column in a step-gradient reversed phase (EAE) and normal phase (BE) elution mode. For fractionations of EAE, the stationary phase (SP) was the upper phase of the solvent system hexane-ethyl acetate-methanol-butanol-water (HEMBWat-v/v/v/v/v)¹ S6 (0:1:0:0:1) and the lower phases of S6 and S8 (1:9:1:0:9), respective. The stationary phase retention (*S_f*) at the first step of the gradient was 73%. To procedures of BE, the SP was the lower phase S6 of HEMBWat systems and the mobile phases were the upper phases of S6, S4 (0:3:0:2:5) and S2 (0:1:0:4:5), in this order and *S_f* = 82%. Fraction rich in phenolic compounds were purified by semi-prep HPCCC, step-gradient and normal elution modes. The sample F14 (122,1 mg) from EAE used S14 (1:2:1:0:2), S12 (1:3:1:0:3), S10 (1:5:1:0:5), S8, S6, S4 and S2 (0:1:0:4:5) systems, and BE fractions F3 (67,9 mg) and F7 (149,4 mg) were processed the using S5 (0:4:0:1:5), S4 and S3 (0:2:0:3:3) systems. These processes resulted in the isolation of five substances **F14-11** (8.9 mg- vanillic acid), **F14-16** (20 mg - protocatechuic acid), **F14-24** (3.2 mg- proanthocyanidin A2) originating from EAA, and **F3-6** (22.4 mg- epicatechin) and **F7-15** (16.7 mg - nudeposide) as of BE. HPCCC performed in two steps the isolations of two phenolic acids, two flavonoids and one lignan from polar extracts showing the versatility of the technique in contributing to the chemical of the genus *Sextonia*.

¹ N. Sumner. Developing counter-current chromatography to meet the needs of pharmaceutical discovery. Journal of Chromatography v. 1218, n. 36, p. 6107-6113, 2011

Keywords: Countercurrent Chromatography, phenolics compounds, HEMBWat solvent systems.





CHEMICAL STUDY AND EVALUATION OF THE ANTIOXIDANT ACTIVITY OF WOOD RESIDUES FROM THE BARK OF *Andira parviflora* Ducke

Letícia Vasconcelos Fernandes^{1*}, *Isadora Moita de Araújo*¹, *João Vitor de Melo Pereira*⁴,
Celina de Jesus Guimarães^{2,4}, *Colin Bright*³, *Claudia Pessoa*⁴, *Gilda Guimarães Leitão*⁵,
*Anderson Cavalcante Guimarães*⁶

[*leticciavasconcelos@gmail.com](mailto:leticciavasconcelos@gmail.com)

1-Departamento de Química, Instituto de Ciências Exatas-UFAM, 69077-00, Manaus, AM, Brazil. 2-Fundação Centro de Oncologia do Estado do Amazonas, 69040-040, Manaus, AM, Brazil. 3-Dynamic Extractions Ltd, Mamhilad House, Rowan Suite, Mamhilad Park Estate, Mamhilad, UK NP4 0HZ., UK. 4-Núcleo de Pesquisa e Desenvolvimento de Medicamentos-UFC, 60020-181, Fortaleza, CE, Brazil. 5- Instituto de Pesquisa de Produtos Naturais-UFRJ, 21941-630, Rio de Janeiro, RJ, Brazil.

The Amazon is recognized as the largest tropical rainforest on the planet, harboring a wide diversity of plant species of economic and medicinal interest. Among them is *Andira parviflora* (sucupira-vermelha), belonging to the Fabaceae family, whose timber exploitation generates large volumes of underutilized residues. In this study, countercurrent chromatography was performed to simplify fractions with antioxidant potential from the ethanolic extract of *A. parviflora* bark and to characterize them using standard techniques. The chloroform (LSV02) and ethyl acetate (LSV03) fractions were evaluated by thin-layer chromatography (TLC) using universal reagents and DPPH radical solution for qualitative radical reduction analysis, and subsequently subjected to fractionation by High-Performance Countercurrent Chromatography (HPLCCC) with seven variations of solvent systems composed of hexane:ethyl acetate:methanol:water (HEMWat) (v/v/v/v). The samples were characterized by mass spectrometry (MS) and nuclear magnetic resonance (NMR). TLC analyses of LSV02 and LSV03 suggested the presence of flavonoids, coumarins, terpenoids, and phenolic compounds, and also revealed yellow spots indicative of DPPH radical inhibition, suggesting antioxidant activity. MS analyses of flavonoid-rich fractions (HPLCCC) indicated the presence of genistein, calycosin, prunetin, medicarpin, and biochanin A, the latter confirmed by NMR and isolated for the first time from the bark of this species. Qualitative TLC analyses revealed distinct chemical classes, highlighting the complexity of the plant matrix. Fractionation by HPLCCC yielded flavonoid-enriched fractions with the isolation of Biochanin A (12 mg) from 200 mg of material injected into the chromatograph. Thus, the research confirmed the antioxidant potential of *A. parviflora* bark and emphasized its relevance as a source of isoflavones and other secondary metabolites of pharmaceutical interest, adding value to a timber residue with possible biotechnological application.

¹ GARCIA, M. G. *et al.* Identification of Isoflavonoids in Wood Residue from *Swartzia laevis* carpa, *Dipteryx odorata*, and *Andira parviflora*. **Chemistry of Natural Compounds**, v. 54, n. 5, p. 856–859, 2018.

² WAGNER, H.; BLADT, S. **Plant Drug Analysis: A Thin Layer Chromatography Atlas**. 2a ed. ed. Berlin: Springer Verlag Berlin Heidelberg, 1996.

Keywords: *Andira parviflora*; Antioxidant activity; Biochanin A; Countercurrent chromatography.





POSTER SESSION ABSTRACT

Session
**Organic Synthesis and
Structural Modification**



SEMISYNTHESIS AND BIOLOGICAL ACTIVITIES OF PALITANTIN DERIVATIVES

Vinícius Gimenes Roqueto^{1*}, Pedro Santucci², Kleber Thiago de Oliveira², Roberto Gomes de Souza Berlinck¹

vini.g_roqueto@usp.br, rgsberlinck@iqsc.usp.br

1-QOSBio, Instituto de Química de São Carlos, IQSC, USP, Avenida Trabalhador são-carlense, 400, Parque Arnold Schmidt, São Carlos, SP, Brazil. 2-LQBO, Departamento de Química de São Carlos, UFSCar, Rodovia Washington Luís, km 235, São Carlos, SP, Brazil.

Palitantin is a secondary metabolite first isolated in 1936 from cultures of *Penicillium palitans*. It exhibits moderate antiparasitic and antifungal activities, and it is a potent inhibitor of acetylcholinesterase. However, synthetic derivatives of this compound have never been described, mainly due to the low overall yield ($\leq 25\%$) obtained by multistep total syntheses. In this study, we aimed to produce (+)-palitantin by a fermentative approach using the fungal strain *Penicillium* sp. (AMF1a), which provided a yield of approximately 160 mg/L, and to explore, through semisynthesis, the generation of new bioactive derivatives by reactions of palitantin with nitrogen nucleophiles, as well as to develop an efficient methodology for the reduction of imine derivatives of palitantin. A total of 2.5 g of (+)-palitantin was isolated from 10 L of 2% malt medium produced by *Penicillium* sp AMF1a. Five imine derivatives of palitantin were obtained: three hydrazones, one sulfonyl hydrazide, and one oxime in yields of 73.1%, 83.4%, 88.3%, 75.7% and 90.4%, respectively. Several reductive conditions were evaluated. Purification methodologies are currently under optimization prior to assessing the biological activities of these derivatives, including antiplasmodial, anti-*Leishmania* spp., anti-*Trypanosoma cruzi*, antibacterial, and cytotoxic assays. All these results will be presented and discussed.

Financial support: FAPESP, CAPES and CNPq.

Keywords: Semisynthesis, (+)-palitantin derivatives, selective reduction of imine derivatives, fungal metabolite.





EUCALYPTOL BIOTRANSFORMATION USING THE FUNGUS ASPERGILLUS NIGER

Viviane da Silva Lobo^{1*}, Carlos Vinicius de Carvalho Matos¹, Mauricio Ferreira da Rosa²

vivianelobo@utfpr.edu.br

1- COEBB, UTFPR Campus Toledo, Toledo, Paraná, 85902-490, Brazil. 2- Curso de Química, Universidade Estadual do Paraná, Campus Toledo, Toledo, Paraná, 85903-220, Brazil.

