

FURANOHELIANGOLIDES FROM *Calea parvifolia* (ASTERACEAE)

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Abstract: Chemical studies on *Calea* have revealed the occurrence of sesquiterpenes, sesquiterpene lactones, as well as of thymol, benzofurans and hydroxyacetophenone derivatives as secondary metabolites. In order to contribute with studies on the *Calea* genus, in this work we report the chemical investigation of aerial parts of *C. parvifolia* (DC.) Baker. The plant material was collected in Ponta Grossa, Parana State, air-dried and extracted with methanol. The methanol extract (24.7 g) was dissolved in MeOH:H₂O 1:1 and partitioned into *n*-hexane, dichloromethane and ethyl acetate. The dichloromethane fraction (2.7 g) was submitted to successive flash column chromatography to afford the pure compounds **1** (6.0 mg), **2** (3.0 mg) and **3** (60.0 mg), and the mixtures of **1** and **4** (68.0 mg), and **5** and **6** (10.0 mg). The structures of isolated compounds (Figure 1) were elucidated by analysis of their one and bi-dimensional NMR data, and comparison with those described in the literature.¹⁻³ The isolated compounds were analyzed by electrospray ionization tandem mass spectrometry (ESI-MS/MS) using a triple quadrupole mass spectrometer. The main ions observed for **1-2** are the fragments at *m/z* 259, 213 and 185, and for **3-4**, the fragments at *m/z* 261, 215 and 187, which corresponds to the initial loss of the acyloxy group at C-8, and subsequent loss of H₂O and/or CO, respectively, from the protonated compounds.⁴ Compounds **5** and **6** that have the tetrahydrofuran-3-one unit, showed two predominant fragments at *m/z* 201 and 229 relative to the loss of [M+H-(C₁₄H₁₇O)]⁺ and [M+H-(C₁₅H₁₇O₂)]⁺, respectively. The analysis revealed that the losses at *m/z* 69 and 71, relative to methacryloxy and isobutyryloxy groups, respectively, are predominant fragmentation processes in the compounds **1-6**.

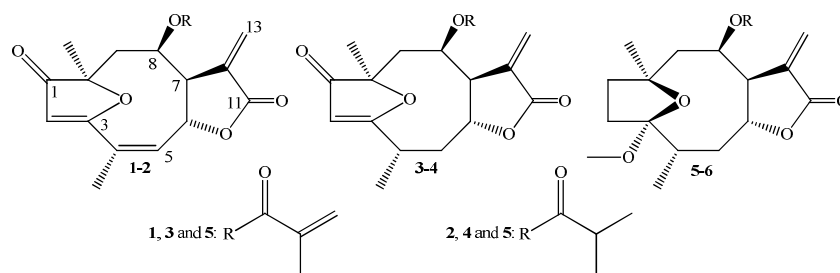


Figure 1. Chemical structures of the compounds **1-6** isolated of *Calea parvifolia*

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