

## ***CHEMICAL PROFILING OF *Picramnia sellowii* (PICRAMNIACEAE): UHPLC-QToF-MS/MS EVIDENCE FOR QUASSINOIDES***

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The family Picramniaceae currently comprises the genera *Picramnia*, *Alvaradoa*, *Nothotalisia*, and the recently described genus *Aenigmanu*, which has not yet been included in the family clade recognized by the Angiosperm Phylogeny Group (APG) (THOMAS et al., 2021). Picramniaceae was segregated from Simaroubaceae, where it was previously classified as the subfamily Picramnioideae. Simaroubaceae is characterized by the presence of quassinoids, which led to the exclusion of the genera belonging to Picramniaceae, as species of this family contain anthraquinones that have not yet been reported in any other group of Simaroubaceae. Until recently, there was no chemical evidence to support the classification of Picramniaceae within Simaroubaceae or in close relationship to taxa associated with Rutaceae and Meliaceae. However, recent investigations have revealed several nortriterpenes with limonoid-like skeletons, as well as the annotation of quassinoids in the genus *Picramnia* (GIMENES et al., 2020; SILVA et al., 2022). Considering the morphological relationship of *Picramnia* with Simaroubaceae, the present study also aimed to explore the chemical diversity of *Picramnia sellowii* and evaluate whether quassinoids were produced in low concentrations. Ethanolic extracts of *P. sellowii* leaves and fractions obtained by SPE column purification (fractions F1–F4) were analyzed by untargeted UHPLC-QToF-MS/MS. The resulting data were processed, deconvoluted, and compared with spectral libraries such as METLIN, GNPS, Fiehn/Vaniya Natural Products Library, and BMDMS-NP for quassinoid annotation. In fraction F2, five quassinoids were annotated in *P. sellowii*, including quassin ( $C_{22}H_{28}O_6$ ;  $m/z$  [M+H]<sup>+</sup> 389.1953,  $m/z$  [M+Na]<sup>+</sup> 411.1776). Efforts are currently being directed toward the isolation of these compounds. This study revealed that the chemical evidence is consistent with the traditional classification of *Picramnia* within Simaroubaceae. The authors thank their institutions for support and CAPES and INCT-CBIP for financial assistance.

**Keywords:** Quassinoids, Picramniaceae, *Picramnia sellowii*, chemosystematic, mass spectrometry, metabolomics

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