Eucalyptol, 1,8-cineole, is the main compound in eucalyptus essential oil and has wide industrial applicability, in addition to its microbiological activities. However, its low chemical reactivity limits its direct use, making the synthesis of derivatives essential to expand its commercial potential and functionality (AZERAD, 2014). Biotransformations have been an alternative to organic synthesis, leading to direct and more sustainable products, and have been gaining more attention in recent years. In this context, the objective of this study was to test the methodology for hydroxylating eucalyptol to produce a derivative with a hydroxyl group in the 2 β or 3 β position, using the fungus *Aspergillus niger*, since traditional organic synthesis methods present challenges in producing them. The medium used for biotransformation was composed of: glucose 10 g L⁻¹, peptone 5.0 g L⁻¹, potassium phosphate bibasic 5.0 g L⁻¹, yeast extract 5.0 g L⁻¹ in 250 mL of distilled water and 100 μ L of eucalyptol PA. The fungi were incubated in this medium under agitation at 200 rpm and 30°C for 7 days (ARRUDA et al., 2018). During this period, daily aliquots were collected and subjected to liquid-liquid extraction with ethyl acetate PA to isolate the product of interest. The aliquots were characterized by Fourier transform infrared spectroscopy (FTIR), and on days 6 and 7, the appearance of a small peak in the 3500 cm⁻¹ range was demonstrated. This result indicates the presence of a hydroxyl group, a group present only in the desired product. Thus, the preliminary data obtained indicate a potential biohydroxylation of eucalyptol with the use of the fungus, however, complete validation requires new processes to confirm the data obtained. The authors thank the institutions CNPq, UTFPR, CA UTFPR TD, and BIOPARK for their support and financial backing for the development of the project.

Keywords: Oxidation, essential oil, 1,8-cineole, alcohol.

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SYNTHESIS OF 2,3-DICARBOXYLATED LUPANES FROM LUPEOL

Lucas Castelão Souza (IC)^{1*}, Mariana Guerra Aguilar (PG)¹, Lucienir Pains Duarte (PQ)¹, Grasiely Faria de Sousa (PQ)^{1*}

*ics2018@ufmg.br, grasielysousa@ufmg.br

¹Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Pentacyclic triterpenes (PTTs) exhibit various biological activities, such as anti-inflammatory and anticarcinogenic properties, as well as protective effects on the cardiovascular, hepatic, and neurological systems.¹ Lupeol, a PTT with a lupane skeleton, stands out for its wide occurrence in plants and significant biological activity. However, its derivatives, despite their therapeutic potential, are found in smaller amounts, which hinders in-depth studies. Structural changes represent a promising strategy to expand research about the impact on the biological activity of these different compounds. Therefore, structural modifications of lupeol were proposed to obtain 2,3-dicarboxylated derivatives in order to further investigate the therapeutic potential of lupeol derivatives, as shown in figure 1.

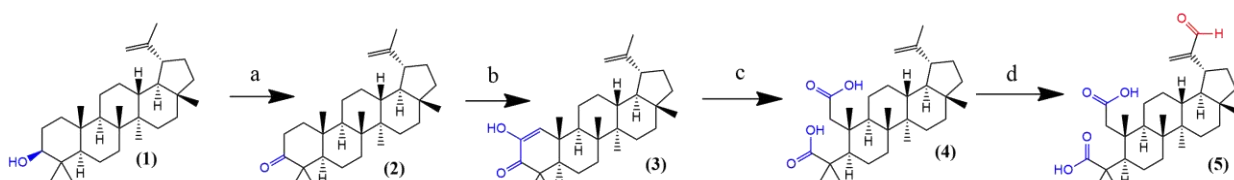


Figure 1: Lupeol structural modifications proposal. Reagents and conditions: (a) CrO₃, H₂SO₄, Acetone, 0°C, 30 min (b) O₂, t-BuOK, t-BuOH, 50°C, 3h (c) H₂O₂, KOH, MeOH, reflux, 100 min (d) SeO₂, EtOH, reflux, 24h

Through NMR experiments, it was possible to monitor the conversions and confirm the formation of the products by comparison with literature data. The synthesis of **2** afforded yields above 85%. The formation of **3** was confirmed by NMR. However, difficulties were encountered during purification, and the crude product was used in the subsequent step without prior purification. In the third step, NMR analysis indicated the formation of **4**, which will be purified and employed in the final step. The results obtained indicate that the proposed synthesis enabled the production of the planned compounds. Despite the absence of the final product, this ongoing study may contribute to adjustments and improvements in the methodology used, aiming for better yields in further trials.

Keywords: Lupeol, A-Seco lupane derivatives, Structural modifications, Triterpenes Pentacyclic

Acknowledgments: CAPES, CNPq, FAPEMIG

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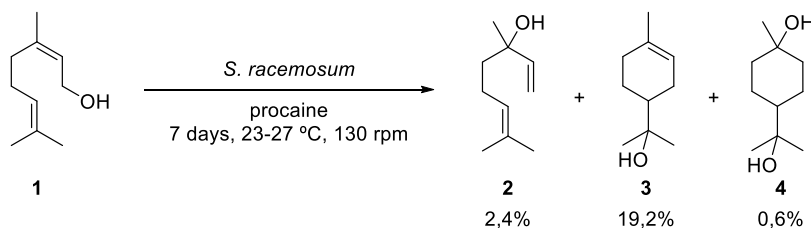
***Syncephalastrum racemosum* BIOTRANSFORMATION UNDER PROCAINE
EPIGENETIC MODULATION OF NEROL LEADS TO α -TERPINEOL**

Laura Lima de Queiroz¹, Jacqueline Aparecida Takahashi¹, Diogo Montes Vidal^{1*}

lauralimadq@ufmg.br, *vidal@ufmg.qui.br

¹Departamento de Química, ICEx, UFMG, Rua Mário Werneck, 2, Belo Horizonte, MG, Brazil

Novel approaches to fungal biotransformation can be a potential strong tool for the acquirement of a wide variety of organic structures. Epigenetics describe modifications in gene expression without alterations in the DNA sequence, and epigenetic modulation is the study of chemical modifications in biosynthetic gene clusters located in inaccessible regions of chromosomes. In this sense, the incorporation of epigenetic modifications to fungal strains under biotransformation processes could help optimize yields and lead to the production of compounds not found in non-modulated processes. Given the importance of monoterpenoids to the flavor and fragrances industry, they are widely employed as substrates for biotransformations. To evaluate the effects of the epigenetic modulator procaine hydrochloride on the biotransformation of nerol (**1**) by the filamentous fungus *Syncephalastrum racemosum*, biotransformation assays were conducted with and without procaine. The assays were performed in triplicate with nerol (**1**) added to grown cultures of *S. racemosum*, under 130 rpm orbital shaking at 23-27 °C. In the epigenetic modulated assays, procaine hydrochloride was added to the culture media during inoculation. After 7 days, the assays were extracted with ethyl acetate and submitted to analyses by gas chromatography coupled to mass spectrometry (GC-MS). Linalool (**2**), α -terpineol (**3**), geraniol, 1,4-mentane-1,8-diol (**4**) were identified as biotransformation products, and there were four unknown products. It was observed that the conversion rate of α -terpineol (**3**) increased from 1,2% to 19,2% in the presence of procaine hydrochloride, while the minor products were obtained between 0,6% and 2,4%. The conversion rates of products without epigenetic modulation did not surpass 6%. Thus, the presence of procaine as an epigenetic modulator not only improved the conversion of products but also made the transformation more selective. These results represent unprecedented data on alterations in the biotransformation pathways of filamentous fungi through the incorporation of epigenetic modifiers.



Keywords: biotransformation, epigenetics, nerol, monoterpenes

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CHEMICAL PROFILE AND BIOLOGICAL EVALUATION OF THE ESSENTIAL OIL FROM *EUGENIA MYRCIANTHES* (MYRTACEAE)

Lucas Ackley Jaime^{1*}, Tainara Aparecida Medina¹, Liza Cristina Gomes Mendonça², Carla Regina Andrighetti², Virgínia Claudia Paulino Silva¹

lucasackley@estudante.ufscar.br

1-Universidade Federal de São Carlos, Centro de Ciências Agrárias, Araras, São Paulo, 13600-970, Brazil. 2-Universidade Federal de Mato Grosso, Campus Universitário de Sinop, Sinop, Mato Grosso, 78556-160, Brazil.

