FACTA UNIVERSITATIS
Series: **Physics, Chemistry and Technology** Vol. 16, N° 1, Special Issue, 2018, p. 17
49th International Symposium on Essential Oils (ISEO2018) • Book of Abstracts

49th ISEO

PL1. Applying organic synthesis in the analysis of essential oils

Nicolas Baldovini[1]*

Keywords: essential oil analysis, organic synthesis, combinatorial synthesis, mass spectral and retention indices databases

Nowadays, the analysis of essential oils (EOs) is usually realized by the use of Gas Chromatography coupled with Mass spectrometry (GC-MS). Indeed, a significant part of the present knowledge on EOs comes from this ingenious association of a highly resolutive separation technique (GC) with the sensitive and informative detection by mass spectrometry. Interesting advances have been proposed to push the boundaries of classical GC techniques (using for example even more resolutive multidimensional GC) or to improve the sensitivity of MS detectors. However, one of the main limitations of this system is linked to the databases used for the identification of the analytes. Hence, the performance of the analysis depends on the reliability and the wealth of information contained in the libraries of mass spectra and retention indices used to identify the constituents. General commercial databases are not always adapted to the characterisation of EO components and the constitution of homemade libraries of authentic compounds is a long and expensive task. In many cases, organic synthesis can be of a great help to address such issues of EO analyses. Hence, the conversion of EO constituents by simple synthetic transformations (hemisynthesis), or even the total synthesis of some components can bring extremely useful information to confirm the identifications. Combinatorial synthesis is another very rapid and useful approach for the preparation of mixtures of homologues which can be used as such to enrich GC-MS libraries as the components of homologous series are usually perfectly resolved on apolar columns. Specific EOs analyses (enantiomeric analyses, characterization of key odorants) are also nicely helped by the syntheses of potent odorants and of racemic and/or enantiopure constituents.

In this presentation, we will describe some of our studies on various EOs and extracts of natural volatiles (sandalwood, vetiver, frankincense, Atlas cedarwood, *Helichrysum* and *Daucus* species etc.) where organic synthesis played a key role for the identification of their constituents and a better characterization of their properties. We hope to convince the community of scientists working in the field of EO analysis that many common problems can be easily solved by simple synthetic procedures which do not necessarily require advanced knowledge or sophisticated equipment.

[1] Institut de Chimie de Nice, CNRS UMR 7272, Université Côte d'Azur, Parc Valrose, F-06108 Nice, France.
**Corresponding author*: baldovin@unice.fr