



CHEMISTRY AND CHEMOTAXONOMY OF Barnadesioideae, THE ANCESTRAL CLADE OF Asteraceae. NEW INSIGHTS FROM THE METABOLIC FINGERPRINT OF SOME *Dasyphyllum* spp.

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Abstract: The species of the subfamily Barnadesioideae (Asteraceae) comprise a monophyletic group with more than 90 species entirely restricted to South America. Barnadesioideae constitutes the basal clade of Asteraceae as demonstrated by phylogenetic studies based on morphology and DNA [1]. Previous reports describe Barnadesioideae as a group of plants with “simple” phytochemistry [2,3]. Therefore our efforts were directed to update the current phytochemical knowledge of Barnadesioideae by constructing a chemical database. The *AsterDB-Barnadesioideae* is a small database embedded in a larger project, the AsterDB, an in-house database of the AsterBioChem research group (<http://www.asterbiochem.org>) exclusively dedicated to the chemistry of the sunflower family. *AsterDB-Barnadesioideae* is offered as a SDF archive where chemical structures are displayed as .mol, .smiles, .inchi and .inchikey file formats (MarvinSketch 15.3.9, ChemAxon Ltd). It also contains essential spectrometric (molecular and monoisotopic mass) and spectroscopic (¹H- and ¹³C-NMR) data of secondary metabolites reported so far in Barnadesioideae. A benzaldehyde, a benzoic acid, a coumarin, two simple acetophenones, 13 flavonoids (glycosides of kaempferol, quercetin and isorhammetin) and 21 triterpenoids (taraxasterol, lupeol, ursane and oleanane derivatives) have been described in 45 species of Barnadesioideae. Triterpenoids and flavonoids constitute almost ubiquitous constituents in Asteraceae. Bohm and Stuessy (1995) describe the phytochemical profile of Barnadesioideae as follows: ‘...no other major taxon within the Asteraceae has such a consistently simple pigment profile...’. This character is suggested to be associated with the basal position of Barnadesioideae inside Asteraceae [3], and could be supported by the similar flavonoid profile between Barnadesioideae and Calyceraceae (sister group to the Asteraceae) [4]. These observations can be reproduced by comparing Calyceraceae and Barnadesioideae with more derived taxa, e.g., Espeletiinae, *Smallanthus* and *Ichthyothere*, demonstrating that even a simple phytochemistry exhibits chemotaxonomic relevance. Additionally, a preliminary HPLC-DAD metabolic fingerprint analysis of some *Dasyphyllum* species (Barnadesioideae) showed the presence of caffeic acid ester derivatives in polar extracts. The occurrence of caffeoyl derivatives is frequently reported in Asteraceae but no report in Barnadesioideae could be found so far. Therefore, these compounds may constitute an early diversifying group of metabolites that have remained constant through time within the Asteraceae family. The isolation and structure elucidation of these secondary metabolites in *Dasyphyllum* spp. and other Barnadesioideae species will be part of further communications.

References:

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