

A photograph of a female scientist in a white lab coat and safety goggles, wearing purple gloves and using a pipette in a laboratory. The background is a blurred laboratory setting with shelves and equipment.

Wiley Science Solutions

Spectral Libraries
and Databases

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Helping laboratories build a better future

Improving data analysis and laboratory efficiency

Wiley Science Solutions provides researchers with superior spectral data collections that improve the quality of the compound analysis and identification processes, ultimately increasing lab productivity and reducing errors.

Wiley's broad and field-tested mass spectral libraries have millions of spectra available, across various applications and techniques, for confident compound identification. Wiley works the way you do by partnering with the leading instrument manufacturers to ensure worry-free installation and implementation within existing workflows.

Efficient

Accurate

Validated

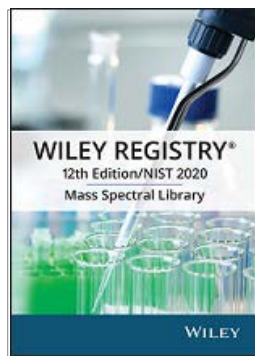
With over 50 years' experience in publishing empirical, experimental, and validated data, Wiley Science Solutions is the most trusted partner in the publishing industry for laboratory data solutions. Our spectral library collections are constantly evolving to increase coverage in order to meet today's rigorous research demands.

Contact us today to learn how Wiley Science Solutions can help save time, increase instrument efficiency, and boost staff productivity.

For more information, contact us and a representative will be in touch to help you find the right solution for your lab.

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Product Showcase



Wiley Registry® 12th Edition / NIST 2020 Mass Spectral Library

Wiley/NIST

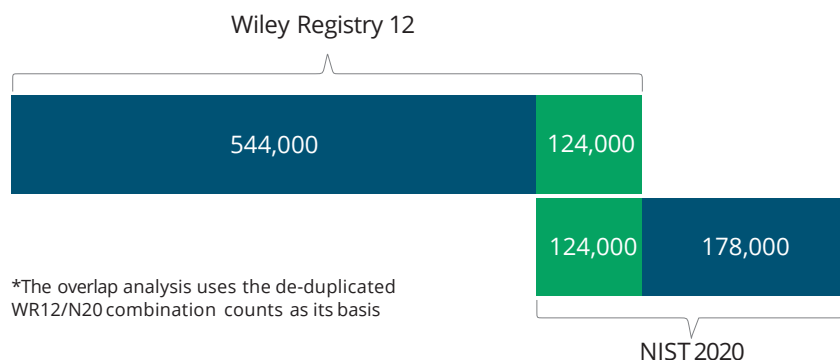
ISBN: 978-1-119-75033-8

The broadest combined library available with over 2 million EI GC-MS and LC-MSⁿ

The combined **Wiley Registry 12th Edition/NIST 2020 Mass Spectral Library** is the most comprehensive mass spectral library commercially available, making it an essential tool for general unknown compound identification. Included in the combination package are:

- Over 1 million EI mass spectra
- Over 1 million searchable chemical structures
- Over 840,000 unique compounds

Overlap Analysis



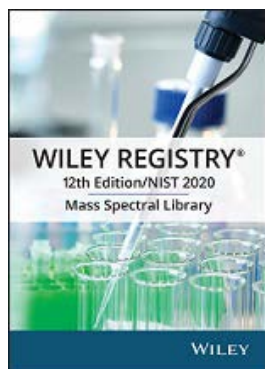
Compatible with most current and legacy mass spectrometry data systems including:

- Agilent (ChemStation, MassHunter, OpenLab)
- Bruker MS Workstation*
- Chromatec Analytic*
- JEOL msFineAnalysis*
- LECO ChromaTOF*
- NIST MS Search
- PerkinElmer TurboMass
- Scion MS Workstation*
- Shimadzu GCMSolutions
- Thermo Chromeleon*, TraceFinder*, Xcalibur
- Waters MassLynx
- Includes complete suite of NIST software tools (AMDIS deconvolution software, MS Interpreter, Lib2NIST).

*Compatible with NIST format

*Wiley Registry is a registered trademark of John Wiley and Sons, Inc.