The Myrtaceae family comprises several species recognized for producing essential oils of economic and pharmacological relevance. Within this family, *Eugenia myrcianthes* Nied. is a South American native tree, widely distributed in Brazil, Paraguay, and Argentina, but still poorly studied in terms of phytochemistry and biological activities. In this study, the essential oil from *E. myrcianthes* leaves was extracted by hydrodistillation using a Clevenger-type apparatus for three hours, yielding 0.03% (w/w) based on dry plant weight. The oil was dried over anhydrous sodium sulfate, filtered, and stored at 4 °C in amber vials until analysis. The chemical composition was determined by gas chromatography–mass spectrometry (GC-MS) and gas chromatography with flame ionization detection (GC-FID). More than 95% of the constituents were identified, showing a predominance of sesquiterpenes. The main compounds were germacrene D (23.2%), α -cadinol (10.8%), α -selinene (8.8%), β -elemene (7.3%), (*E*)-caryophyllene (6.8%), and δ -cadinene (5.5%), along with minor constituents such as spathulenol, globulol, and nerolidol. This profile is consistent with other *Eugenia* species, which often contain high levels of bioactive sesquiterpenes. Biological evaluation included cytotoxic assays against human tumor cell lines (HeLa, MCF-7, U-251MG) and non-tumoral fibroblasts (GM07492A), as well as leishmanicidal activity against *Leishmania* (*L.*) *amazonensis* promastigotes and virucidal activity against Mayaro virus (MAYV). The essential oil showed higher cytotoxicity toward fibroblasts ($IC_{50} = 16.6 \pm 2.2 \mu\text{g/mL}$) than toward tumor cells, indicating a lack of tumor selectivity. In antiparasitic assays, the oil exhibited weak leishmanicidal activity ($EC_{50} > 50 \mu\text{g/mL}$) with inhibition below 40%. Virucidal assays also showed low activity, with $17.2\% \pm 4.8$ inhibition of MAYV replication at $13.4 \mu\text{g/mL}$. In conclusion, the essential oil of *E. myrcianthes* is chemically rich in sesquiterpenes and contributes to the scarce phytochemical knowledge of this species. Although the biological activities evaluated here were of low potency and without tumor selectivity, the predominance of bioactive sesquiterpenes suggests that this oil may display stronger effects in other pharmacological models not yet explored. Moreover, since several major constituents (e.g., germacrene D, α -cadinol, (*E*)-caryophyllene) are reported as insecticidal, the oil may also hold potential against agricultural pests such as caterpillars and leaf-cutting ants, warranting further investigations.

Keywords: *Eugenia myrcianthes*; Myrtaceae; essential oil; sesquiterpenes; biological activities





**CHEMICAL DIVERSITY AND BIOLOGICAL ACTIVITIES OF ESSENTIAL OILS
FROM TWO *Cordia* SPECIES**

Izabela Fernanda Francisco^{1*}, Isabel Fernanda Guimarães¹, Letícia Alves Dente², Beatriz Lima Guerra², Carla Regina Andrichetti², Virgínia C. Paulino Silva¹

izabelafrancisco@estudante.ufscar.br

1-Universidade Federal de São Carlos, Araras, São Paulo, 13600-970, Brazil. 2-Universidade Federal de Mato Grosso, Campus Universitário de Sinop, Sinop, Mato Grosso, 78556-160, Brazil.

The genus *Cordia* (Boraginaceae) comprises more than 300 tropical species and is considered promising for pharmacological applications due to its chemical diversity and therapeutic uses. Despite this potential, few species have been investigated in detail, and there is still scarce knowledge about their essential oil (EO) composition and bioactivity. Among them, *Cordia glabrata* Cham. and *Cordia superba* Cham. are South American native trees with limited phytochemical and biological data. This study aimed to characterize the chemical composition of their leaf EOs and to evaluate cytotoxic, antimicrobial, and antiviral activities. Thirty-six compounds were identified in *C. glabrata* (89.7% of the total composition), dominated by hydrocarbon sesquiterpenes (42.2%) and oxygenated sesquiterpenes (35.6%), with selina-11-en-4- α -ol (17.8%), germacrene D (14.6%), δ -cadinene (8.1%), germacrene A (8.0%), and β -elemene (7.0%) as major constituents. In *C. superba*, 31 compounds were identified (95.6%), mainly oxygenated diterpenes (42.8%), oxygenated sesquiterpenes (16.2%), and oxygenated monoterpenes (6.9%), with phytol (42.8%), *n*-hexadecanoic acid (8.4%), and intermedeol (4.8%) as the main components. Comparative analysis revealed clear chemical differences: *C. glabrata* exhibited a sesquiterpene-centered profile, whereas *C. superba* was characterized by a diterpene-rich composition. Biological evaluation showed distinct activity profiles. The EO of *C. glabrata* (OECG) exhibited cytotoxicity against HeLa (IC₅₀ = 39.9 μ g/mL) and U-251MG (IC₅₀ = 42.0 μ g/mL), but low activity against MCF-7 (>100 μ g/mL). The EO of *C. superba* (OECS) displayed moderate cytotoxicity (HeLa IC₅₀ = 55.1 μ g/mL; U-251MG IC₅₀ = 90.5 μ g/mL). Antimicrobial assays indicated weak effects, with MIC values of 250–500 μ g/mL for both oils against *Staphylococcus aureus*, *Candida tropicalis*, and *Fusarium oxysporum*. In antiviral assays, OECG showed the highest virucidal potential, with selectivity index (SI) = 11 for HSV-1 and 12 for MAYV, while OECS showed lower potency (SI = 2 for both viruses). In conclusion, the essential oils of *C. glabrata* and *C. superba* present distinct chemical signatures associated with different biological activities. Although both oils exhibited modest cytotoxic and antimicrobial effects, the promising virucidal selectivity of *C. glabrata* highlights its pharmacological potential, while the diterpene-rich profile of *C. superba*, dominated by phytol, suggests alternative applications that warrant further investigation.

Keywords: *Cordia glabrata*, *Cordia superba*, essential oils, cytotoxicity, antiviral activity





EVALUATION OF THE INHIBITORY ACTIVITY OF SEMISYNTHETIC DERIVATIVES AGAINST HISTONE DEACETYLASE II

Thays Eller Vasconcelos de Lima³, Lucas Inacio dos Santos Ferreira², Ludmila Vieira Moura², Maria Eduarda Caretta³, Heberth de Paula³, Valdemar Lacerda Júnior², Pedro Alves Bezerra Morais*^{1,2}

thayseller22@gmail.com

¹ Programa de Pós-Graduação em Agroquímica, Universidade Federal do Espírito Santo, 29.500-000, Alegre - ES, Brazil; ² Programa de Pós-Graduação em Química, Universidade Federal do Espírito Santo, 29.075-910, Vitória - ES, Brazil. ³ Departamento de Farmácia e Nutrição, Universidade Federal do Espírito Santo, 29.500-000, Alegre - ES, Brazil;

The regulation of gene expression keeping the DNA sequence is related with epigenetic mechanisms. Epigenetic is associated with important physiological processes such as homeostasis, embryonic development, and cell differentiation. Bennett and Licht (2018) described that chromatin consists of a complex of proteins and nucleic acids. When it presents a condensed structure with inactive genes, it is called heterochromatin. On the other hand, euchromatin is characterized by a less condensed organization, allowing genes to be expressed for protein synthesis. The epigenetic mechanisms gene regulated usually involve DNA methylation and post-translational modifications of histones, which are essential regulators of chromatin organization and, consequently, of gene expression. Failures in epigenetic mechanisms lead to disruptions in normal cellular physiology and resulting in the development of several pathologies. Histone proteins play an important role in regulating epigenetic mechanisms, as their profile is targeted by several enzymes that add or remove modifications to these proteins (DE OLIVEIRA, 2012). The proteins responsible for removing acetyl groups are known as histone deacetylases (HDACs). LI et al. (2018) describe that the reduction in acetylation levels caused by anomalous HDAC activity plays a crucial role in carcinogenesis, carrying out gene alteration and, consequently, promoting changes in the cellular phenotype. This work aims the synthesis of twenty semisynthetic triazole derivatives, using isatin, adamantane, monoglycoside and phenolic natural products as building blocks, through Copper(I)-Catalyzed Alkyne–Azide Cycloaddition (CuAAC) “Click” Reaction, and evaluation of inhibitory activity on HDAC using the HDAC-Glo™ I/II system (Promega). The enzyme and substrate/ATP solutions will be prepared in a specific buffer, while the compounds will be solubilized in DMSO at different concentrations. The reactions will occur in 384-well plates, with subsequent addition of ADP-GLO® and Kinase Detection Reagent®, allowing luminescent analysis and determination of IC₅₀ values. The semisynthetic triazole derivatives have already been prepared in a wide range of yield (30-80%) and their structures were confirmed by NMR 1H and 13C analyses. The enzymatic inhibitory activity against HDAC class I/II is on going.

