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THE USE OF qNMR SPECTROSCOPY FOR ANALYTICAL EVALUATION OF LAVENDER EXTRACTS. DETERMINATION OF ROSMARINIC ACID

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NMR spectroscopy is a powerful method for structural identification of both individual compounds and complex natural products mixtures. The main advantages of this modern analytical tool are, among others, high resolution power, as well as simultaneous qualitative and quantitative evaluation of the investigated sample [1].

The current work presents the determination of rosmarinic acid (RA) content in lavender extracts basing on fast and reliable 2D NMR correlations. Few data on the quantitative determination of RA in lavender are known in the literature, even though it is an abundant and highly valuable secondary metabolite [2]. A pure sample of RA was isolated from dried leaves of lemon balm (*Melissa officinalis L.*) and its ^{1}H and HSQC spectra recorded. Purity grade of the obtained sample was calculated basing on ^{1}H NMR and internal standard (IS) method. Methyl 4-nitrobenzoate was used as an IS, both for ^{1}H and HSQC measurements. Two diagnostic signals of RA have been chosen on the basis of their separation from the IS peaks. The HSQC relaxation delay parameter (D_1) was optimized basing on the relaxation times T_1 determined for both diagnostic signals. The calibration curve was drawn on the basis of HSQC correlation, plotting the peak volumes of the chosen diagnostic peak, normalized to the peak volume of IS versus molar ratio between RA and IS. A perfect linearity was achieved. The quantitative determination of RA in a lavender extract was easily performed, thanks to an excellent resolution of RA diagnostic signals from all other extract components cross peaks. The elaborated method can be routinely used for the quality control of herbal pharmaceuticals or related products. The analysis time is comparable with the time of an average HPLC experiment. The sample preparation procedure and interpretation of results are very simple and can be easily adapted for any modern analytical laboratory.

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