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PHYTOCHEMISTRY OF MOQUINIASTRUM SORDIDUM: GNPS-GUIDED DEREPLICATION, TWO NEW METABOLITES, AND STEREOCHEMICAL ELUCIDATION USING IPAP/PIP-HSQMBC

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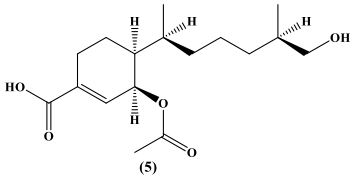
Recent taxonomic revisions based on molecular phylogenetics transferred species from *Gochnatia* to *Moquiniastrum*, which now includes 22 species, 19 in Brazil's Cerrado and Atlantic Forest. Here, we report a phytochemical study of *Moquiniastrum sordidum*. The plant was extracted with ethanol, yielding a crude extract partitioned into hexane, dichloromethane, ethyl acetate, and hydromethanolic fractions. Dereplication was performed using UHPLC-HRMS with molecular networking. Chromatographic separation afforded nine compounds, including two new metabolites: a sesquiterpene (**5**) and a phenolic glycoside (**8**). Known compounds identified were simiarenol (**1**), oleanolic acid (**2**), hispidulin (**3**), tyrosol (**4**), genkwanin (**6**), and apigenin (**7**). The relative configuration of compound **5** was established using *pip*-HSQMBC-IPAP NMR, which afforded accurate long-range $^{2,3}J_{CH}$ coupling constants. With four stereogenic centers, conformational searches (CREST) followed by DFT calculations (ORCA) were performed. Comparison between Boltzmann weighted theoretical parameters and experimental data enabled assignment of the absolute configuration as 1*R*, 6*S*, 7*S*, 11*R*. Dereplication enabled the putative identification of 45 metabolites: 12 flavonoids, 10 chlorogenic acid derivatives, 5 hydroxycinnamic acid derivatives, 9 terpenes, and 9 others. Manual inspection of fragmentation patterns, supported by GNPS2 tools, facilitated recognition of structural families within the molecular network. Preliminary cytotoxic screening against HCT-116 cells showed that the dichloromethane fraction inhibited proliferation by 92% at 50 µg/mL, while activity dropped below 50% at 5 µg/mL.



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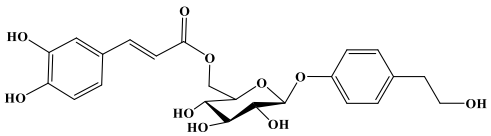

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Keywords: *Moquiniastrum sordidum, Gochnatia sordida, dereplication, diagnostic fragment ions.*