WILEY-VCH

WILEY

Spectral Libraries and Databases

Techniques:

GC-MS

LC-MS^n

NMR

Raman

IR/UV-Vis

Wiley Spectra Lab

Spectroscopy Solved

NEW!
Sigma-Aldrich Libraries

The world's largest spectral database with over 2 million spectra

What is Wiley Spectra Lab?

Wiley Spectra Lab is an expert spectral data system that uses empirical spectral data and advanced software to help chemists, toxicologists, and life scientists confidently identify chemical substances.

How can I use it?

Customize your spectral search to meet your needs with combinations of over 175 spectral databases sourced from Wiley, **Bio-Rad Sadtler™**, Sigma-Aldrich and others to provide the focus required by technique and analyte.

What spectra are available?

Currently available are the MS collection, with over 825,000 mass spectra covering geochemicals, metabolites, poisons and esters; the NMR collection, featuring over 921,000 spectra covering multiple atomic centers, and the IR collection with over 345,000 IR, ATR-IR, Raman, UV-Vis, FT-IR and Near-IR spectra.

www.wileyspectralab.com

Wiley Spectral Libraries -
Illuminating Discoveries

Fast, reliable analysis solutions for industry, research and public safety.

In the modern analytical and bio-analytical laboratory, rapid and accurate identification and reliable analysis of drugs, poisons, pollutants, metabolites and other substances has never been more crucial or complex. **Spectral libraries from Wiley** provide the research community with high-quality data collections that help reduce errors and increase productivity for toxicology, food, environmental, medicinal, and analytical laboratories.

Wiley's Spectral Libraries and Databases are constantly evolving to increase coverage for meeting today's research demands and offer millions of spectra for confident compound identification across various techniques including NMR, IR, UV-Vis, Raman and mass spectrometry (LC-MS, GC-MS).

Available in the most popular instrument formats, Wiley works with leading manufacturers to ensure worry-free installation that supports existing workflows. Equipping laboratories with Wiley's broad and field-tested spectral libraries saves time, increases instrument efficiency and boosts staff productivity.

Applications

Name	Technique	Size	Uniqueness compared to WR 11e	Uniqueness compared to NIST 2017
Wiley Registry: Mass Spectral Library 11th Edition	GCMS	775,500+	–	79%
Wiley Registry: Mass Spectral Library 11th Edition/NIST 2017	GCMS, LC-MS^n	1.6 mil +	15%	67%
NIST/EPA/NIH Mass Spectral Library 2017	GCMS, LC-MS^n	306,600	46%	–
NIST/EPA/NIH MS/MS Mass Spectral Library 2017	LC-MS^n	652,475	64%	54%
Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds 3rd Edition	GCMS	3,400+	23%	22%
LIPIDS Mass Spectral Database	GCMS	430	27%	20%
Mass Spectra of Pesticides with Retention Indices, 2nd Edition	GCMS	1,300+	22%	11%
Mass Spectra of Volatiles in Food (SpecData) 2nd Edition	LC-MS^n	1,500+	–	–
Mass Spectra of Pesticides 2009	GCMS	1,200+	24%	20%
Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites, 5th Edition	GCMS	10,400+	67%	66%
Mass Spectra of Designer Drugs 2018	GCMS	26,000+	74%	71%
Mass Spectra of Physiologically Active Substances: Including Drugs, Steroid Hormones and Endocrine Disruptor 2011	GCMS	4,000+	66%	66%
Wiley Registry of Tandem Mass Spectral Data, MS for ID	LC-MS^n	10,000	–	–
METLIN Mass Spectral Database	LC-MS^n	1.2 mil	88%	87%
AntiBase: The Natural Compound Identifier	Natural	43,700+	85%	93%
Sigma-Aldrich Library of Raman Spectra	Raman	6,400+	–	–
Sigma-Aldrich Library of ATR-IR Spectra	ATR-IR	19,000+	–	–
Sigma-Aldrich Library of FT-IR Spectra	FT-IR	20,000+	–	–
13C-NMR of Organic Compounds	NMR	155,000	–	–
1H-NMR of Organic Compounds	NMR	228,000	–	–

Clinical	Forensics	Environmental	Toxicology	Food Safety	General Library	Specialty Library	Metabolomics	Page no.
	✓	✓	✓	✓	✓			6
✓	✓	✓	✓	✓	✓			6
✓		✓		✓	✓		✓	6
✓		✓			✓			6
	✓			✓		✓		7
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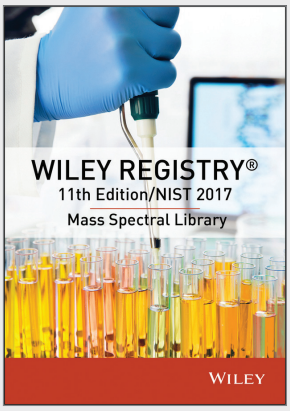
GC-MS

