LRI-filtered identification of essential oil constituents by using a novel MS database

Mariarosa Maimone, Peter Q. Tranchida, Luigi Mondello

Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali,
University of Messina – Polo Annunziata, viale Annunziata, 98168 Messina, Italy
mmaimone@unime.it

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The linear retention index (LRI) approach can be used in combination with conventional mass spectral searching, with the goal of boosting the identification of "challenging" molecules, occurring in flavours and fragrances. To this end, a GC-MS database (*FFNSC* library), collecting around 3000 spectra derived from pure chemicals, essential oils and perfumes, has been built-up providing each spectrum with mass fragments and structural information, but also with the experimental value of LRI. In the present study such powerfull tools were used to perform the chemical investigation of the essential oils obtained from Iranian plants of *Artemisia kopetdaghensis* Krasch ex Poljakov, *Artemisia oliveriana* J. Gay ex Besser, *Artemisia austriaca* Jacq. and *Artemisia diffusa* Krasch ex Poljakov. Accurate GC-FID and GC-MS analyses were carried out. Quantitative analysis was based on both the internal standard method and the measurement of FID response factors. LRIs were used to eliminate database matches with high similarity scores but with LRI values far from the target ones.

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