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Chemical comparative study of *Byrsonima verbascifolia* (L.) DC and *Byrsonima sericea* DC and its flavonoids by molecular networking

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The genus *Byrsonima*, popularly known as murici, is widely used in folk medicine due to its anti-inflammatory and anti-ulcer activities, which justify its traditional use in the treatment of gastrointestinal disorders. Species of this genus frequently contain flavonoids derived from quercetin, proanthocyanidin derivatives, galloylquinic acid derivatives, and amentoflavone. However, some species of *Byrsonima* are considered neglected, meaning their industrial, nutritional, and chemical potential has been little explored. This is the case of *Byrsonima verbascifolia* and *Byrsonima sericea*, two species whose chemical arsenal remains poorly studied. One approach for evaluating the chemical profile of plants is the use of liquid chromatography coupled with mass spectrometry. Chromatographic peak areas and fragmentation profiles obtained by HPLC-ESI-IT-MS/MS can be processed in GNPS (Global Natural Products Social Network) to construct molecular networks, a resource that allows the visualization of structural relationships among detected compounds. In this way, it was possible to generate and compare the networks of hydroethanolic leaf extracts of *B. verbascifolia* and *B. sericea*, highlighting the diversity and relative abundance of their secondary metabolites. The molecular network comprised 57 nodes, with 32 indicating molecules exclusive to *B. verbascifolia*, 12 to *B. sericea*, and 13 shared between both species. Two clusters were formed, corresponding to the classes of terpenes and flavonoids. The terpenes identified included myrcene (m/z 159) and ebelactone and its derivatives. The main class of metabolites identified was flavonoids, particularly glycosylated quercetin derivatives, characterized by the aglycones at m/z 301 (quercetin), m/z 299 (diosmetin), and m/z 300 (peonidin), followed by the loss of sugars: -132 Da for pentoses ($-Xyl$, $-Ara$), -146 Da for deoxyhexoses ($-Rha$), -162 Da for hexoses ($-Glu$), or the loss of galloyl groups (-152 Da). The results are consistent with what is expected for the genus, as other *Byrsonima* species, such as *B. crassa*, *B. intermedia*, and *B. fagifolia*, have been reported to contain diverse glycosylated and galloylated quercetin derivatives. However, no reports of diosmetin or peonidin derivatives have been made in the genus. The data indicate a greater chemical diversity and molecular abundance in the hydroethanolic leaf extracts of *Byrsonima verbascifolia*, especially flavonoids, which may account for the biological activity of the extract, since both quercetin and diosmetin derivatives exhibit strong anti-inflammatory potential.

Keywords: *Byrsonima verbascifolia*, murici, GNPS, molecular networking, flavonoids.



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