



FIRST REPORT OF THE ISOLATION AND CHARACTERIZATION OF ENT-16 α ,17-DIHYDROXY-KAURAN-3-ONE FROM *EUPHORBIA TIRUCALLI* LEAVES (EUPHORBIACEAE)

Anndreisa Christiny Monteiro^{1*}, Simone Grecco dos Santos¹, Patricia Sartorelli¹

anndreisa.monteiro@unifesp.br

1- Instituto de Ciências Ambientais, Químicas e Farmacêuticas, UNIFESP, 09972-270, Diadema-SP, Brasil.

Euphorbia tirucalli is a species belonging to the Euphorbiaceae family, popularly known as aveloz¹. It is a plant widely used in folk medicine to treat various diseases, due to its numerous reported medicinal properties². To contribute to the phytochemistry from the genus *Euphorbia*, the present study aims to isolate and identify the chemical constituents from *E. tirucalli* leaves. The leaves of *E. tirucalli* were collected from the medicinal garden of the Eldorado campus of UNIFESP, followed by drying, grinding, and extraction until exhaustion with *n*-hexane and, subsequently, with methanol. The methanolic extract was subjected to a liquid-liquid partition procedure with *n*-hexane, DCM and EtOAc, to afford its respective partition phase fractions. The dichloromethane phase was fractionated on a silica gel column, with DCM/EtOAc, with an increasing polarity gradient, obtaining 18 fractions. Fractions ET-C8 to ET-C11 were combined and subjected to a new chromatographic fractionation with the same previous conditions, and at subfraction 21 was possible to observe a pure compound. The compound was analyzed by UHPLC-DAD-ESI-QTOF-HRMS/MS, ATR-FTIR, and NMR (¹H, ¹³C, DEPT 135, HSQC and HMBC), to perform its complete chemical characterization. The MS spectra displayed ions with *m/z* 321.2418 [M+H]⁺, 303.2316 [M-H₂O+H]⁺ and 285.2218 [M-2(H₂O)+H]⁺, corresponding to C₂₀H₃₂O₃ molecular formula. The ¹H and ¹³C NMR spectra revealed signals corresponding to a kaurane diterpene derivative, evidenced by the characteristic signals at δ_H 2,46 (t, *J*= 14,8 Hz, H-2) and δ_H 3,51 (q, *J*= 10,7 Hz, H-16 e H-17), and at δ_C 79,80 (C-O; C-16), δ_C 70,00 (CH₂OH; C-16) and δ_C 218,3 (C=O). The presence of carbonyl was only confirmed in HMBC and at ATR-FTIR spectrum with an absorption band at 1700 cm⁻¹, characteristic of a ketone carbonyl group. After comparing the experimental data with the literature, it was possible to confirm the identification of the compound as *ent*-16 α ,17-dihydroxy-kauran-3-one, being the first time reported at *Euphorbia tirucalli*.

Keywords: *Euphorbia tirucalli*, Kaurane diterpene, chemical characterization, chromatographic isolation

References:

- [1] SALEHI, B. et al. *Euphorbia-Derived Natural Products with Potential for Use in Health Maintenance* *Biomoléculas* 2019, 9(8), 337; <https://doi.org/10.3390/biom9080337>
[2] HIROTA, B. C. K. et al. *Phytochemistry and biological activities of the genus Jatropha: Mini-review*. *Visão Acadêmica*, Curitiba, v.11, n.2, p.103-112, 2010.