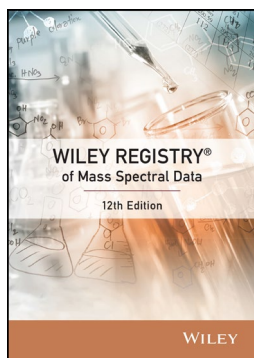
Wiley Registry® 12th Edition/NIST 2020 Mass Spectral Library

Wiley/NIST

ISBN: 978-1-119-75033-8

Experience improved spectral search performance with the *Wiley Registry 12th Edition/NIST 2020 Library*. Replicate spectra and over 3 million chemical names and synonyms provide a higher rate of correct identification and ensure that this library can aid in classical EI, exact mass, and other methods of identification.

Over 1 million EI mass spectra
Over 1 million chemical structures
Over 840,000 unique compounds



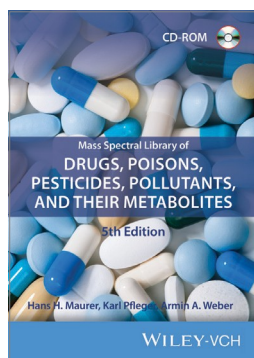
Wiley Registry of Mass Spectral Data, 12th Edition

Wiley

ISBN: 978-1-119-17102-7

The field-tested *Wiley Registry of Mass Spectral Data, 12th Edition* is the largest mass spectral library commercially available, providing over double the compound coverage of our competitors. Applications include untargeted GC-MS screening and accurate mass workflows with MS-TOF instruments. Now with chemical classifications, calculated Kovats retention indices and splash IDs.

Over 817,000 spectra
Over 785,000 chemical structures
Over 668,000 unique compounds



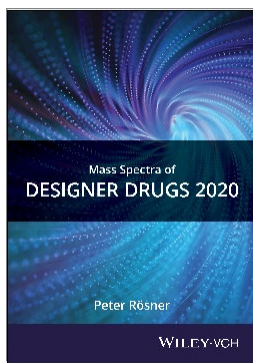
Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites, 5th Edition

Hans H. Maurer, Karl Pflieger, Armin A. Weber

ISBN: 978-3-527-34327-0

Developed by renowned toxicologist Hans H. Maurer and his team, the *Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites, 5th Edition* sees the addition of 1,780 carefully evaluated data sets, bringing the total to 10,430 mass spectra and GC retention indices. Featured compounds from 175 categories include psychoactive substances, almost all relevant therapeutic drugs, and 7,800 of their metabolites.

10,430 spectra
Over 8,400 unique compounds



Mass Spectra of Designer Drugs 2020

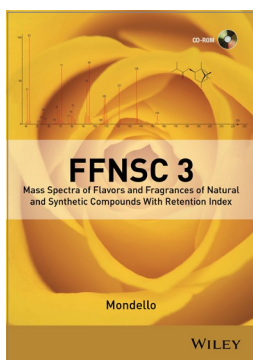
Peter Rösner

ISBN: 978-3-527-34813-8

The *Mass Spectra of Designer Drugs 2020* is the largest collection of chemical signatures of NPS and drugs of abuse in the world. The 2020 edition features the addition of over 1,300 new mass spectra and over 700 new, unique compounds in over 30 different classification groups such as fentanyls, synthetic cannabinoids, and opiates.

Over 29,000 spectra

Over 22,000 unique compounds



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

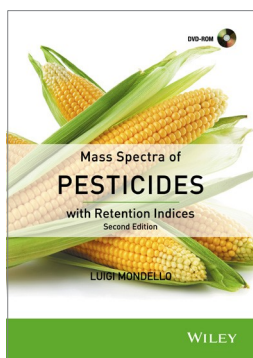
Luigi Mondello

ISBN: 978-1-119-06984-3

Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition contains over 3,000 mass spectra, LRI retention data, calculated Kovats RI, and searchable chemical structures of compounds of interest for the flavors and fragrances industry. This innovative library for natural and synthetic products makes the identification of unknown compounds in complex mixtures easier, faster, and more reliable.

