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A comprehensive LC-MS/MS method validation for the quantitative investigation of 37 fingerprint phytochemicals in *Achillea* species: A detailed examination of *A. coarctata* and *A. monocephala*

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Research Highlights

- A comprehensive LC-MS/MS method validation to quantify 37 phytochemicals in plants.
- The developed method is applicable to all plant species as well as *Achillea*.
- The studied species might be a source for chlorogenic acid, rutin and apigenin.
- *A. monocephala*; promising species in terms of antioxidant and cytotoxic activities.

Abstract

The current study aims to optimize and validate a comprehensive LC-MS/MS method for the quantification of 37 phytochemicals (15 phenolic acids, 17 flavonoids, 3 non-phenolic organic acids, 1 phenolic aldehyde and 1 benzopyrene) in *Achillea* species. Though *Achillea* species were chosen as real life samples, the current method is applicable to a wide range of plant species. The developed method was fully validated in terms of linearity, accuracy (recovery), inter-day and intra-day precision (repeatability), limits of detection and quantification (LOD/LOQ) and relative standard uncertainty (U% at 95 % confidence level (k=2)). Reversed-phase ultrahigh performance liquid chromatography was optimized to achive optimum separation for 37 phytochemical compounds and to overcome the suppression effects. MS detection was performed using a triple quadrupole mass spectrometer and negative or positive ionization