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PHYTOCHEMICAL INVESTIGATION AND CYTOTOXIC ASSESSMENT OF *Jacaranda caroba*

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The genus *Jacaranda* comprises approximately 49 species distributed across Central America, South America, and the Caribbean. Among them, *Jacaranda caroba*, commonly known as "caroba-do-campo," is traditionally used as a diuretic and for the treatment of syphilis. Its leaves, macerated in sugarcane spirit, are applied topically as a wound-healing agent or ingested for the treatment of ulcers. In this study, a phytochemical prospecting guided by cytotoxicity bioassays was conducted against the tumor cell lines MDA-MB-231 (metastatic breast adenocarcinoma) and A431 (epidermoid carcinoma), as well as the non-tumorigenic mammary epithelial cell line MCF-10, employed for selectivity analysis, using chloroform and methanolic leaf extracts. Chromatographic fractionation of the extracts yielded 11 fractions from the chloroform extract (1–11) and 6 from the methanolic extract (12–17), which were evaluated for cell viability using the MTT assay after 72 h of exposure. Among the samples of the chloroform extract, fraction 6 stood out, which after purification, resulted in the white solid 6.1. These samples presented the lowest inhibitory concentrations. Subfraction 6.1 exhibited IC_{50} values of 2.60 ± 0.003 µg/mL for MDA-MB-231 and 2.45 ± 0.001 µg/mL for A431. Despite the pronounced inhibitory potential, both showed low selectivity (SI ≈ 1.1). Chemical characterization of subfraction 6.1 by infrared spectroscopy and nuclear magnetic resonance revealed the presence of a mixture of uvaol, erythrodiol, and ursolic acid lactone. Fractions 7 and 8 of the chloroform extract, as well as ursolic acid isolated from both extracts, exhibited IC_{50} values around 11 µg/mL with SI ≈ 1.0. Fraction 14 of the methanolic extract emerged as the most active against the MDA-MB-231 cell line, displaying an IC_{50} of 24.17 ± 0.001 µg/mL and SI = 2.8, and its characterization revealed the predominant presence of 3-*O*-acetylursolic acid. Additionally, three pentacyclic triterpenes were isolated, including corosolic acid and a mixture of 3*β*-hydroxy-urs-21-en-28,20*β*-lactone with 3,28*β*-dihydroxy-urs-21-ene, the latter being reported for the first time in the genus. The cytotoxic activity observed was mainly associated with pentacyclic triterpenes, with a possible synergistic effect among compounds. These findings highlight the potential of *J. caroba* as a source of pharmacologically relevant molecules and reinforce the need for further studies aimed at improving selectivity and elucidating mechanisms of action.

Keywords: *Jacaranda caroba, cytotoxic assessment, MDA-MB-231, A431*