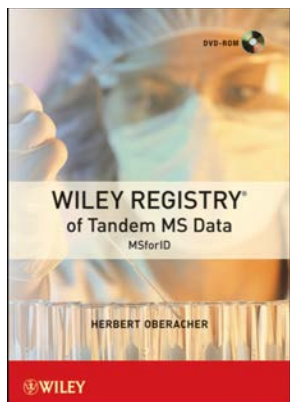


Wiley Registry[®] of Tandem Mass Spectral Data: MS for ID

Herbert Oberacher



High Mass-Accuracy LC-MS/MS Library

The *Wiley Registry of Tandem Mass Spectral Data: MS for ID* consists of 12,048 positive and negative mode spectra of over 1,000 compounds of interest for forensics, toxicology, and pathology. Covering areas such as illicit drugs, pharmaceutical compounds, pesticides, and other small bioorganic molecules, this database is a reliable tool for the identification of small molecules with specificity usually about 95% and sensitivity exceeding 92%.

Each compound was carefully measured by the Oberacher team at the Institute of Legal Medicine, Innsbruck Medical University. A series of controlled conditions ensured accurate, reliable, and reproducible search results in a variety of settings. The library demonstrates high transferability to a variety of tandem mass spectrometric instruments.

The Wiley Registry of Tandem Mass Spectral Data: MS for ID comes bundled with one of the most accurate search algorithms developed for LC-MS/MS providing fast, reproducible, and stable search results.

Specifications

- Mass Spectra: 12,048
- Searchable Structures: 12,048
- Unique Compounds: 1,163

Compatibility

- Agilent MassHunter*, OpenLab*
- Bruker MetaboScape, ToxTyper 2.0
- Proteome Scaffold Elements*
- NIST MS Search
- Scripps XCMS
- Shimadzu LabSolutions
- Thermo Chromeleon™*, LCQUAN™, Mass Frontier™*, mzCloud™, TraceFinder™*, ToxFinder™*, ToxID™*, xCalibur™*
- Waters UNIFI

Ordering Information

Wiley Registry of Tandem Mass Spectral Data: MS for ID
DVD-ROM ISBN: 979-1-1190-3744-7

*Compatible with the NIST format

<https://sciencesolutions.wiley.com>

WILEY