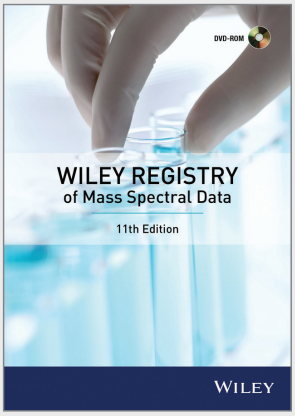


Wiley Registry 11th Edition/NIST 2017 Mass Spectral Library

Wiley/NIST, August 2017

ISBN 978-1-119-41223-6

The *Wiley Registry 11th Edition/NIST 2017* provides an essential tool for general unknown identification in analytes ranging from aerosols and VOCs to complex biologicals and organics. Consistently evolving to increase coverage, this library is the most important tool available to the modern laboratory, increasing instrument efficiency and boosting staff productivity.

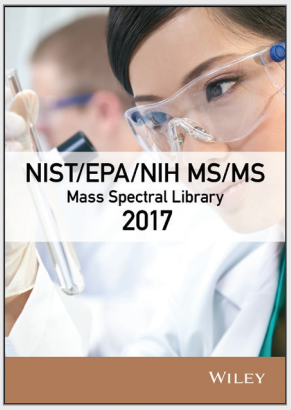


Wiley Registry of Mass Spectral Data, 11th Edition

Wiley, March 2016

ISBN 978-1-119-17101-0

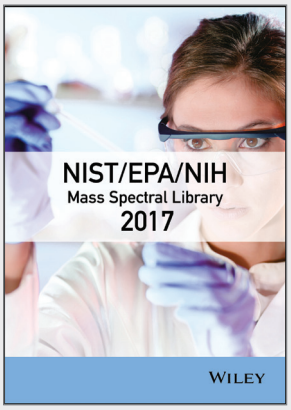
The *Wiley Registry 11th Edition* is the most comprehensive mass spectral library on the market. Applications include untargeted GCMS screening and accurate mass workflows with MS-TOF spectra. Included in the 11th edition are over 775,500 mass spectra, over 741,000 searchable chemical structures, and over 599,700 unique compounds.



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

NIST/Wiley, August 2017

ISBN 978-1-119-37673-6



NIST/EPA/NIH Mass Spectral Library 2017

NIST/Wiley, July 2017

ISBN 978-1-119-37674-3

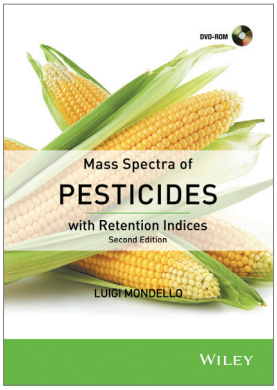
GC-MS

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

Luigi Mondello, October 2015

ISBN 978-1-119-06984-3

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) data, can be used to filter MS results, enabling the more reliable peak assignment of components in complex mixtures. This software contains >3,400 mass spectra, LRI retention data, calculated kovats RI, and searchable chemical structures of compounds of interest for the flavors and fragrances industry.

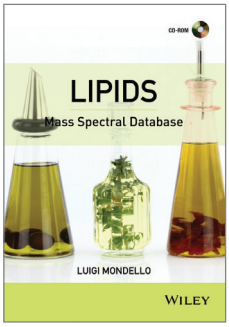


Mass Spectra of Pesticides with Retention Indices, 2nd Edition

Luigi Mondello, July 2016

ISBN 978-1-119-28404-8

This database contains 1,300 pesticide molecules classified in 20 different classes. This edition features 342 new pesticides compounds, 1,300 LRI values on a SLB-5ms column, and 147 LRI values on a EQUITY-1 column. Mass spectra, relative to standard and well-known simple matrix components, were obtained and recorded through GC-qMS separation/identification.