Over 3,400 mass spectra

Over 3,300 unique compounds



Mass Spectra of Pesticides with Retention Indices, 2nd Edition

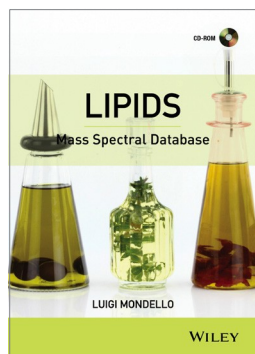
Luigi Mondello

ISBN: 978-1-119-28404-8

The *Mass Spectra of Pesticides with Retention Indices, 2nd Edition* contains 1,300 pesticide molecules sorted in 20 different classes. This 2nd edition features 342 new pesticides compounds, 1,300 LRI values on a SLB-5ms column, and 147 LRI values on an EQUITY-1 column. The GC-MS-based pesticides library provides significant support for peak assignment in complex mixtures.

1,300 spectra

Over 1,200 unique compounds



LIPIDS Mass Spectral Database

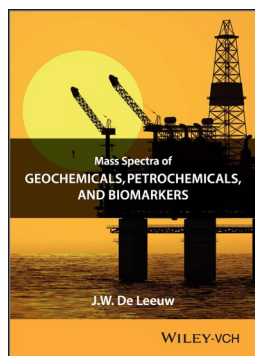
Luigi Mondello

ISBN: 978-1-119-28938-8

The *Lipids Mass Spectral Database* contains 430 GC mass spectra registered from a pure standard and categorized into 11 classes of lipids. The database provides significant support for peak assignment in complex mixtures, making it a valuable tool in many research areas such as food analysis and clinical and medical applications.

430 spectra

428 unique compounds



Mass Spectra of Geochemicals, Petrochemicals, and Biomarkers (SpecData)

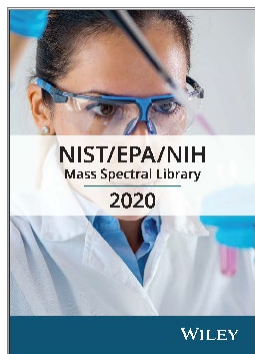
J.W. De Leeuw

ISBN: 978-0-471-64798-0

Mass Spectra of Geochemicals, Petrochemicals and Biomarkers (SpecData) is a high-quality database for organic, geo, and/or petrochemist featuring 1,093 mass spectra of well-defined compounds. Chemical structures elucidated, if necessary, by a variety of techniques including NMR spectroscopy and single-crystal x-ray structure analysis.

1,093 spectra

Over 1,000 compounds



NIST/EPA/NIH Mass Spectral Library 2020

NIST/Wiley

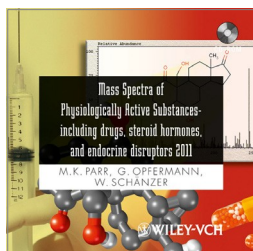
ISBN: 978-1-119-75029-1

The *NIST/EPA/NIH Mass Spectral Library 2020*, the successor to the NIST 2017, is a fully evaluated collection of electron ionization (EI) and MS/MS mass spectra, with chemical and GC data, plus search software to identify your own unknown spectra. NIST 20 contains over one million mass spectra including 350,000 EI spectra for 306,000 compounds and 1,320,000 tandem MS/MS spectra.

350,643 EI spectra

306,869 EI compounds

1,320,389 MS/MS spectra



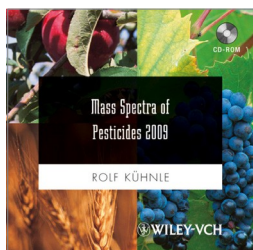
Mass Spectra of Physiologically Active Substances: Including Drugs, Steroid Hormones, and Endocrine Disruptors 2011

Maria Kristina Parr, Georg Opfermann, Wilhelm Schanzer, Hugh L. J. Makin

ISBN: 978-3-527-32727-0

In collaboration with the Institute of Biochemistry and German Sport University of Cologne, the *Mass Spectra of Physiologically Active Substances* features 4,182 mass spectra and chemical structures of androgens and estrogens, as well as their trimethylsilyl-, O-methoxyoxime-, and acetal derivatives and beta-2-agonists.

Over 4,100 spectra
Over 3,900 unique compounds



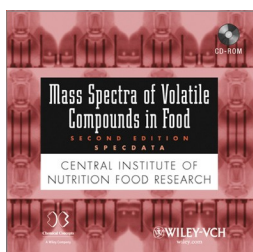
Mass Spectra of Pesticides 2009

Rolf Kühnle

ISBN: 978-3-527-32488-0

Developed by Rolf Kühnle, the *Mass Spectra of Pesticides 2009* includes 1,007 high-quality mass spectra of pesticides such as insecticides, acaroids, nematicides, fungicides, rodenticides, and over 900 unique compounds.

