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PHYTOCHEMICAL PROFILING AND NS2B-NS3 DENGUE VIRUS PROTEASE INHIBITION BY Banisteriopsis SPECIES

Jorge Luiz Souza Simão[1*], Isabella Marques do Nascimento[1], Ana Carolina Souza Parreira[1], Jéssica Cristina Amaral[2], Collin Zimmer[3], Tanja Schirmeister[3], Lorena Ramos Freitas de Sousa[4], Vanessa Gisele Pasqualotto Severino[1]

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 Diseasses, 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 λ = 380 nm and an emission of λ = 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 *Banisteriospis* 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*

[1] WHO. Dengue and severe dengue. 2024; [2] Maus *et al*. *Bioorg. Med. Chem*, vol. 47, 116392, 2021; [3] Saqallah *et al*. *Phytochemistry*, vol. 202, 113362, 2022.