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ANTIOPHIDIC POTENTIAL OF Mimosa gracilis var. capillipes AND Mimosa modesta var. ursinoides: METABOLOMIC AND IN SILICO APPROACHES AGAINST Bothrops AND Crotalus VENOMS

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Snakebite envenomation, recognized by the WHO as a neglected tropical disease (NTD), affects approximately 5 million people worldwide annually, with nearly 1 million reported cases[1]. In South America, the genera *Bothrops* and *Crotalus* are responsible for most envenomation cases. Among their toxins, phospholipase A_2 (PLA_2) plays a central role in inflammatory responses, while proteases contribute to local tissue damage and coagulation disorders. Although antivenom serum remains the primary treatment, it shows limited effectiveness against local damage, highlighting the need for complementary therapies. In this study, ethanolic extracts of *M. gracilis* var. *capillipes* and *M. modesta* var. *ursinoides* collected in Goiás, Brazil, authenticated with numbers 60.375 and 37.079, respectively, and extracted by maceration in ethanol, were investigated. The extracts were subjected to antioxidant activity evaluation (DPPH· method), in vitro antivenom assays-proteolytic, PLA_2, and coagulant inhibition LC-MS/MS, molecular networking via the GNPS platform, and molecular docking. Metabolomic analysis enabled the putative annotation of 77 compounds from various classes of secondary metabolites, including gallic acid, catechin, luteolin, kaempferol, and apigenin, all recognized for their antioxidant and anti-inflammatory properties. *In vitro* assays showed that *M. gracilis* leaf extracts and *M. modesta* root extracts exhibited high antioxidant activity, with EC_{50} values of 1.25 and 3.25 µg/mL, respectively, and complete inhibition (100%) of proteolytic, PLA_2, and coagulant activities at concentrations of 1 mg/mL. The interaction between the extracts and venom proteins was confirmed by SDS-PAGE, with the disappearance of characteristic venom bands. Molecular docking indicated that, among the annotated compounds, six flavonoids exhibited higher predicted binding affinities to PLA_2 (PDB IDs: 1pa0, 3t0r, and 2qog) than rutin, a reference compound with demonstrated *in vivo* antivenom activity[2]. To validate these findings, further in vitro and *in vivo* assays with the six selected flavonoids will be conducted to assess efficacy, toxicity, drug-likeness, and molecular dynamics. This study contributes to advancing the development of complementary therapies to conventional treatment for snakebite envenomation.

Keywords: Antivenom activity, Metabolomics, *Mimosa*, Phospholipase A_2 (PLA_2), Molecular docking, Snakebite envenomation.

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