Book of Abstracts

Poster Presentations

Low-Resolution Mass Spectrometry study on *ortho*-menthane irregular monoterpenes as an initial step to build-up a library

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Summary: *Irregular* ortho-*menthane monoterpenes are in general poorly represented in commercial mass spectral libraries. In this work, we recorded and interpreted low-resolution mass spectra of seven members of this group, as an initial step to build-up a new library.*

Keywords: ortho-*menthanes; low-resolution mass spectrometry; fragmentations*

1. Introduction

Irregular *ortho*-methane monoterpenes are a small group of natural products found concentrated in the essential oil of *Baccharis trimera* (Less.) DC (Asteraceae) (BTEO) [1,2]. Except for the well-known *o*-cymene, carquejyl acetate (I.) and carquejol (II.) (Fig. 1), commercial libraries usually do not contain mass spectra of other *ortho*-menthane derivatives. As a continuation of our work on *ortho*-menthanes [1,2], we present here some low-resolution mass fragmentation patterns and their interpretation schemes, as an initial step to build-up a mass library of this interesting group. were distinctive, showing typical fragmentation patterns derived from their structures: i.e., McLafferty/Retro-Diels-Alder rearrangements, as well as σ-, i- and α-cleavages. With these results, a careful search in the GC-MS chromatograms of BTEO allowed to identify V. (carquejiphenol) as a natural product not previously informed. Comparisons between spectra obtained from the two analyzers, evidenced intensity differences in some fragments. This should be taken into account when performing automated searches and comparisons.

2. Experimental

Natural and semi-synthetic *ortho*-menthanes with different chemical functionalities (Fig. 1: I.-VI.) were obtained starting from BTEO, following original protocols [2]. ^{1}H and ^{13}C-NMR allowed to confirm their structures. Their low resolution-mass spectra were acquired with GC-MS instruments, using EI ionization (20/70 eV) with two different mass analysers: 1) single quadrupole (HP6890/HP-5973), and 2) ion trap (Trace 1300/ITQ-900). The stationary phase of the capillary columns was (5%-phenyl)-methylpolysiloxane for both cases. Mass scan range: 50-350 uma. Interpretation of the spectra were according to the literature [3].

3. Results

The mass spectra recorded for each one of the seven ortho-menthanes studied (Fig. 1: I.-VII.)

4. Conclusions

Ortho-menthanes are an interesting group to build-up a new library of EI-MS that will eventually assist in the secure identification of thesecompounds in complex compositions, like BTEO.

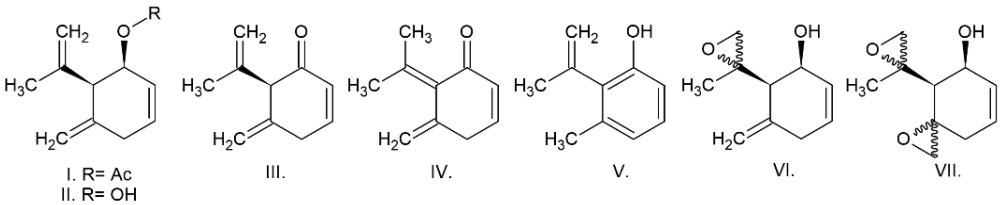

Fig. 1. Irregular ortho-*methane monoterpenes for which low-resolution mass spectra were recorded and interpreted.*

References

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