Over 1,000 spectra
Over 900 unique compounds



Mass Spectra of Volatiles in Food, 2nd Edition

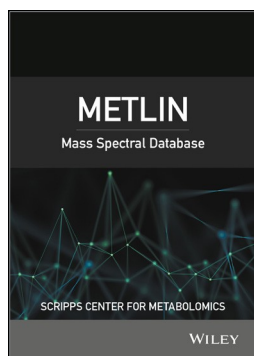
Central Institute of Nutrition and Food Research

ISBN: 978-0-471-64825-3

The *Mass Spectra of Volatile Compounds in Food* collection includes 1,620 reference mass spectra and covers the whole range of volatile compounds in food. Created by the Central Institute of Nutrition and Food Research, the database also features derivatives of non-volatile compounds, such as sugars or polyhydroxyphenols.

Over 1,600 spectra

LC-MS and Screening

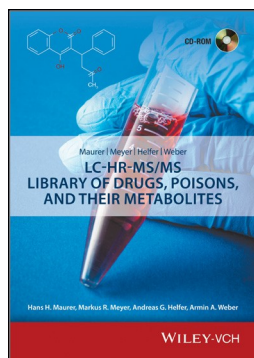


METLIN Mass Spectral Database

Scripps Center for Metabolomics, Gary Siuzdak, H.P. Benton
ISBN: 978-1-119-37705-4

The *METLIN Mass Spectral Database*, bundled with the 2017 edition of the NIST MS/MS library, is a feature-rich, comprehensive metabolite and tandem mass spectrometry database designed for untargeted metabolomic analysis. Featuring over 942,000 spectra, METLIN is an essential resource in pharmaceuticals, preventive healthcare, and agricultural research.

942,942 spectra
942,940 compounds

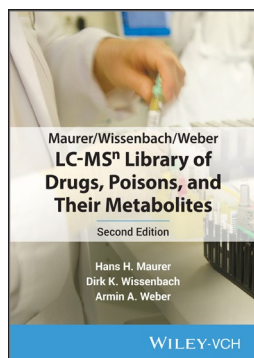


LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites

Hans H. Maurer, Markus R. Meyer, Andreas G. Helfer, Armin A. Weber
ISBN: 978-3-527-34338-6

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.

Over 5,000 spectra
Over 2,200 unique compounds

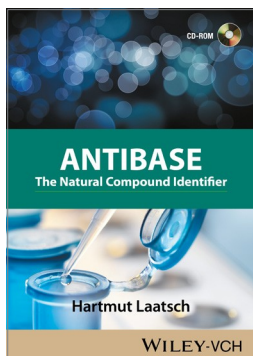


LC-MSⁿ Library of Drugs, Poisons, and Their Metabolites, 2nd Edition

Hans H. Maurer, Dirk K. Wissenbach, Armin A. Weber
ISBN: 978-3-527-34649-3

The Maurer/Wissenbach/Weber *LC-MSⁿ Library of Drugs, Poisons, and Their Metabolites, Second Edition* provides a proven metabolite-based LCMSⁿ screening method and MS² and MS³ spectra of over 2,270 parent compounds and over 3,600 of their metabolites, making it one of the only LC-MSⁿ screening libraries that focuses on metabolite spectra.

Over 13,000 spectra
Over 2,270 toxicologically relevant compounds



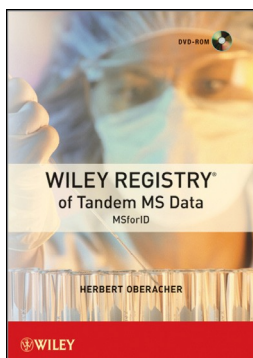
AntiBase: The Natural Compound Identifier

Hartmut Laatsch

ISBN: 978-3-527-34359-1

AntiBase: The Natural Compound Identifier is a compilation of natural products featuring properties of more than 40,000 compounds and over 41,000 chemical structures. This indispensable database provides researchers with a convenient way of checking if a compound with antimicrobial effects has already been studied and provides insights into biological activity correlated to structural information.

