

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, Lívia 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).

1- Groppo, M. et al. Molecular Phylogenetics And Evolution, 2021. DOI: 10.1016/j.ympev.2020.106971.

Keywords: *Chemophenetic, Conchocarpus, Dryades, Cytotoxicity, Alkaloids*

