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Chemometric analysis of NMR and GC datasets for chemotype characterization of essential oils from different species of *Ocimum*

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Abstract

The genus *Ocimum* (Labiatae) comprises 30 species found in tropical and subtropical regions of the planet, of which species *O. basilicum* L. and *O. gratissimum* are widely used in food and traditional medicine. Phytochemical studies on *Ocimum* have revealed a number of essential oil chemotypes, for example, eugenol, methyl chavicol, linalool, and methyl cinnamate. Since essential oils are commercially assessed according to their content, the aim of this study was to develop a simple and precise method for their qualitative and quantitative analysis using NMR spectroscopy combined with chemometrics. Seven essential oils from different species of *Ocimum*, an unknown sample, and a commercial sample were evaluated and the results compared to those from established and precise GC-MS and GC-FID methods. Chemometric evaluation from both ¹H NMR and GC-MS data revealed three chemotypes: eugenol for *O. gratissimum*, *O.*

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