# A comprehensive metabolite profiling of Isatis tinctoria leaf extracts



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**Author(s)** Mohn, T.; Plitzko, I.; Hamburger, M.
**Author(s) at UniBasel** Hamburger, Matthias ;
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A broad-based characterisation of a pharmacologically active dichloromethane extract from Isatis tinctoria leaves was carried out. For a comprehensive picture we also included the polar constituents of I. tinctoria (MeOH extract) and for comparative purposes, the taxonomically closely related plant I. indigotica. Diode array detector, evaporative light scattering detector, atmospheric pressure chemical ionisation and electrospray ionisation mass spectrometry, and electrospray ionisation time-of-flight mass spectrometry detectors were used in parallel to ensure a wide coverage of secondary metabolites with highly diverging analytical properties. Off-line microprobe nuclear magnetic resonance spectroscopy after peak purification by semi-preparative high-pressure liquid chromatography served for structure elucidation of some minor constituents. More than 65 compounds belonging to various structural classes such as alkaloids, flavonoids, fatty acids, porphyrins, lignans, carotenoids, glucosinolates and cyclohexenones were unambiguously identified, and tentative structures were proposed for additional compounds. Numerous compounds were identified for the first time in the genus Isatis, and an indolic alkaloid was discovered.
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