Keywords: Epigenetics, Histones deacetylases, Inhibitory activity, Semi-synthetic products, Triazole compounds





MYRICITRIN ACYLATED DERIVATIVES: ENZYMATIC SYNTHESIS, ADMET PROPERTIES, AND DOCKING STUDIES

Natalie Giovanna da Rocha Ximenes^{1,4*}, Nátalie Tavares Delgado¹, João Pedro Neves de Mello², Paula Alvarez Abreu², Marcelo Mignoni³, Shaft Corrêa Pinto⁴, Michelle Frazão Muzitano⁴, Ivana Correa Ramos Leal¹

natalieximenes@gmail.com

1 - Laboratório de Produtos Naturais e Ensaios Biológicos (LaProNEB), Departamento de Produtos Naturais e Alimentos, Centro de Ciências da Saúde, UFRJ. Avenida Carlos Chagas Filho, 373, Rio de Janeiro, RJ, 21941-599, Brazil. 2 - Laboratório de Modelagem Molecular e Pesquisa em Ciências Farmacêuticas. UFRJ- Campus Macaé, Av. São José do Barreto 764, São José do Barreto, Macaé, RJ, Brazil. 3 - URI, Av. Sete de Setembro, 1621 - Fátima, Erechim - RS, 99709-910, Brazil 4 - Instituto de Ciências Farmacêuticas, Centro Multidisciplinar UFRJ Macaé, Av. Aluizio da Silva Gomes, 50, RJ, 27933-378 - Brasil.

Flavonoids constitute one of the largest classes of secondary metabolites and are notable for their pharmacological properties. However, their applicability is limited due to their hydrophilic nature. The use of lipases for enzymatic acylation of these compounds has resulted in greater stability and solubility. This study aims to perform transesterification reactions using nine vinyl esters with Novozyme®435 followed by the isolation of the products. It also aims to perform their ADMET properties and docking evaluation. Each reaction mixture consisted of 22.5 mg of myricitrin, 4.5 - 11.25 mg of the enzyme (Novozyme® 435 lipase (1531 U/g) (from *Pseudozyma antarctica*) (20-50% relative to the amount of flavonoid), and 1.5 mL of the vinyl ester. Exceptionally, the reaction with vinyl benzoate (40 MI) was carried out for 288 h and 29.93 mg of enzyme. For propionate and pivalate reactions, isopropanol (0.5 mL) was used as solvent. The ionic liquid [C₄mim][BF₄] was used alternatively. The reactions were monitored by TLC and the kinetics were established through the obtained relative area percentages by UHPLC-DAD. The highest conversion percentages to monoesters were reached after 144 h, except for the reaction with vinyl propionate, in which the maximum peak was achieved at 72 h. The products furnished isolated yields of 20.20%, 47.91% and 9.8% for myricitrin benzoate, butyrate, and pivalate, respectively; 27.06%, 47% and 30.2% for myricitrin cinnamate, laurate, and neodecanoate, respectively; and 23.1%, 62.7% and 32.8% for myricitrin decanoate, propionate, and stearate, respectively. The structures of the products were elucidated by NMR and Mass Spectrometry, and their ADMET properties were evaluated using ADMETlab 3.0 and VegaHub softwares. Myricitrin propionate and benzoate showed the highest drug score and drug likeness values, and predicted low toxicity in mammalian cells. Docking studies with the enzyme myeloperoxidase — a target of great biological relevance — are currently in progress, as well as their *in vitro* evaluation. The authors would like to acknowledge CAPES, CNPq, and FAPERJ.

Keywords: ADMET, docking, ionic liquids, lipase, myeloperoxidase





Structural elucidation of unknown byproduct from Marker degradation of diosgenin

Camila Garcia Magalhães¹, Lucas Penha Dutra¹, Lucienir Pains Duarte¹, Diogo Montes Vidal^{1*}

*vidal@qui.ufmg.br

1-NEPLAM - Departamento de Química, ICEx, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil.

Diosgenin is a steroidal sapogenin found in plants, such as those of the genus *Dioscorea*. It is a crucial product for pharmaceutical industry, since it is used as starting material to synthesize several types of steroids, including progesterone, and anti-inflammatory corticosteroids, such as dexamethasone¹. Marker degradation is the first step in the conversion of diosgenin into valuable steroidal derivatives. In the classical method a mixture of diosgenin and acetic anhydride is heated under 200 °C in a sealed vessel for opening the spirostan ring (E and F), furnishing the corresponding pseudodiosgenin, which the corresponding bisacetylenoether of diosgenin acetate. Over the years, several alternatives have been proposed for this reaction employing milder conditions with improved yields. Addition of ammonium chloride and pyridinium chloride is one of most common modifications². However, the role of these reagents and the mechanism of this reaction remain unknown. Here, it is reported the conversion of diosgenin into its bisacetylenoether, along with a previously undescribed side-product. The reaction was accomplished by dissolving diosgenin, ammonium chloride and dimethylaminopyridine in acetic anhydride in 1:1.5:1.5 molar ration. The reaction was kept under reflux overnight. The product was subject to purification by column chromatography, yielding compound **1a** as the major product (67%) and **1b** as a byproduct (9%). They were characterized by FT-IR, GC-MS and ¹H and ¹³H NMR experiments. Compound **1b** was also analyzed by 2D NMR. Based on spectroscopy and spectrometric data analyses, compound **1a** was identified as bisacetylenoether of diosgenin, as supported by literature comparison. A spectroscopy and spectrometric literature review indicates that compound **1b** is novel, and its full structural characterization is in progress. Analyses of 2D NMR spectra revealed no change in rings A, B, and C. Key COSY and HMBC correlations suggest that tetrahydropyran ring (F) remained intact, while ring E had opened.

Keywords: Marker degradation, diosgenin, steroid, spirostan.

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POSTER SESSION ABSTRACT

Session
Chemical Ecology



**SEASONAL INFLUENCE ON PHENOLIC COMPOUNDS OF *Eugenia punicifolia*
ASSESSED BY NMR-BASED METABOLOMICS**

Kidney O. G. Neves^{1*}, Samuel O. Silva¹, Marinildo S. Cruz¹, Francisco Célio M. Chaves², Marcos B. Machado¹, Alan Diego C. Santos³

alandiegormn@gmail.com

1-Central Analítica, Universidade Federal do Amazonas, 69067-005, Manaus, AM, Brazil. 2-Empresa Brasileira de Pesquisa Agropecuária - Embrapa Amazônia Ocidental, 69010-970, Manaus, AM, Brazil. 3-Núcleo de Pesquisa de Produtos Naturais, Universidade Federal de Santa Maria, Santa Maria, RS, 97105-900, Brazil.

Eugenia punicifolia DC., popularly known as “vegetable insulin,” is a medicinal plant native to the Amazon and widely used in traditional medicine for the treatment of type 2 diabetes. Its pharmacological properties are mainly associated with its content of flavonoids and other bioactive phenolics, whose biosynthesis can be modulated by environmental factors. This study investigated the influence of seasonality on the chemical profile of *E. punicifolia* leaf extracts obtained with a methanol:ethanol:water (3:1:1) mixture, using ¹H NMR spectroscopy integrated with multivariate analysis. Samples were collected monthly over a 12-month period, enabling the correlation of metabolic profiles with climatic data (temperature, precipitation, relative humidity, and solar radiation). Principal Component Analysis (PCA) and Partial Least Squares Discriminant Analysis (PLS-DA) revealed groupings corresponding to rainy, dry, and transitional periods, with robust models ($R^2 > 0.85$; $Q^2 > 0.85$). Quercetin, myricetin, gallic acid, catechin, and epigallocatechin were identified as the main seasonal markers. Quercetin production showed a positive correlation with solar exposure ($r = 0.60$) and negative correlations with relative humidity ($r = -0.59$), precipitation ($r = -0.62$), and the number of rainy days ($r = -0.64$). Gallic acid exhibited the opposite pattern, being favored by high humidity ($r = 0.66$), greater precipitation ($r = 0.62$), and more rainy days ($r = 0.74$), while being reduced by increased solar radiation ($r = -0.56$). Catechin and epigallocatechin maintained relatively stable levels, with a slight increase between September and November, the months with the highest average temperature. Our findings suggest one way in which seasonality may modulate the biosynthesis of flavonoids and phenolic acids in *E. punicifolia*, consistent with adaptive responses to environmental stresses such as fluctuations in UV radiation, water availability, and biotic pressure. The integration of NMR-based metabolomics and climatic data proved to be an effective approach for understanding how abiotic factors may influence the secondary metabolism of this species. This study provides a scientific basis for management strategies and the optimization of harvest timing to maximize the pharmacological potential of *E. punicifolia*, thereby contributing to the sustainable use of medicinal plants from Amazonian biodiversity.

