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

Section: 01

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

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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