Over 44,000 spectra
Over 40,000 natural product compounds



Wiley Registry of Tandem Mass Spectral Data, MS for ID

Herbert Oberacher

ISBN: 978-1-118-03744-7

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%.

Over 12,000 spectra
Over 1,000 unique compounds



NIST/EPA/NIH MS/MS Mass Spectral Library 2017

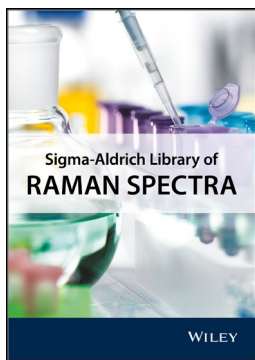
NIST/Wiley

ISBN: 978-1-119-37673-6

The *NIST/EPA/NIH MS/MS Mass Spectral Library 2017* software contains over 234,000 spectra of over 42,000 ions. The new MS/MS library also contains metabolites, peptides (including biologically active peptides and all di-peptides and tryptic tri-peptides), contaminants, lipids, and more.

234,000 spectra of over 42,000 ions

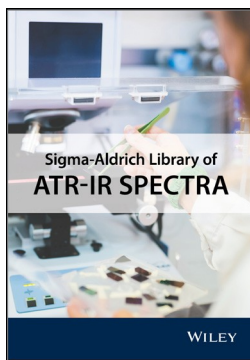
Confident identification with the NEW Sigma-Aldrich collections



Sigma-Aldrich Library of Raman Spectra

ISBN: 978-1-119-37678-1

6,487 Raman Spectra



Sigma Aldrich Library of ATR-IR Spectra

ISBN: 978-1-119-37680-4

19,503 ATR-IR Spectra



Sigma Aldrich Library of FT-IR Spectra

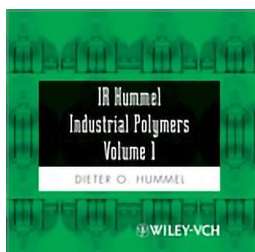
ISBN: 978-1-119-37678-8

11,270 FT-IR Spectra

The Sigma-Aldrich* libraries are a world-class collection of Raman, FT-IR, and ATR-IR spectra sourced from the laboratories of Sigma-Aldrich by Merck KGaA Darmstadt, Germany. Each spectra library includes Sigma-Aldrich catalog numbers, ensuring quick and accurate ordering of standards from Sigma-Aldrich.

*Sigma-Aldrich is now Millipore Sigma.

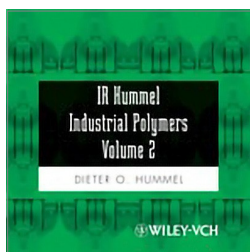
Comprehensive collection of IR industrial polymers



IR Hummel Industrial Polymers- Volume 1

ISBN: 978-0-471-66221-1

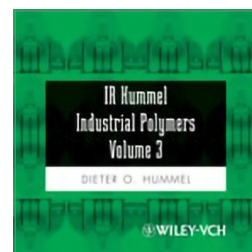
1,900 Spectra



IR Hummel Industrial Polymers- Volume 2

ISBN: 978-0-471-66222-8

1,570 Spectra



IR Hummel Industrial Polymers- Volume 3

ISBN: 978-0-471-66223-5

1,520 Spectra

The IR Hummel Industrial Polymer collection is an extensive collection of high-quality FT-IR spectra for polymers, elastomers, and fibers. Full compound coverage can be found at www.compoundsearch.com.

Purchasing Information

For your convenience, we've built lasting partner relationships with the following instrument manufacturers, resellers, lab service companies, and software vendors to ensure that our products are available globally wherever you are already purchasing your lab equipment.

Equipment Manufacturers:

Agilent Technologies
Bruker Daltonics
DANI
JEOL
JSC Chromatec
LECO
PerkinElmer Scion
Instruments SCIEX
Shimadzu
TA Instruments
Thermo Scientific
Waters
YL Instruments

Resellers & Lab Service Companies:

Adaptive Solutions
Digital Data Management Corporation
MSWil GmbH
Peak Spectroscopy Quantum Analytical
Stanton Scientific
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Software Vendors:

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