Keywords: *Eugenia punicifolia*, metabolomics, NMR, seasonality, flavonoid.





METRONIDAZOLE IN SOIL: IMPACTS ON GERMINATION AND BIOASSIMILATION IN TOMATO (L. esculentum) AND BASIL (O. basilicum)

Gabriela do N. Camargo^{1*}, Débora F. de Andrade¹, Rodolfo S. Barboza¹

camargogabi.97@gmail.com

1- Instituto de Química, Centro de Ciências Matemáticas e da Natureza, Universidade Federal do Rio de Janeiro, 21941-909, Rio de Janeiro – RJ, Brasil.

The presence of emerging contaminants, such as pharmaceutical products (PPs), represents a global concern due to their potential adverse ecological effects and human health risks¹. The release of these compounds into the environment, often through agricultural waste and sewage sludge, can lead to their uptake and accumulation in cultivated plants, thus introducing PPs into the human food chain^{1,2}. Metronidazole (MNZ), a widely used nitroimidazole antibiotic, is a contaminant of interest due to its persistence and capacity to interact with living organisms³. In this study, we investigated the impact of MNZ contamination on the early developmental stages of tomato (*Lycopersicum esculentum*) and basil (*Ocimum basilicum*). Seeds were germinated and specimens cultivated in soils containing MNZ at concentrations of 250, 500, and 750 mg kg⁻¹ and compared to a control group (uncontaminated). Germination and survival rates were evaluated, and the results showed they were similar between the plants in contaminated environments and the control. The ability of both species to germinate and develop even in the presence of the contaminant suggests the existence of tolerance or degradation mechanisms, making them promising for future investigations into detoxification and bioaccumulation. To assess contaminant assimilation, methanolic extracts from roots and aerial parts (stem+leaf) were analyzed by thin-layer chromatography, using a mobile phase of BuOH:CH₃COOH:H₂O (4:1:1,v/v/v), detection was performed under UV light at 254 nm. Through image densitometry, it was possible to semi-quantify the MNZ, confirming its presence in tomato specimens at all levels of contamination and in basil only at the 750 mg kg⁻¹. The results indicated a predominance of the contaminant in the roots, with evidence of its translocation to the aerial parts, demonstrating that root uptake is a key pathway for assimilation. This study highlights the importance of monitoring the presence of PPs in soil and evaluating the risks associated with their uptake by edible plants.

1 Keerthan S, et. al. (2021) *Crit. Rev. Environ. Sci. Technol.* 51, 1221–1258.

2 Pérez-Lucas G, Navarro S (2024) *J. Xenobiot.* 14,1343–1377

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Keywords: Metronidazole, Pharmaceuticals products, *Lycopersisum esculentum*; *Ocimum basilicum*.





A STUDY OF THE VOLATILE ORGANIC COMPOUNDS PRODUCED BY PLANTS OF DROSERA FAMILY

Samuel Henrique de Melo Santos¹, Rafael Rios Ribeiro², Laura Lima de Queiroz¹, Bruna Luiza Marinho Silva², Yumi Oki², Geraldo Wilson Fernandes², Diogo Montes Vidal^{1*}

*vidal@qui.ufmg.br

1- NEPLAM, Departamento de Química, Instituto de Ciências Exatas, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte, MG, Brazil. 2- Instituto de Ciências Biológicas, UFMG, Av. Antônio Carlos, 6627, Belo Horizonte.

Carnivorous plants are a class of plants capable of attracting, capturing, and digesting small animals to obtain nitrogenous compounds, which are essential for the synthesis of chlorophyll and other metabolites. Since they live in nutrient-poor soils, these organisms have developed, over the course of evolution, strategies to capture their prey more effectively, such as the use of chemical attractions and physical traps. Plants of the Droseraceae family are known for having glandular trichomes that secrete a sticky substance capable of capturing their prey and holding them until digestion occurs^[1]. Thus, this work aims to extract and analyze volatile compounds present in the mucilage produced by the tentacles of three species of the Droseraceae family: *Drosera intermedia*, *Drosera graomogolensis* and *Drosera hirtella*. For this purpose, several extraction attempts were carried out, including dynamic headspace, solid-phase microextraction (SPME), manual collection with a capillary tube, and solvent dipping extraction, to identify the profile of volatile compounds present in the plant's excretion as a way to better understand its attraction mechanism. After gas chromatography analysis of the various extraction methods mentioned earlier, the results suggest that *D. intermedia* is the plant with the highest expression of volatile compounds, due to the predominant presence of a naphthoquinone known as plumbagin in its extracts. The other species presented only trace compounds; therefore, it is necessary to develop methodologies to achieve a greater concentration of the compounds in order to carry out proper structural elucidation. As reported in the literature^[2], the compound found in *D. intermedia* may be related to the plant's defense mechanism against predators due to its high redox potential; however, there are no studies on its possible influence as a potential attractant to insects.

Keywords: Droseraceae, Carnivorous plant, Gas chromatography, volatile compounds.

Acknowledgements: CAPES, CNPq, FAPEMIG.

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Volatile Compounds and Enzymatic Activity in the Biocontrol of Yellow Wilt in *Piper nigrum* by *Bacillus velezensis* PN2-45

Lais Sousa Almeida^{1*}, Suzana Kaory G. Inoue¹, Sara Cristine F. de Oliveira¹, Victor Augusto S. Borges¹, Pablo Luís B. Figueiredo², Joyce Kelly R. da Silva¹

lais.almeida@icb.ufpa.br

1-LABITPNA, Laboratório de Bioprospecção e Inovação Tecnológica de Produtos Naturais da Amazônia, ICB, UFPA, R. Augusto Corrêa, 01, Belém, PA, Brazil. 2-Laboratório de Química Dos Produtos Naturais, UEPA, Belém, PA, 66087-670, Brazil.

Black pepper (*Piper nigrum*), an important spice of high commercial value with Brazil and Pará state as one of the world's leading producers. However, its cultivation is severely affected by yellow wilt caused by *Fusarium oxysporum*. In this sense, this study evaluates the potential of *Bacillus velezensis* PN2-45 to control *F. oxysporum* infection in *P. nigrum* plants. Previously, the strain *B. velezensis* PN2-45 inhibited 72.9% of the mycelial growth of *F. oxysporum* in vitro by dual culture assay and the GC-MS analysis identified its volatile compounds reported as antifungal agents, including dodecanal, n-decanal, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-3-buten-2-one, and 2-ethyl-hexanol. *Piper nigrum* cv. Bragantina plants were coinoculated with *B. velezensis* PN2-45 and *F. oxysporum* under greenhouse, and the samples were collected at 3 and 9 weeks after inoculation. Co-inoculation reduced yellow wilt symptoms in *P. nigrum* seedlings, while infected plants exhibited leaf yellowing and premature defoliation. Leaf volatiles included α -muurolol, γ -cadinene, bicyclogermacrene, and *epi*- α -muurolol, whereas root volatiles comprised β -caryophyllene, δ -elemene, camphene, and α -muurolol. The co-inoculation altered the seedlings' volatile chemical profile: the levels of β -caryophyllene were significantly impacted by fungal infection, showing an increase after 3 weeks (from 16.96% to 29.33%) and after 9 weeks (from 19.51% to 33.16%) compared to control. In contrast, co-inoculation led to a significant reduction in β -caryophyllene levels in root samples compared to pathogen-infected seedlings. After 3 weeks, the levels decreased from 29.33% to 21.89%, and after 9 weeks, they reduced from 33.16% to 26.29%. High amount of β -caryophyllene is associated with increased susceptibility to fungal infection, also low levels of this sesquiterpene in vitro (100 ng. μ L⁻¹) promote the faster hyphal growth of *F. graminearum*, suggesting that some pathogens can modulate the host's synthesis of this compound for their own benefit¹. These results suggest that the inhibition of this compound's synthesis by the PN2-45 strain may aid in the biocontrol of yellow wilt. Inoculation with *B. velezensis* PN2-45 stimulated the activity of phenylalanine ammonia-lyase (44.8-60.9 U.mL⁻¹) and the lipooxygenase (4.2-6.5 M.s⁻¹) pathway in leaves after 9 weeks and highly increased the total phenolic content in roots samples, ranging from 3.8 mgEAG.g⁻¹ to 14.79 mgEAG.g⁻¹ after 3 weeks. These results suggest a potential role in resistance induction in *P. nigrum*. In conclusion, the *B. velezensis* PN2-45 strain shows great potential for agronomic applications in the biocontrol of yellow wilt.

