

FFNSC 2 - Flavors and Fragrances of Natural and Synthetic Compounds - Mass Spectral Database



by Prof Luigi Mondello

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Software

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Advanced Component Identification in Complex Mixtures

2nd Edition Expanded by 64%

Prepared by the Prof. Luigi Mondello under rigorous measurement conditions, the mass spectral library contains compounds central to flavor and fragrance research.

Essential oils are mixtures consisting of monoterpene and sesquiterpene hydrocarbons, their oxygenated derivatives, and aliphatic oxygenated compounds. The difficulties that arise in the GC-MS peak identification of these complex samples is due to the fact that many terpenes have identical mass spectra. This is a consequence of similarities both in the initial molecule, or in the fragmentation patterns and rearrangements after ionization. Hence, MS identification of these compounds should always be accompanied by retention time information that may support the MS library search results.

This innovative MS library for natural and synthetic products (essential oils, perfumes, etc.) makes the identification of unknown compounds in complex mixtures easier, faster and more reliable.

The use of chromatographic information, such as Linear Retention Index (LRI), can be used to filter MS results, enabling the more reliable peak assignment of components in complex mixtures.

Mass spectra, relative to standard and well-known simple matrix components, were obtained and recorded through GC-MS separation/identification. Furthermore, traditional information relative to each component (CAS number, common name, CAS name, molecular weight, compound formula, chemical class) plus linear retention index values are entered.

Applications: Flavors and Fragrances of Natural and Synthetic Compounds, 2nd edition contains 3000 mass spectra, LRI retention data, calculated Kovats

RI, and searchable chemical structures of compounds of interest for the flavors and fragrances industry.

Available Formats

Formats included on the disc include **Agilent** Chemstation and Masshunter, **ACD/Labs** MS Manager, **NIST** software (compatible with **JEOL**, **Leco**, **Bruker**, **Thermo** xCalibur), **PerkinElmer** TurboMass, **Thermo** Spectral ID, **Waters** MassLynx.

Shimadzu

Shimadzu GCMS Solution format is available exclusively from [Shimadzu](#).