

Área: ORG

A novel sesquiterpene lactone from *Disynaphia littoralis*

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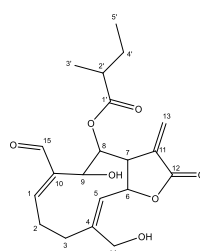
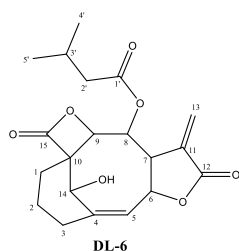
Palavras Chave: Asteraceae, flavonoids, quinic acid derivatives, dereplication.

Highlights

A novel sesquiterpene lactone from *Disynaphia littoralis*. Five known metabolites isolated from *D. littoralis*. Ten compounds identify by UHPLC–HRMS/MS dereplication. Expanded chemodiversity of *D. littoralis*.

Abstract

An important class of specialized metabolites frequently isolated from the *Disynaphia* genus is sesquiterpene lactones. This genus includes 14 species, of which only three have been previously studied: *D. filifolia*, *D. multicrenulata*, and *D. halimifolia*. In addition to sesquiterpene lactones, these species have also been reported to produce flavonoids, benzofuran derivatives, and terpenes. This work aimed to investigate the chemical composition of the aerial parts of *Disynaphia littoralis*, a species native to the Campos Gerais region in Paraná State, Brazil, using classical fractionation techniques combined with dereplication workflows. Chromatographic separations on silica gel and Sephadex LH 20 yielded five known triterpenes and one novel sesquiterpene lactone. The structures of the compounds were elucidated through comprehensive analysis of 1D and 2D NMR data, supported by comparisons with published spectroscopic values. The triterpenes were identified as lupeol (DL-1), α -amyrin (DL-2), β -amyrin (DL-3), taraxerol (DL-4), and pseudo taraxasterol (DL-5). Compound DL-6 was obtained as a colorless oil, and its molecular formula was established as C₂₀H₂₄O₇, based on the ion peak observed at m/z 377.1598 [M+H]⁺ (calcd. m/z 377.1595 [M+H]⁺) in the UHPLC–HR–MS/MS. The NMR spectrum revealed characteristic signals corresponding to a germacranolide-type skeleton, similar to a sesquiterpene lactone previously isolated from *D. halimifolia*. However, DL-6 differed structurally by the presence of an isopentyloxy substituent at C-8 (Figure 1). Ultra-high performance liquid chromatography coupled with high-resolution tandem mass spectrometry (UHPLC–HRMS/MS), processed through the Global Natural Products Social Molecular Networking (GNPS2) platform and visualized in Cytoscape, allowed the putative identification of two quinic acid derivative, caffeoylquinic acid (DLMN-1) and dicaffeoylquinic acid (DLMN-2); three flavonoids, eupafolin (DLMN-3), hispidulin (DLMN-4), and quercetin (DLMN-5); two monoterpene lactones, loliolide (DLMN-6) and dihydroactinidiolide (DLMN-7); two sesquiterpenes, caryophyllene epoxide (DLMN-8) and α -cyperone (DLMN-9); and finally, a germacranolide-type sesquiterpene lactone (DLMN-10) with a structure similar to that of DL-6 (Figure 1). Among the identified metabolites, eupafolin (DLMN-3) and hispidulin (DLMN-4) were previously isolated from *D. littoralis*. All other compounds are being reported for the first time in this species. This study reinforces the importance of investigating Asteraceae species endemic to the Campos Gerais region of Paraná and highlights their potential as a source of structurally unique and biologically relevant specialized metabolites.



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