Keywords: black pepper, biological control, *Fusarium oxysporum*, antibiosis

¹ Fantaye, C.A., et al. *Journal of Chemical Ecology*, v. 41, p. 213-223. 2015.





**(1R,2S)-GRANDISOIC ACID AS A MALE-SPECIFIC VOLATILE RELEASED BY THE
WEEVIL *Homalinotus coriaceus* (Coleoptera: Curculionidae)**

Sabrina Cruz de Souza^{1*}, João Marcus Rocha Fraga², Daiane Szczerbowski¹, Jacqueline
Aparecida Takahashi¹, Diogo Montes Vidal¹

diogomvidal@gmail.com

¹ Departamento de Química, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil.

² Independent researcher, Itaguaí, RJ, Brazil.

According to the FAO, Brazil is the fourth largest producer of coconut (*Cocos nucifera*) worldwide¹. However, the country still imports these fruits due to losses caused by pathogens and insect pests. *Homalinotus coriaceus* is the most prevalent coleoptera in the southeastern region, where adults bore holes into the floral peduncle, disrupting sap flow and causing the abscission of flowers, fruits, and sometimes entire clusters². Integrating behavioral, biological, and chemical studies for the use of semiochemicals, especially pheromones, offers a complementary approach to cultural and chemical practices, enabling more selective and environmentally sustainable pest management. In this context, the present study aimed to identify the pheromone components of *H. coriaceus* for potential application in integrated pest management programs. Headspace volatile extracts from males and females, obtained via aeration³, revealed two male-specific compounds, which were identified by chromatographic analyses, microderivatizations, and co-injections with synthetic standards using a GC-MS system (EI-Q). The major component was 1-methyl-2-(1-methylethenyl)cyclobutanecarboxylic acid (grandisoic acid), and the minor component was (*E*)-2-(3,3-dimethylcyclohexylidene)acetic acid. Enantioselective gas chromatography confirmed that natural grandisoic acid corresponds to the (1R,2S) stereoisomer. Although these compounds have been reported as aggregation pheromones in other curculionids, this is the first report for *H. coriaceus*. Future bioassays will clarify their role in the species chemical ecology.

Keywords: Gas chromatography, headspace volatiles, pheromones, semiochemicals

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¹ FAO. Crops and livestock products, 2023.

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³ Zarbin *et al.* *Quim Nova*, 22 (2), 1999.





SPATIAL METABOLOMICS REVEALS THE ROLE OF PENICILLIC ACID IN CHEESE RIND MICROBIOME DISRUPTION BY A SPOILAGE FUNGUS

Carlismari Oliveira Grundmann^{1*}, Christopher Tomo², Julia Hershelman², Benjamin Wolfe², Laura Sanchez¹

cgrundma@ucsc.edu

1- Department of Chemistry and Biochemistry - University of California Santa Cruz, UCSC, 1156 High Street, Santa Cruz, CA, USA. 2- Department of Biology, Tufts University, 200 College Avenue, Medford, MA, USA.

Microbial interactions in cheese rinds influence community structure, fermentation, and the development of sensory properties such as flavor, aroma, and texture^{1,2}. However, the chemical mechanisms mediating these interactions in cheeses and other fermented foods remain poorly understood. Here, we investigated how the spoilage mold *Aspergillus westerdijkiae* chemically inhibits beneficial cheese-rind bacteria using microbial community assays, transcriptomics, MALDI-MSI, LC-MS/MS, and genome mining. In cheese rind community and co-culture experiments, *A. westerdijkiae* strongly inhibited bacterial growth, with pronounced effects on *Staphylococcus equorum* and *Brachy bacterium alimentarium*. In co-culture with *S. equorum*, transcriptomic profiling revealed broad changes, including upregulation of a putative *bceAB* gene associated with resistance to antimicrobial compounds. The integration of MALDI-MSI, fungal genome mining, and LC-MS/MS revealed spatially localized production of bioactive metabolites at the fungal–bacterial interface, such as notoamides and circumdatins. Additionally, the mycotoxins penicillic acid and ochratoxin B showed broader spatial diffusion compared to the other metabolites, suggesting their primary role in community disruption. The presence of these mycotoxins was confirmed by LC-MS/MS comparison with commercial standards, with penicillic acid concentrations increasing 2.5-fold in co-culture with *B. alimentarium* compared to monoculture. In contrast, interactions with *S. equorum* did not show the same increase but triggered production of distinct metabolites, such as notoamides, underscoring a partner-specific metabolic response. To validate ecological function, purified penicillic acid was tested in cheese curd agar bioassays. After 10 days of exposure, increasing concentrations (10, 100, 1000 µM) produced progressively stronger inhibition of *B. alimentarium*, with only minor effects on *S. equorum* at these concentrations. These results show that *A. westerdijkiae* deploys a context-dependent arsenal of mycotoxins and indole alkaloids, with responses varying by bacterial partner, suggesting species-specific chemical strategies. Together, our findings show that fungal chemical mechanisms disrupt cheese-rind communities by inhibiting beneficial bacteria, leading to likely negative sensory outcomes with implications for microbial ecology and food safety.

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Keywords: natural rind cheese, fungal-bacterial interaction, mycotoxins, imaging mass spectrometry





UNVEILING THE CHEMICAL AND BIOLOGICAL INTERPLAY OF PHYLLOSTICTA SPP.: INSIGHTS INTO ENDOPHYTIC-PHYTOPATHOGENIC FUNGAL INTERACTIONS IN CITRUS.

Josiel Nascimento Amazonas^{1*}, Taicia Pacheco Fill¹

j272416@dac.unicamp.br, taicia@unicamp.br

1- Laboratório de Biologia Química Microbiana-LaBioQuiMi, IQ, UNICAMP, Campinas, SP, Brazil.

Phyllosticta spp. comprises several fungal species, among which *P. citricarpa* and *P. capitalensis* stand out as antagonists sharing the same citrus host. Citrus Black Spot (CBS), caused by *P. citricarpa*, is responsible for necrotic lesions, premature fruit drop, and severe economic losses in citrus production worldwide. Although some virulence factors have been described, the chemical arsenal of this pathogen remains poorly characterized. In contrast, *P. capitalensis* is a nonpathogenic endophyte frequently reported in the literature for its antagonistic activity against *P. citricarpa*, highlighting its potential role in biocontrol. However, little is known about the molecular basis of this interaction, particularly regarding the Specialized Metabolites (SMs) involved. In this study, the inhibitory potential of *P. capitalensis* against *P. citricarpa* was evaluated in dual-culture assays on potato dextrose agar (PDA). Morphological analysis revealed a significant reduction in pathogen growth, with marked hyphal alterations and an inhibition rate of 67.32%. Metabolites from mono- and co-cultures were extracted with ethyl acetate (AcOEt) and analyzed by LC-HRMS (Orbitrap). Data were processed using MZmine 4.5 for feature-based molecular networking, MetaboAnalyst 6.0 for multivariate statistics, and SIRIUS for propagation of annotation. Annotation propagation in SIRIUS revealed characteristic metabolites of *P. capitalensis*, including 2-pyrone derivatives and guignardone-type meroterpenes. In contrast, *P. citricarpa* exhibited predicted families of modified and glycosylated terpenes. Notably, these same ions contributed most strongly to the separation observed in principal component analysis (PCA), confirming their role as discriminant metabolic features between experimental groups. To validate the production of these metabolites, the endophyte was cultured in three different liquid media (Potato-Dextrose, Czapek and Yeast Broth) for periods of 10, 14 and 21 days. Screening demonstrated that Czapek medium was suitable for the biosynthesis of 2-pyrones and guignardones. To validate the biological relevance of these metabolites, the antifungal activity of the extracts of Czapek obtained at different cultivation times against the phytopathogenic isolate CBS of *P. citricarpa* was evaluated. In the assays performed at 500 and 250 ppm, the 14-day extract showed the highest antifungal activity, with an effect comparable to the positive control (Imazalil). Overall, these results highlight the chemical potential of *P. capitalensis* as a source of bioactive specialized metabolites, provide insights into the metabolic basis of endophyte-pathogen interactions, and point to promising candidates for the development of novel antifungal agents for CBS management.

Keywords: *Phyllosticta*, citrus black spot, endophytic fungi, Citrus.





