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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 Garcia[1], Paulinne Moreira Lima[1], Catarina Silva Guimarães[1], Teonildes Sacramento Nunes[2], Danielle Rocha Pinho[3], Norberto Peporine Lopes[3], Gabriel Azevedo de Brito Damasceno[1], Angélica Ferraz Gomes[1], Juliano Geraldo Amaral[1]

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; Passiflors ssp.; MolnetEnhancer; Electrospray; Molecular Networking*