Wiley Science Solutions
Spectral Libraries and Databases
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.

[sciencesolutions.wiley.com](http://sciencesolutions.wiley.com)
**Product Showcase**


Wiley/NIST
ISBN: 978-1-119-41223-6

The broadest combined library available with over 1.6 million EI GC-MS and LC-MS mass spectra

The combined *Wiley Registry 11th edition/NIST 2017 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 973,000 searchable chemical structures
- Over 770,000 unique compounds

**Overlap Analysis**

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<th>Wiley Registry 11</th>
<th>NIST 2017</th>
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*The overlap analysis uses the de-duplicated WR11/N17 combination counts as its basis*

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 GCMSsolutions
- Thermo Chromeleon, TraceFinder, Xcalibur
- Waters MassLynx
- Includes complete suite of NIST17 software tools (AMDIS deconvolution software, MS Interpreter, Lib2NIST).

*Wiley Registry is a registered trademark of John Wiley and Sons, Inc.*
Wiley/NIST
ISBN: 978-1-119-41223-6

Experience improved spectral search performance with the Wiley Registry 11th edition/NIST 2017 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 770,000 unique compounds

Wiley Registry of Mass Spectral Data, 11th Edition
Wiley
ISBN: 978-1-119-17101-0

The field-tested Wiley Registry of Mass Spectral Data, 11th 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.

Over 775,000 spectra
Over 632,000 unique compounds

Hans H. Maurer, Karl Pfleger, 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

sciencesolutions.wiley.com
Mass Spectra of Designer Drugs 2019
Peter Rösner
ISBN: 978-3-527-34685-1

The Mass Spectra of Designer Drugs 2019 is the largest collection of chemical signatures of NPS and drugs of abuse in the world. The 2019 edition features the addition of over 1,500 new mass spectra and over 1,250 new, unique compounds in over 30 different classification groups such as fentanyl, synthetic cannabinoids, and opiates.

Over 28,000 spectra
Over 21,000 unique compounds

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

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
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

The *NIST/EPA/NIH Mass Spectral Library 2017*, the successor to the NIST 2014, 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 17 contains nearly a million mass spectra including 306,000 EI spectra for 267,000 compounds and 652,000 tandem MS/MS spectra.

306,622 EI spectra for over 267,000 compounds
652,475 MS/MS spectra for over 15,243 compounds
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

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
**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

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**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

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**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

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**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

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**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
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
- Sci-X
- 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 GC Image

**Software Vendors:**
- ACD/Labs
- Bio-Rad Informatics
- MestreLab
- MSP Kofel
- Proteome Software

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