Qualitative and quantitative analysis of volatile components of Teucrium massiliense L. – identification of 6-methyl-3-heptyl acetate as a new natural product

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Abstract :

Volatile components extracted from the aerial parts and separated organs of Corsican and Sardinian *Teucrium massiliense* have been studied. The chemical composition of essential oils obtained by hydrodistillation (HD) has been investigated using GC–RI, GC–MS (EI and CI modes) and ^{13}CNMR spectroscopy. For the first time, a real concentration via calibration curves and response factor calculations has been determined for each oil component. The concentrations of the major components were 6-methyl-3-heptyl acetate (23.83–18.16 g/100 g), 3-octyl acetate (10.55–6.95 g/100 g), isobutyl isovalerate (7.67–2.91 g/100 g), germacrene D (6.13–1.01 g/100 g) and linalool (6.63–5.23 g/100 g). To the best of our knowledge, the occurrence of 6-methyl-3-heptyl acetate as a natural product is reported for the first time. Furthermore, the chemical composition of volatile fractions emitted from the aerial parts and separated organs of *T. massiliense* L. has been studied by HS–SPME/GC–RI and GC–MS after optimization of SPME parameters. Concerning the contribution of plant organs to the aromatic plant fingerprint, we noted that the flowers produced more volatiles than other organs. The volatile fractions obtained from the different organs were qualitatively quite similar to each other but differed in the percentages of their major components. Also, the influence of HS–SPME extraction parameters (equilibrium and extraction times and temperature) on the chemical composition of the plant volatile fraction is discussed.

Keywords : Teucrium massiliense L; volatile components; HS–SPME; GC–MS; 6-methyl-3-heptyl acetate.

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