

Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition

Luigi Mondello



Introduction

Essential oils are mixtures consisting of monoterpene and sesquiterpene monocarbons, 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 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 (chemical structure, CAS number, common name, CAS name, molecular weight, compound formula) plus linear retention index values are entered.

Key Benefits

- Prepared by Prof. Luigi Mondello under rigorous measurement conditions, the mass spectral library contains compounds central to flavor and fragrance research
- Includes a 30-day trial version of Cromatoplus software

Specifications

- Spectral Records: 3,462
- Chemical Structures: 3,462
- RI1 = measured on SLB-5MS (Hydro): 3,462
- RI2 = measured on SLB-5MS (FAMES): 2,516
- RI3 = measured on Supelcowax-10 (FAMES): 1,466 (same records as RI4)
- RI4 = measured on Supelcowax-10 (FAEEs): 1,466 (same records as RI3)
- RI5 = measured on Equity-1 (Hydro): 646

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Compound Coverage

Compound coverage for individual compounds can be verified at www.compoundsearch.com

What's New

- Compound coverage is increased by 15% over FFNSC2
- With the addition of more columns, retention index data has been more than doubled.
- Experimental RI data has been indexed in NIST and Agilent formats, making this available for all NIST and Agilent based data systems.
- Retention index functionality has been improved for Agilent Chemstation and MassHunter.

Compatibility

Compatible with most current and legacy mass spectrometry data systems, including:

- Bruker
- Leco
- JEOL
- Agilent (Chemstation, MassHunter)
- PerkinElmer TurboMass
- Waters MassLynx
- ACD ND9
- Cromatoplus (30-day trial version included)

Author Biography

Professor Dr. Luigi Mondello is a prominent figure in the flavors and fragrances research industry as the Editor of the *Journal of Separation Science* published by John Wiley & Sons and Editor in Chief of the *Journal of Essential Oil Research* published by Taylor & Francis. He received a degree in Chemistry from the University of Messina, Italy in 1991 and is now a Full Professor of Analytical Chemistry in the Department of Chemistry Science, Biological Science, Pharmaceutical Science and Environmental Science for the University. Prof. Mondello is currently the author of 292 scientific papers, 63 book chapters, and 25 reviews. His research interests include chromatography techniques and the advancement of coupled techniques such as LC-GC-MS, GC-GC, GCxGC, LCxLC, LCxGC and their applications in the study of natural and synthetic complex matrices. Prof. Mondello is also the author of *Flavors and Fragrances of Natural and Synthetic Compounds 3*, *FAMEs Fatty Acid Methyl Esters: Mass Spectral Database* and *Mass Spectra of Pesticides with Retention Indices*.

Ordering Information

Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition
CD-ROM ISBN: 978-1-119-06984-3

Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition Upgrade
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