Reliable identification of plant and marine constituents by using dedicated MS databases.

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Gas chromatography combined with mass spectrometry (GC-MS) is a very powerful two-dimensional method, commonly used for the identification of unknown compounds. Peak assignment is usually performed through MS database matching. However, there are drawbacks related to such an approach. In first instance, when dealing with classes of compounds characterized by similar structures (e.g., sesquiterpenes in essential oils, fatty acids in fish oils, etc.), the fragments generated by the ionization process are very similar, thus leading to the acquisition of nearly-identical spectra for different compounds. In such cases, the occurrence of incorrect cases of peak identification is, by no means, not rare. Additionally, many commonly used GC-MS databases contain thousands of compounds, the spectra of which are often of poor quality, with no hint on the applied acquisition conditions. Such issues have enhanced the need for a novel GC-MS databases, such as the “FFNSC” (Flavour and Fragrance Natural and Synthetic Compounds) and “FAMEs” (Fatty Acid Methyl Esters), constructed with spectra derived from essential oils and pure standard compounds. Each compound in the database is accompanied by one (or more) linear retention index (LRI) value. The innovative feature of the FFNSC and FAMEs databases lies in the “LRI filter” option provided by the software (GCMS solution). In fact, the software can automatically calculate LRI values for each peak in the chromatogram, and use such values interactively, as a filter, during MS database matching. Possible matches, with a non-compatible LRI value, are automatically excluded from the “hit list”, greatly increasing the reliability of peak assignment. Furthermore, many other parameters can be set in the interactive windows of the software, such as the minimum degree of similarity between the target and the database spectrum. The FFNSC and FAMEs databases contain around 3,500 and 250 spectra, respectively; each is provided with CAS registered information and LRI value(s). Applications on fish lipid FAMEs and essential oils are shown and discussed.

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