10th Brazilian Conference on Natural Products
XXXVI RESEM
4-7 November 2025, Belo Horizonte, MG, Brazil

Section: 05

METABOLOMICS FOR AGRICULTURE APPLICATIONS AND DRUG DISCOVERY

Ana Cláudia Chagas de Paula Ladvocat[1], Paula Carolina Pires Bueno[2], Danielle Ferreira Dias[3], Marisi Gomes Soares[3], **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.*