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ANOTATION OF IRIDOIDS AND SECO IRIDOIDS IN KUTCHUBAEA INSIGNIS AND FERDINANDUSA HIRSUTA (RUBIACEAE)

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Iridoids are a class of secondary metabolites with biological potential that are reported in several plants. In the Rubiaceae species, they are mainly reported in the Ixoroideae subfamily, which includes plants of the *Kutchubaea* and *Ferdinandusa* genera, for which there are very few reports of phytochemical studies. Considering this gap, the objective of this study was to investigate the chemical constituents of these species. Initially, we performed a clean-up step using a Sep-Pak C18 (2 g/12 mL) on methanolic extracts from leaves, branches, and fruits that were analyzed by liquid chromatography coupled to mass spectrometry (LC-MS), with fragmentation (MS2) spectra converted to mzML format for molecular network analysis on the GNPS2 platform. To create the network and library match, it was set a minimum 0.50 cosine between the spectral library and the ions, a tolerance of 0.02 was used between the fragment ions and the precursor ions because the experiments were acquired on a high-resolution spectrometer. To verify the annotations, the fragmentation patterns were checked manually. Of the metabolites annotated in these species, eight iridoids were putatively identified: genipin, monotropein methyl ester (galioside), geniposide, sweroside, epivogeloside, secologanin, swertiamarin, and secologanin 7-methyl ester. Furthermore, molecular network analysis revealed that each species had unique biosynthesis for each subclass of these iridoids, since iridoids were annotated in *Kutchubaea insignis* and seco iridoids in *Ferdinandusa hirsuta*. These results demonstrated the potential for isolating these iridoids in these species. The authors would like to thank the funding agencies FAPEAM, CAPES, CNPq, and FINEP for their financial support, and CA-LTQPN/INPA for the mass spectrometry analyses.

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