

Área: ORG

Expanding the Chemical Profile of *Campovassouria cruciata* (Asteraceae)

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Highlights

Expanding the Chemical Profile of *Campovassouria cruciata* (Asteraceae). Seven known metabolites isolated from *C. cruciata*. UHPLC–HRMS/MS dereplication via GNPS 2.0. Expanded chemodiversity of *C. cruciata*.

Abstract

Continuing our investigation of Asteraceae from the Campos Gerais region (Paraná, Brazil), we selected a species of the genus *Campovassouria* for phytochemical study. This genus comprises only two species, and *Campovassouria cruciata* has been previously investigated, mainly revealing terpenes, especially diterpenes. More recently, a sesquiterpene lactone was isolated from specimens collected in Minas Gerais, Brazil. The aim of this study was to characterize the chemical composition of the aerial parts by classical fractionation and dereplication workflows. Chromatographic separations on silica gel and Sephadex LH 20 afforded seven known compounds. Their structures were elucidated by comparison of 1D/2D NMR data with literature values. Compounds **1** to **3** are kaurane-type diterpenes: *ent*-kauronic acid (**1**), grandifloric acid (**2**), and 17-Hydroxy-*ent*-kaur-15-en-19-oic acid (**3**). Compounds **4** and **5** were identified as umbelliferone (a coumarin, **4**) and rutin (a flavonoid, **5**). Compounds **6** and **7** were characterized as quinic acid derivatives: chlorogenic acid (**6**) and 3,5-*O*-dicaffeoylquinic acid (**7**). Ultra-high-performance liquid chromatography coupled with high-resolution tandem mass spectrometry (UHPLC–HRMS/MS), processed through the Global Natural Products Social Molecular Networking platform (GNPS2) and visualized in Cytoscape, enabled the putative identification of three kauranes, four coumarins, and three quinic acid derivatives (**Figure 1**). Although this species has been previously investigated, we expand its chemical profile by reporting additional metabolites. Except for *ent*-kauronic acid and umbelliferone, all other metabolites are reported from *C. cruciata* for the first time, underscoring the species' potential as a source of bioactive natural products.

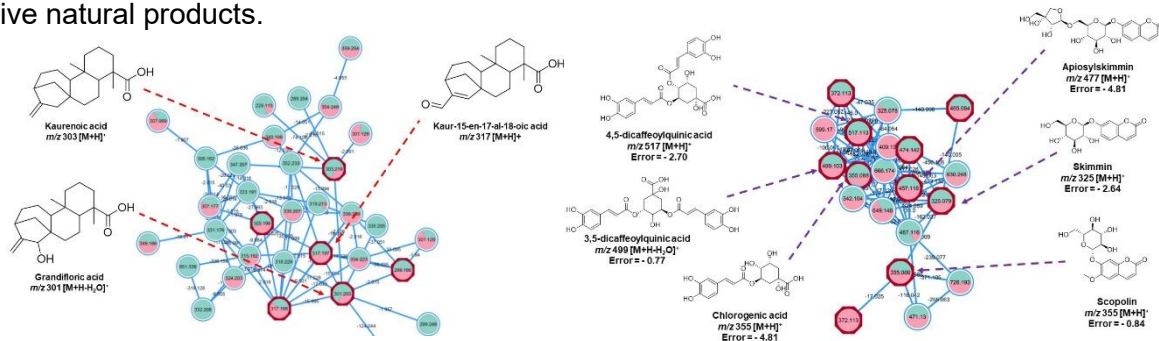


Figure 1: Molecular networking of the crude extract (blue nodes) and ethyl acetate fraction (pink nodes) of *C. cruciata* analyzed by UHPLC-HRMS in positive mode.

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