CHIRAL ANALYSIS OF BIOLOGICALLY RELEVANT SAMPLES USING BROADBAND ROTATIONAL SPECTROSCOPY

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Terpenes are the main constituents of essential oils and are responsible for their chemical and biological activities. Additionally, terpenes found in essential oils are often structurally similar, like thymol, carvacrol, p-cymene and terpinen-4-ol in the case of thyme essential oil. These oils are likely to be enantio-enriched because of their natural origin [1]. Broadband rotational spectroscopy offers unparalleled features that make it a unique tool to analyze complex molecular mixtures as those present in essential oils. Even structurally similar molecules as diastereoisomers can be easily detected as they would show a different rotational spectrum. Additionally, the combination of the microwave three-wave mixing (M3WM) technique with the broadband capabilities allow one to distinguish enantiomers within a mixture of chiral molecules and to determine their enantiomeric excess in the gas phase.

Here, we present recent results on the analysis of two thyme essential oils from Spain obtained from the leaves of *Thymus vulgaris* and using the above-mentioned techniques. It is important to bear in mind that the chemical composition of the essential oils coming from the same plant species shows variations according to the environment, growth region and cultivation practices. In our case, terpene compositions of the two studied thyme oils change, even coming from the same country. Linalool is mainly present in one of the oils, whereas thymol is present in the other. The analyses of essential oils with these techniques could extent the use of rotational spectroscopy as a chemical analytical tool (a new application still to be explored in more detail).

[1] V. A. Shubert, D. Schmitz, C. Pérez, C. Medcraft, A. Krin, S. R. Domingos, D. Patterson, M. Schnell, *J. Phys. Chem. Lett.* 7 (2016) 341−350.