LIPIDS Mass Spectral Database

Luigi Mondello, July 2016

ISBN 978-1-119-28938-8

Mass Spectra of Volatiles in Food, 2nd Edition

Central Institute of Nutrition and Food Research, December 2003

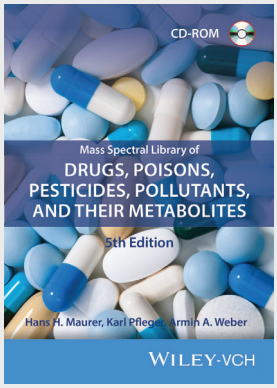
ISBN 978-0-471-64825-3

Mass Spectra of Pesticides 2009

Rolf Kühnle, January 2009

ISBN 978-3-527-32488-0

GC-MS

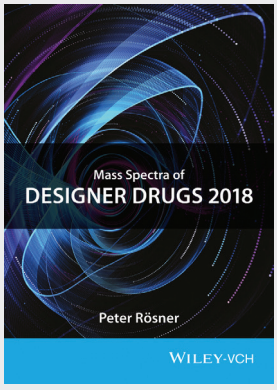


Mass Spectral and GC Data of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites, 5th Edition

Hans H. Maurer, Karl Pfleger, Armin A. Weber, December 2016

ISBN: 978-3-527-34327-0

This innovative reference library for clinical and forensic toxicologists has once more been extensively updated. The *5th Edition of Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants and their Metabolites* sees the addition of 1,780 data sets, bringing the total to 10,430 mass spectra and GC retention indices. Of the 175 categories included, This library showcases both past and present psychoactive substances, along with almost all relevant therapeutic drugs and 7,800 of their metabolites. This library comes as a set bundled with two hardcover volumes and CD software compatible with most instrumentation manufacturers.



Mass Spectra of Designer Drugs 2018

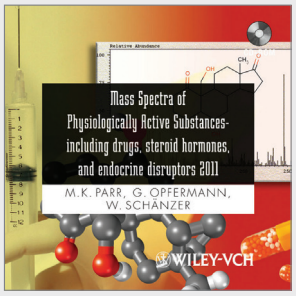
Peter Rösner, February 2017

ISBN 978-3-527-34527-4

Mass Spectra of Designer Drugs is the largest collection of chemical signatures of NPS and drugs of abuse in the world. This impressive mass spectral library was developed to support forensics and toxicology labs to combat this global health epidemic.

The 2018 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, 415 fentanyles, 1,042 synthetic cannabinoids, and 344 opiates.

With an average quality index per spectrum of 949.4 and 17,114 kovats retention indices this spectral library provides comprehensive data on the most up-to-date list of novel psychoactive substances.



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, March 2011

ISBN: 978-3-527-32727-0

LC-MS^n, Natural

METLIN Mass Spectral Database

Scripps Center for Metabolomics, Gary Siuzdak , H. P. Benton

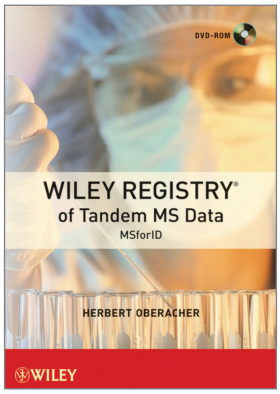
ISBN 978-1-119-37705-4

METLIN is a feature-rich, comprehensive metabolite and tandem mass spectrometry database designed for untargeted metabolomic analysis.

The database is an essential resource in pharmaceutical, preventive healthcare, and agricultural research, providing compound information for most of the 958,000 chemical structures. Data fields include name, structure, elemental formula, mass, CAS number, systematic name, KEGG ID, HMDB ID, PubChem ID, and commercial availability. Data were generated using multiple instruments, including Agilent, Bruker and Waters QTOF mass spectrometers.

Wiley's version of METLIN Mass Spectral Database comes bundled with the 2017 edition of the NIST MS/MS library featuring 652,475 spectra for 15,243 compounds and 123,881 ions.

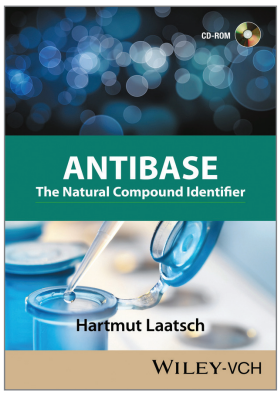
LC-MS^n



Wiley Registry of Tandem Mass Spectral Data, MS for ID

Herbert Oberacher, March 2012

ISBN 978-1-118-03744-7



AntiBase: The Natural Compound Identifier

Hartmut Laatsch, April 2017

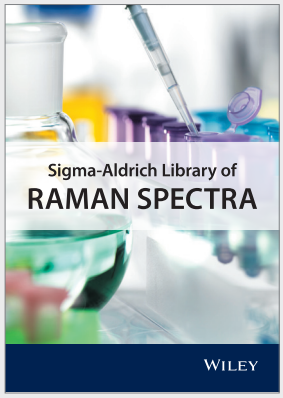
ISBN 978-3-527-34359-1

AntiBase is a comprehensive compilation of natural products featuring properties of more than 43,700 compounds. In addition to providing researchers the convenience of checking if a compound with antimicrobial effects has already been studied, *AntiBase* also provide insights into biological activity correlated to structural information as well. Antimicrobial activity is a key feature in translational and precision medicine making *AntiBase* an indispensable tool for emerging genomic and metabolomic research.

