B043 Quantitative analysis of metabolite profiling of root extracts from *Lithospermum erythrorhizon*

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The root extracts of *Lithospermum erythrorhizon* has been used as by itself or in combination with other herbal extracts for wound healing, anti-inflammation, anti-infection and as a dye for staining textiles and pigment for food coloring. Shikonin, the red naphthoquinone pigment, and acetylshikonin have been identified as the bioactive principles in *L. erythrorhizon*. However, a quantitative metabolite profiling analysis of *L. erythrorhizon* root extracts has not yet been reported. In nutraceutic and pharmaceutic point of views, it is important to develop an optimal and reproducible extraction procedure as well as quantitative methods for analyzing index and/or active compounds in order to best quality control in herbal manufacturing. In this paper, we demonstrated that using *n*-hexane as extraction solvent and under optimized extraction conditions the yield of root extract reached approximately 4% (weight/dry weight of root tissues). Thin-layered chromatography, high performance liquid chromatography, IR, and 1D- and 2D-NMR were performed in this study to analyze and identify the compound profile of root extract of *L. erythrorhizon*. In addition to shikonin, we have obtained seven shikonin derivatives, namely acetylshikonin, β-acetoxyisovaleryshikonin, isobutyrylshikonin, β,β-dimethylacrylshikonin, isovalerylshikonin, β-hydroxy-isovalerylshikonin, and deoxyshikonin. The contents of shikonin, acetylshikonin, β-acetoxyisovaleryshikonin, isobutyrylshikonin, β,β-dimethylacrylshikonin, and isovalerylshikonin in the total root extract were 1%, 6%, 5%, 19%, 10%, and 12% (w/w), respectively, as determined using HPLC analysis. These compounds are potentially good candidates as the referencing/index compounds of root extract of *L. erythrorhizon* and four out of the six compounds are first time to be quantitatively characterized. Antioxidant activity of total extracts, shikonin and its derivatives were evaluated and compared using 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging activity assay.

B044 On-line identification of unstable iridoids from *Jamesbrittenia fodina* by LC-MS and LC-NMR

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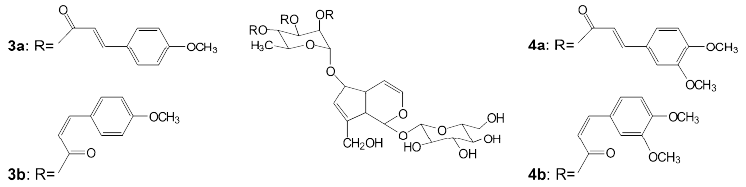
LC-UV-MS analysis of the methanol extract of *Jamesbrittenia fodina* Wild (Scrophulariaceae) revealed the presence of different iridoid cinnamic acid esters. Isolation of these constituents was prevented by instability problems. LC/UV/MS and LC/NMR analysis of the mixtures obtained after a tentative isolation revealed that, in a first instance, instability was due to a light induced *cis/trans* isomerisation of the cinnamoyl moiety (1). Further investigation of related compounds showed an additional instability linked to other chemical transformations. A detailed LC/NMR/MS study of these fractions demonstrated that the modifications occurred on the rhamnose moiety of these iridoids. It could be concluded that the second type of instability was attributable to trans-esterification of the cinnamoyl moiety on the rhamnose unit. The recording of stop-flow LC/NMR spectra on specific LC-peaks permitted the direct monitoring of these transformations. Based on these on-line data, four new unstable aucubin derivatives were efficiently characterised.



Reference: 1. Cogne A.-L. et al. (2002) Phytochem. Anal., in press.