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Isolation and characterization of novel limonoids in *Trichilia pallida* (Meliaceae) guided by LC-MS/MS

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The Meliaceae family is widely recognized not only for the quality of its timber but also for its ability to biosynthesize tetranortriterpenes (limonoids), a class of secondary metabolites that exhibit a broad spectrum of biological activities, including insecticidal, bactericidal, antifungal, and anticancer properties. Several genera within this family have been extensively investigated owing to the bioactive potential of their constituents, with particular emphasis on *Melia* L., *Toona* (Endl.) M. Roem., *Azadirachta* A. Juss., and *Trichilia* P. Browne[1,2]. In the present study, an analytical strategy was established based on the monitoring of diagnostic ions in tandem mass spectrometry (MS/MS) fragmentation spectra, with the aim of identifying putative limonoids and guiding the selection of *Trichilia pallida* extracts and fractions for metabolite isolation. All extracts and fractions were analyzed by ultra-high-performance liquid chromatography (UHPLC) coupled with high-resolution mass spectrometry (HRMS). MS/MS spectra displaying diagnostic ions were employed to direct fraction collection by high-performance liquid chromatography (HPLC), with monitoring at 215 nm. This approach enabled the isolation and structural elucidation—through one-dimensional (1D) and two-dimensional (2D) nuclear magnetic resonance (NMR) spectroscopy—of eleven limonoids and two norlimonoids. Three isolated limonoids were further evaluated for their cytotoxic potential using the MTT assay against the MRC-5 (non-tumoral), A549 (lung cancer), A2780 (ovarian cancer), and B16F10 (murine melanoma) cell lines. Notably, promising activity was observed against B16F10 cells, in which the limonoids induced the expression of the *Caspase-3* gene, a key effector directly associated with apoptosis. Collectively, these results underscore the potential of limonoids as lead candidates for the development of novel antitumor agents, highlighting their relevance as promising scaffolds in oncological drug discovery.

Keywords: *Limonoids, mass spectrometry, molecular network.*

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