Natural

Raman, ATR-IR, FT-IR and NMR*

Wiley, on behalf of Merck KGaA Darmstadt, Germany, releases the Sigma-Aldrich Raman, ATR-IR, and FT-IR Collections which can be accessed through Wiley Spectra Lab



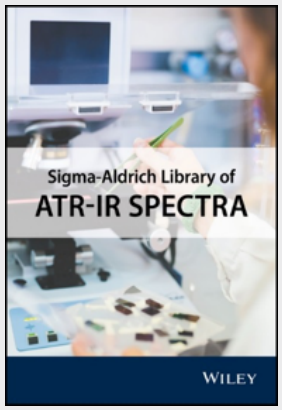
Sigma-Aldrich Library of Raman Spectra

ISBN 978-1-119-37678-1

Raman scattering is used in biomedical research, pharmacology, metabolomics, and more, giving researchers the ability to investigate the chemical composition and fingerprint of a vast range of both liquid and solid materials. Raman Spectroscopy is a non-invasive, non-destructive technique that offers many advantages, including handling a wide range of sample types with minimal sample processing, ability to couple to optical fibers and combine with microscopy for spatial resolution, and providing quantitative biomolecular information.

Raman

- Raman Spectra (in spectral range: 4000 to 100 cm-1): 6,487
- Distinct Sigma-Aldrich catalog numbers: 6,487
- Searchable Chemical Structures: 6,464
- Unique Compounds: 6,100
- Structures with InChI key: 6,279
- CAS Registry numbers: 6,438



Sigma-Aldrich Library of ATR-IR Spectra

ISBN 978-1-119-37680-4

Attenuated total reflection (ATR) sampling technique when coupled with IR has revolutionized solid and liquid testing by providing faster sampling rates, improved sample-to-sample reproducibility, and minimized user to user spectral variation allowing for more precise material verification and identification. ATR-IR spectroscopy is optimal for testing of solids like laminates, paints, plastics, and rubbers, as well as viscous liquids and biological materials. With strong advantages such as minimal sample preparation and analysis of samples in their native state, ATR-IR can be a valued technique in obtaining chemical images of pharmaceutical tablets for pharmacological research, analysis of automotive paint in forensics, determination of trans fat content in manufactured food products, and more.

ATR-IR

*Available with

Wiley Spectra Lab

Spectroscopy Solved

Sigma-Aldrich Library of FT-IR Spectra

ISBN 978-1-119-37678-8

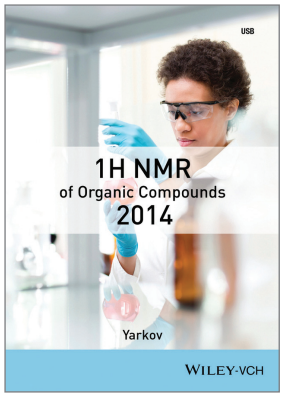
The data collection speed of FTIR analysis makes it the method of choice for identification of unknown materials and confirmation of production materials, while the sensitivity and spectral quality empowers many advanced research applications. Benefits of this sampling technique are evident in the reproducibility of data, and ease of maintenance and use. FTIR offers both qualitative and quantitative analysis of a wide range of organic and inorganic samples. Applications can include monitoring air quality to address environmental concern, identify seized drugs in forensics, molecular degradation assessment of polymers and plastics and more.

FT-IR

13C NMR of Organic Compounds 2014, 2nd Edition

Wolfgang Robien, February 2014

ISBN 978-3-527-33858-0



1H NMR of Organic Compounds 2014

Alexander Yarkov, October 2014

ISBN 978-3-527-33856-6

NMR

Partner Information

In addition to being directly available from **Wiley, Spectral Libraries** are available for purchase from the following companies.

Equipment Manufacturers

Including:

- Agilent Technologies
- PerkinElmer
- Shimadzu Scientific Instruments
- Thermo Scientific
- Waters
- Brukar Daltonics
- DANI
- JEOL
- LECO
- TA Instruments

Software Vendors

Including:

- ACD/Labs
- Bio-Rad Informatics
- MSP Kofel

Resellers and Lab Service Companies

Including:

- Scientific Instruments Services
- Quantum Analytical
- Proteome Software

For a full list, please visit
www.wiley.com/go/databases

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