Microbiome-Guided Discovery of Colletotrichum sp. as an Antagonist of Penicillium italicum in Citrus sinensis Using an Untargeted Metabolomic Approach

José Rodrigo Ferreira Maciel^{1*}, Júlio César Barbosa¹, Paula de França¹, Evandro Aparecido da Silva², Tatiane Maria Malara Cardamoni³, Nelson Arno Wulff³, Roberto Gomes de Souza Berlinck², Taicia Pacheco Fill¹

j231033@dac.unicamp.br e taicia@unicamp.br

1-LaBioQuiMi, Institute of Chemistry, UNICAMP, Brazil. 2-Fund for Citrus Protection, Brazil. 3-University of São Paulo - São Carlos Brazil.

Citrus fruits, such as sweet oranges (*Citrus sinensis*), are highly susceptible to postharvest losses caused by fungal pathogens. Green mold (*Penicillium digitatum*) and blue mold (*P. italicum*) are the predominant decay agents, leading to considerable economic impact. In this study, we employed metagenomics to characterize the microbial communities present on orange peels from healthy fruits and from fruits infected with *P. digitatum* strain Pd1 or *P. italicum* strain PHI-1 (4 days post-inoculation), using 16S rRNA and ITS sequencing. Infection by *P. italicum* resulted in a marked reduction of microbial diversity, with most bacterial and fungal ASVs being suppressed. Within the fungal community, the genus *Colletotrichum* exhibited the most pronounced decrease in abundance. Guided by metagenomic profiling, we isolated 93 cultivable microorganisms from orange peels, including a *Colletotrichum* sp. Furthermore, we performed untargeted metabolomic analyses to investigate the chemical interactions between *Colletotrichum* sp. in association with *P. italicum*. PCA analysis showed a clear trend of separation between groups: co-culture and monocultures. The PCA plot revealed that the quality control (QC) samples clustered closely together, clearly separating from the experimental groups. Additionally, the Random Forest analysis identified 15 variables as key contributors to the discrimination between groups. Furthermore, we used the molecular networking tool of the GNPS online platform to facilitate the metabolic dereplication process. The MS/MS spectral data from the cocultures of wild-type *P. italicum*, and *Colletotrichum* sp., along with their respective monocultures, were integrated into the molecular network, resulting in a total of 3,494 nodes. In co-culture, a significant rise in the relative abundance of *P. italicum*-associated metabolites, including deoxybrevianamide E, brevianamide F, and austamide, was detected. Our results indicate that *P. italicum* modifies the citrus microbiota, leading to a reduction in certain taxa, including fungi of the genus *Colletotrichum*. The isolation of this antagonist, together with metabolomic analyses, revealed an increased abundance of pathogen-derived metabolites as well as the induction of additional compounds during co-cultivation, underscoring the chemical basis of the inhibitory interaction. These findings highlight the chemical basis of fungal interactions and provide insights into potential strategies for postharvest disease control in citrus. **Keywords:** *Citrus x sinensis*, Microbiota, *Colletotrichum*, co-culture, untargeted metabolomics





**POLYSUBSTITUTED BENZENES AS DEFENSE COMPOUNDS OF THE
SPRINGTAIL CERATOPHYSELLA DENTICULATA**

Marc Tschiersch,^{1*}, Anton Möllerke, Stefan Schulz¹

m.tschiersch@tu-bs.de

*1-Institute of Organic Chemistry, Technische Universität Braunschweig, 39106 Braunschweig,
Germany.*

Collembola are soil-inhabiting arthropods and closely related to the Insecta, from which they diverged about 400 mya. It is assumed that Collembola, similarly to insects, use semiochemicals for communication and defensive purposes. However, our understanding of the collembolan chemistry is limited. The primary defense mechanism of Collembola, or springtails, is their ability to catapult themselves out of danger using their furca, a tail-like appendage. However, soil-dwelling or soil-inhabiting species have a reduced or absent furca and rely more on chemical defenses for protection. To learn more about the chemical defenses of *Ceratophysella denticulata*, we utilized a combination of GC/MS and GC/IR, supplemented by synthesis. This approach allowed us to elucidate the structure of a group of novel, highly substituted benzenes. Total synthesis confirmed the proposed structure and enabled us to perform bioactivity assays. These demonstrated a deterrent effect on predatory insects. Although highly hetero-atom substituted benzenes have been reported as natural products in bacteria and marine invertebrates, there have been no previous reports in insects and other arthropods, to our knowledge. The high abundance of these compounds in *C. denticulata* indicates their importance for the springtail. We have identified earlier 4-methoxy-5-(methylthio)benzo[d][1,3]dioxole, 5-ethyl-7-methoxy-6-(methylthio)benzo[d][1,3]oxathiole, and 5,6,7-trimethoxybenzo[d][1,3]oxathiol-4-amine, the latter being the first fully hetero-substituted benzene from nature.

A further, a more detailed analysis of the Collembola contents revealed three additional benzenes. The structure was deduced from HR-MS data, because the concentration was too low for GC/IR analysis. Therefore, a trial-and-error synthetic approach was used. This approach led to the identification of benzo[1,2-d:4,5-d']bis([1,3]dioxole), the obvious precursor benzo[d][1,3]dioxole-5,6-diol, and 7-methoxy-6-(methylthio)benzo[d][1,3]dioxol-4-amine. In summary, the defense system of *C. denticulata* uses a diverse array of benzenes. Whether they also play a role in intraspecies communication, as has been shown for 1,3-dimethoxybenzene, remains unclear.

Keywords: *Substituted benzenes, Collembola, defense, synthesis, mass spectrometry*





Study on the Influence of Temperature and pH on the Secondary Metabolism of *Vibrio coralliilyticus* and *Vibrio shiloi*

Ana Luiza Suhet^{1*}, Jacqueline S. Cruz², Fabiano L. Thompson³, Lidilhone Hamerski¹

1-Instituto de Pesquisas de Produtos Naturais Walter Mors - Universidade Federal do Rio de Janeiro-IPPNUFRJ. 2. Seção de Engenharia Química - Instituto Militar de Engenharia - IME.

3-Instituto de Biologia-Universidade Federal do Rio de Janeiro –IB/UFRJ

analuizasuhet@gmail.com

Coral reefs are among the most complex, diverse, and productive ecosystems on the planet, home to approximately 25% of all marine species. They play a significant economic role, providing goods and services through activities such as fishing, tourism, and coastal protection. However, the survival of coral reefs is under threat due to the decline in reef cover caused by changes in environmental conditions (rising ocean temperatures, sea level rise, deoxygenation, and ocean acidification) and human activities (industrialization, urbanization, agriculture, pollution, and overfishing). These factors place stress on the ecosystem and accelerate processes such as coral bleaching, making corals more susceptible to pathogen infections and mortality. These diseases include bacterial infections. Although the mechanisms of these infections are not yet fully understood, species of the bacterial genus *Vibrio* are considered major agents causing temperature-related diseases in marine organisms. The aim of this study was to investigate the influence of temperature and pH on the secondary metabolism of two species of the genus *Vibrio*, *Vibrio coralliilyticus* and *Vibrio shiloi*, in order to relate it to coral pathogenesis. The *V. coralliilyticus* and *V. shiloi* strains were cultivated in SYP liquid medium (Starch, Yeast, Peptone) at temperatures of 22, 25, and 28°C and at pH 5 and 7, in triplicate, and maintained under agitation for 10 days. An extraction was performed with ethyl acetate, and the organic phase was concentrated using a rotary evaporator to obtain the crude extracts. The samples were analyzed by HPLC using a Phenomenex Luna PhenylHexyl column, with an elution system of acetonitrile and water in a 10–100% acetonitrile gradient. The statistical analysis of the chromatographic data was conducted using the MetaboAnalyst 6.0 platform, based on retention times and peak areas of the chromatographic signals. The analysis of the chromatographic profiles of the crude extracts of *V. coralliilyticus* and *V. shiloi* revealed that changes in temperature and pH in the culture medium can influence the secondary metabolism of both species, potentially affecting the process of coral pathogenesis. The authors thank their institutions for support and acknowledge the financial assistance provided by CAPES, CNPq, and FAPERJ.

Keywords: *Vibrio*, *Vibrio coralliilyticus*, *Vibrio shiloi*, coral bleaching, marine species





CHEMICAL COMPOSITION OF *Physalaemus* FOAM NESTS BY GC-MS: A NEGLECTED BUT RELEVANT DIMENSION?

