

PP89. The content of α - and β - thujones in essential oils: the qNMR approach

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The two diastereomeric thujones, (–)- α -thujone and (+)- β -thujone, are cyclopropane-containing monoterpene ketones that naturally occur in a number of higher plants. As components of essential oils of several genera, the most noteworthy ones are *Artemisia*, *Thuja*, and *Salvia*, thujones are often used in perfumery and are the legally limited components of the renown alcoholic drink absinthe.

The unspecific titration methods for the determination of total thujone content in various samples prompted the development of GC-MS and GC-FID methods that are today the most common ones for its quantitation. Although very precise, these methods require pure standards which are not easily obtainable. It has been recently reported that the content of thujone in absinthe can be determined using ¹H NMR spectroscopy [1].

Herein, we wish to report on the development of a new and fast method, that does not require expensive pure standards of thujones, for the determination of both contents of α - and β -thujone in essential oils using ¹H qNMR spectroscopy. NMR spectra of essential-oil samples recorded in CDCl₃ containing pentachloroethane (as an internal standard) were used for quantitation purposes. In contrast to the previously proposed NMR methodology, wherein the relevant signals fall in a usually crowded interval of chemical shift values, our newly developed method makes quantitative use of the well-separated signals at δ 0.1241 ppm (*dd*, *J* = 5.6, 4.0 Hz, 1 H) and/or –0.0389 ppm (*dd*, *J* = 5.8, 4.0 Hz, 1 H). The values of the integrals of these signals, originating from hydrogen atoms of the cyclopropane ring of α - and β - thujones, respectively, in respect to the integral of the signal of the standard, allowed an easy determination not only the total thujone content but also the content of the two separate diastereomers. We successfully applied this methodology for the determination of thujone content in several essential oils samples, containing total thujones in the range of 4-70% (*w/w*).

References:

[1] Monakhova, Y.B. et al., 2011. *Int. J. Spectrosc.* 2011, 171684.

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