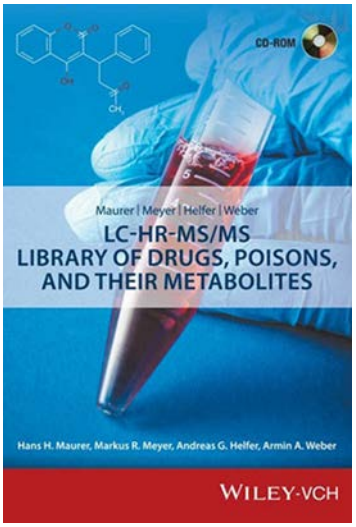
LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites

Heighten screening sensitivity with metabolite-based LC-HR-MS/MS library



Developed by toxicologist Hans H. Maurer and his team, the Maurer/Meyer/Helfer/Weber *LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites* consists of 5,006 spectra, over 2,000 parent drug or poisons, and over 3,000 of their metabolites or artifacts in over 95 compound classification groups. This metabolite-based library helps minimize the risk of false negative LC-MS results.

LC-high-resolution tandem mass spectrometry (LC-HR-MS/MS) provides various advantages for screening approaches, such as higher versatility, sensitivity, and specificity. This library is the basis for metabolite-based screening procedures described for various drug classes. Data fields within the library include compound name, empirical formula, exact molecular mass, exact precursor mass, polarity, retention time, CAS number, and category.

Compatibility

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

*Compatible with the NIST format

Specifications

- Spectra: 5,006
- Structures: 3,144
- Unique Compounds: 2,299
- Metabolites/Artifacts: > 3,000
- Endogenous Molecules: 70

Ordering Information

LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites
DVD-ROM ISBN: 978-3-527-34338-6

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