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

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

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Wiley's Spectral Libraries and Databases

Techniques:

GC-MS

LC-MS^n

NMR

Wiley Spectral Libraries -

Illuminating Discoveries!

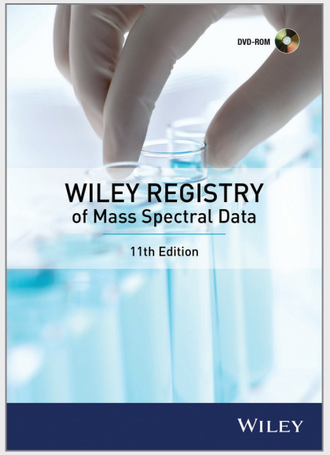
Fast, reliable analysis solutions for industry, research and public safety.

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.

GC-MS



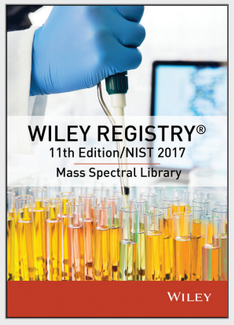
Wiley Registry of Mass Spectral Data, 11th Edition

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.

Improvements to the *Wiley Registry* include removal and sequestration of suspect spectra from the main library and partition of excess replicate spectra (beyond 4 replicates) into a separate replicate library. The result is a main library that has increased overall breadth and improved spectral search performance.

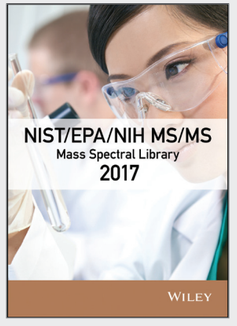


Wiley Registry 11th Edition/NIST 2017 Mass Spectral Library

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, The *Wiley Registry/NIST* is the most important tool available to the modern laboratory, increasing instrument efficiency and boosting staff productivity.



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

www.wiley.com/go/databases

GC-MS

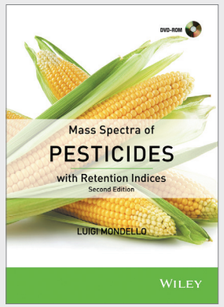
Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds, 3rd Edition

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.

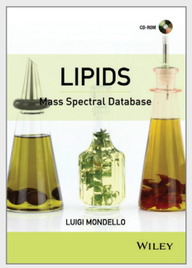
Mass Spectra of Pesticides with Retention Indices, 2nd Edition



Luigi Mondello, July 2016

ISBN 978-1-119-28404-8

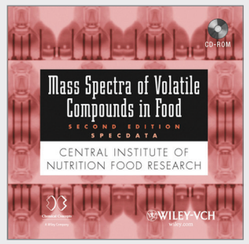
The *Mass Spectra of Pesticides with Retention Indices, 2nd Edition*, contains 1,300 pesticide molecules classified in 20 different classes. This edition features 342 new pesticides compounds, 1,300 LRI values on a SLB-5ms column, and 147 LRI values on a EQUITY-1 column. Mass spectra, relative to standard 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 (SpecData), 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

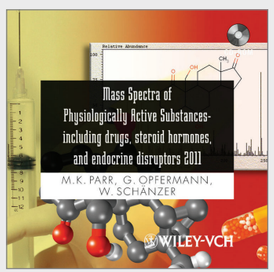
This innovative reference library for clinical and forensic toxicologists has once more been extensively updated. The *5th Edition of Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants and their Metabolites* sees the addition of 1,780 data sets, bringing the total to 10,430 mass spectra 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 2017

Peter Rösner, February 2017

ISBN 978-3-527-34379-9

Compiled by Dr. Peter Rösner, *Designer Drugs 2017* has been reviewed extensively by mass spectral experts Giselher Fritschi and Thomas Junge. This library now features 25,114 mass spectra and 19,665 unique compounds in over 30 classification groups. Showcasing the largest collection of chemical signatures for both novel psychoactive substances (NPS) and drugs of abuse in the world, *Designer Drugs 2017* better equips labs to combat the opioid and novel psychoactives epidemics currently threatening public health.



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

Applications

Name	Technique	Size	Uniqueness compared to WR 11e	Uniqueness compared to NIST 2014	Clinical	Forensics	Environmental	Toxicology	Food Safety	General Library	Specialty Library
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 / 652,475	46%	–	✓		✓		✓	✓	
NIST/EPA/NIH MS/MS Mass Spectral Library 2017	MS/MS	652,475	–	–	✓		✓			✓	
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	GC-MS	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 2017	GCMS	25,000+	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	–	–	✓	✓	✓				✓
13C-NMR	NMR	268,000	–	–	✓			✓		✓	
1H-NMR	NMR	157,000	–	–	✓			✓		✓	

LC-MS^n, NMR, Natural

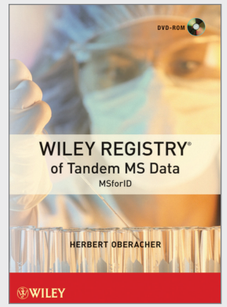
LC-MS

Wiley Registry of Tandem Mass Spectral Data, MS for ID

Herbert Oberacher, March 2012

ISBN 978-1-118-03744-7

This database contains 10,000 positive and negative mode spectra of over 1,200 compounds of interest for forensics, toxicology, and pathology. The *Registry* comes bundled with one of the most accurate search algorithms developed for LC-MSMS and is also available in formats compatible with current LC-MSMS software systems.



NMR

13C NMR of Organic Compounds 2014, 2nd Edition

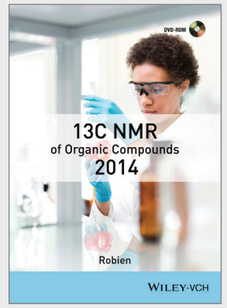
Wolfgang Robien, February 2014

ISBN 978-3-527-33858-0

1H NMR of Organic Compounds 2014

Alexander Yarkov, October 2014

ISBN 978-3-527-33856-6



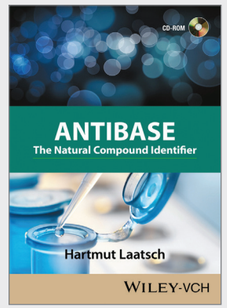
Natural

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.



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