Jamicelly Rayanna Gomes da Silva^{1*}, Andrés Eduardo Brunetii¹, Norberto Peoporine Lopes¹

*Jamicelly.rayanna@gmail.com

1- University of São Paulo, Ribeirão Preto School of Pharmaceutical Sciences

The Amphibia class contains 8,911 documented species, distributed into three orders: Gymnophiona, Caudata, and Anura. Anurans represent the most diverse order (7,858 species), and their secretions contain specialized metabolites such as peptides, biogenic amines, and alkaloids contributing to several aspects of their biology. Despite their significance, the role of these compounds in reproductive context are little understood. The construction of foam nests by few lineages like those in the family Leptodactylidae stands out, as this reproductive mode provides key functions to embryos including protection against predators, gas exchange regulation, and embryonic dehydration. However, the chemical composition and function of the metabolites present in foam nests have been only partially described. Thus, this study aims to provide a comprehensive characterization of nonpolar metabolites from the foam nests of *Physalaemus* spp. from the Leptodactylidae family. To this end, lyophilized samples of foam nests of four species (i.e., *P. cristinae*, *P. olfersii*, *P. obtectus*, and *P. cuvieri*) were extracted, concentrated, resuspended, and analyze using Gas Chromatograph coupled to a quadrupole Mass Spectrometer (GC-MS). The data generated was analyzed using MZmine 4.7 and Metaboanalyst, and also through manual annotations. Our findings identified that Fatty Acid Methyl Esters (FAME) constitute the most abundant chemical class, with the highest concentration (51.72%) in *P. obtectus*. Free fatty acids are also high concentrations, with considerable variation between species. Strikingly, steroids were also recovered at high levels, suggesting they play crucial functions, likely related to the nest structure. Minor metabolites, such as aldehydes, hydrocarbons, vitamins, ketones, alcohols, and terpenoids, occurred in lower proportions but were consistently found in the nests. Overall, this study represents a unique contribution for understanding the contributions of non-polar metabolites in the structural and functional composition of amphibians' foam nests, possibly mediating embryo protection and foam stability. These findings reinforce the importance of further studies on the ecological and evolutionary role of nonpolar metabolites in anuran foam nests.

Keywords: *Leptodactylidae*; *Physalaemus*; GC-MS.





METABOLOMIC PROFILE OF MARINE BACTERIA CULTIVATED UNDER CONDITIONS THAT MIMIC THE EFFECT OF CORAL BLEACHING

Mariana Rocha^{1*}, Ana Paula Muche Schiavo¹, Bianca Del Bianco Sahm², Leticia Veras Costa Lotufo², Anelize Bauermeister¹

mari_rocha.12@usp.br; anelize@iq.usp.br

1-Instituto de Química da Universidade de São Paulo, Av. Professor Lineu Prestes, 748, São Paulo, SP, Brazil. 2- Instituto de Ciências Biomédicas da Universidade de São Paulo, Av. Professor Lineu Prestes, 2415, São Paulo, SP, Brazil

Coral reefs are extremely diverse ecosystems, essential for the life of countless marine species, and of great economic importance to coastal communities. However, the maintenance of these ecosystems is being threatened by damage caused by the rising of the ocean surface water temperatures and acidification, both reflections of the climate changes caused by global warming. Understanding the impacts of these environmental changes on corals microbiome is essential for finding ways to mitigate the bleaching. Corals harbor a diverse range of microorganisms that form their holobiont, making it essential to investigate how the microbiota and its metabolic products can be affected under stressful environmental conditions. Therefore, this study aims to isolate and cultivate bacteria associated with the coral *Mussismilia hispida*, a coral widely spread in Brazilian coast, in order to investigate the metabolites produced by the associated microorganisms and evaluate the effect on their production under conditions that mimic coral stress, such as variations in temperature and pH. To date, 119 bacteria strains have been isolated based on their morphological aspect, as well as colony color and shape. The investigation of their metabolites production and the taxonomic identification are still ongoing. Metabolite analysis has been performed on an ultra-high-performance liquid chromatography coupled with mass spectrometry (UHPLC-MS), applying an untargeted method. The data will be analyzed in GNPS (Global Natural Products Social Molecular Networking) platform and the microbeMASST tool. The authors thank the support from their institution, the Coordination of Superior Level Staff Improvement (CAPES) for the fellowship, and FAPESP for the grant (process 2024/05211-4).

Keywords: metabolomics, natural products, specialized metabolites, chemical ecology, marine microorganisms.





*Unraveling the Chemical Ecology between *Fusarium* sp. and *Citrus sinensis*: Integrating Genomics, Metabolomics, and Biological Assays*

Mayra Pinheiro^{1*}, Paula de França¹, Daniel Akiyama¹, Júlio Cesar Jeronimo Barbosa¹, Rodrigo Maciel,¹ Leandro Wang Hantao¹, Taicia Pacheco Fill¹.

m234915@dac.unicamp.com

¹State University of Campinas, Institute of Chemistry, CEP, 13083-970 Campinas, SP, Brazil

Brazil, the world's largest producer and exporter of oranges, faces major challenges in its citrus industry due to diseases caused by microorganisms¹. *Fusarium* species, known for producing mycotoxins harmful to human, animal, and plant health, represent a major threat². Recently, we isolated a species responsible for causing irreversible damage to the citrus industry in the Northeast. However, both the disease and the pathogen remain unexplored regarding the chemical and ecological aspects of its secondary metabolism and its role in the pathogen-host interaction. In this study, the pathogen was isolated and subjected to molecular identification. To characterize its biosynthetic potential, complete genome sequencing was performed using the Illumina NovaSeq platform and the genome was assembled using Qiagen CLC Genome Workbench 21.0, with gene cluster analysis performed using fungiSMASH 7.0. To investigate the metabolites involved in host-pathogen interactions, a metabolomics workflow based on untargeted mass spectrometry was applied. Two groups were evaluated at different periods (5, 10, and 15 days): in vitro-inoculated *C. sinensis* plants and healthy plants (controls). In parallel, the same experiment was performed to analyze volatile compounds by solid phase microextraction (SPME) and comprehensive two-dimensional chromatography coupled to quadrupole time-of-flight mass spectrometry (GCxGC-TOFMS). Its biological activity was assessed through antifungal assays and *C. sinensis* seed germination tests. Genome sequencing and assembly resulted in 39 contigs with a total size of 37.28 Mb and a GC content of 48.61%. The fungiSMASH analysis identified 35 Biosynthetic Gene Clusters (BGCs), distributed as follows: 34.29% NRPS, 20% Terpene, 14.29% PKS, 5.71% PKS-Terpene, 8.57% PKS-NRPS, 5.71% Isocyanide, 5.71% RiPP, and 5.71% other compounds. Multivariate PCA analysis revealed a clear discrimination between control and infected plants. In the infected group, a higher abundance of plant defense metabolites was observed, such as phenylalanine (m/z 166.0865) and the flavonoid nobiletin (m/z 403.1388), which has previously been reported as a defense metabolite in citrus. Other compounds were also observed exclusively in infected samples, including peptides, organic acids, and mycotoxins (m/z 338.3417) and (m/z 374.2331). The analysis of VOCs revealed significant differences in the chemical profile between healthy and inoculated plants. The SPME technique coupled with GCxGC-TOFMS enabled the identification of a wide variety of VOCs, highlighting the class of sesquiterpenes. To evaluate the influence of the metabolite m/z 374.2331 (obtained through in vitro extract isolation) on the pathogen-host interaction, we conducted a germination assay to test its phytotoxicity on citrus seeds. The metabolite m/z 374.2331 exhibited a moderate phytotoxic effect at a concentration of 500 ppm and high phytotoxicity at a concentration of 1000 ppm on seed germination. Our biological assays suggest that the metabolite m/z 374.2331 may play a significant role in the virulence of the new phytopathogen. Moreover, the mycotoxin inhibited the growth of endophytic fungi isolated from *Citrus sinensis*, belonging to the genera *Colletotrichum* and *Diaporthe*, with minimum inhibitory concentrations (MIC) of 6.25 ppm and 12.5 ppm, respectively. Thus, the obtained results elucidate key aspects of the chemical ecology in pathogen-host interactions, providing a molecular foundation for future investigations.

Keywords: chemical ecology, citrus, phytopathogen, metabolomics, genomic, interaction, Mycotoxin.

¹Mayra Pinheiro, et al. Microbial Specialized Metabolites in Phytopathogen-Host Citrus Interactions, Annual Review of Microbiology, 2025.

²Munkvold GP, et al. Mycotoxin production in *Fusarium* according to contemporary species concepts. Phytopathol. 2021.

