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Mass Spectral Library

2023

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Wiley Registry®/NIST Mass Spectral Library 2023

User Manual

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PUBLISHER'S NOTE

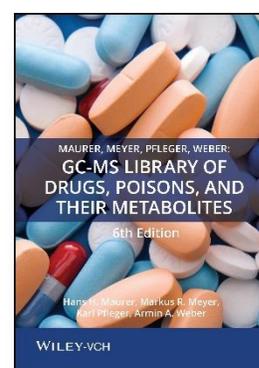
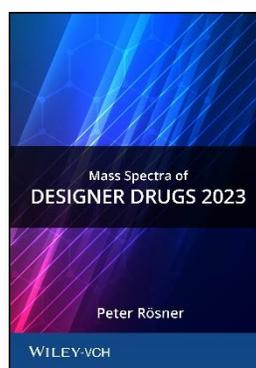
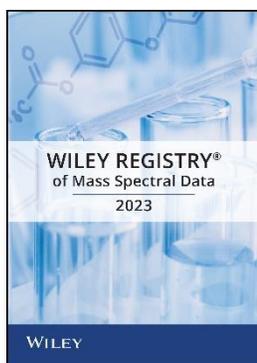
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries scientists have come to rely on.

The Wiley Registry/NIST combination library is consistently the most important tool available to the modern laboratory for the identification of global unknowns. Its breadth and scope guarantee the highest likelihood of identifying global unknown compounds. Containing the complete de-duplicated Wiley Registry 2023 and the latest 2023 update of the complete NIST EI and MSMS libraries, the Wiley Registry/NIST combination library provides the most up-to-date software and spectra available. The Wiley Registry/NIST 2023 library contains over 1 million mass spectra collected by the NIST Mass Spectrometry Data Center and Wiley Science Solutions.

SPECTRABASE

Address: <https://spectrabase.com/>

SpectraBase is a free web-based database that provides free instant access to the latest compounds covered by Wiley spectral libraries.



CONTACT INFORMATION

Editorial Correspondence

Wiley welcomes contributions of spectra for compounds, especially novel compounds not presently covered in the spectral library. Wiley can handle data in any machine-readable format. Data submissions, editorial notes, and corrections should be sent to the address below:

Wiley Science Solutions

c/o John Wiley & Sons, Inc.

111 River Street

Hoboken, NJ 07030-5774 USA

Telephone: +1-201-748-6000

Fax: +1-201-748-8888

Email: dbinquiry@wiley.com

Website: <https://sciencesolutions.wiley.com/>

Customer Care

Customer care is available online or through correspondence at:

Customer Care Center – Consumer Accounts

10475 Crosspoint Blvd.

Indianapolis, IN 46256 USA

<https://support.wiley.com/s/>

COMPLIANCE

Products manufactured by WTS are in compliance with Directive 2011/65/EU of the European Parliament and of the Council of 8 June 2011 on the restriction of the use of certain hazardous substances in electrical and electronic equipment (also known as “RoHS Recast”). In addition, this declaration of conformity is issued under the sole responsibility of WTS. Specifically, products manufactured do not contain the substances listed in the table below in concentrations greater than the listed maximum value.

Substance	Maximum Limit (ppm)
Lead (Pb)	1000
Cadmium (Cd)	100
Mercury (Hg)	1000
Hexavalent Chromium (Cr6+)	1000
Poly Brominated Biphenyls (PBB)	1000
Poly Brominated Diphenyl ethers (PBDE)	1000

GETTING STARTED

Hardware and Software Recommendations

- Operating System: Microsoft Windows (Windows 10 or 11 recommended)
- CPU: AMD or Intel processor, preferably multiple core
- Software: 32-bit or 64-bit software
- Memory: At least 2GB
- Disk Space: At least 2GB free space

The library is provided in multiple formats, but is not supplied with manufacturer software. Mass spectrometry software should be installed prior to installing the mass spectrometry library, in any format.

If you have questions about the format of the database or need to order a replacement, please contact Wiley Customer Care at <https://support.wiley.com/s/>.

Registration Code

A registration code accompanies the packaging provided with the flash drive. This database may be installed on only one machine.

License

Unless specified otherwise in writing, this product is sold as a single computer license (for the avoidance of doubt, not networked). Multiple license and network licenses are available. For additional licenses, please contact your sales representative or e-mail dbinquiry@wiley.com.

Help keep the cost of libraries down by reporting all copyright and license violations to the publisher at dbinquiry@wiley.com.

COMPATIBILITY

Wiley has provided you with a selection of native manufacturer formats to aid you in your installation. Please consult your software manufacturer's documentation and customer support before contacting Wiley Customer Support. This flash drive contains the following manufacturer formats:

- Agilent ChemStation
- Agilent MassHunter
- NIST MS Search
- PerkinElmer TurboMass
- Shimadzu GCMSsolution
- Thermo Xcalibur™
- Waters MassLynx

DIRECTORY ASSISTANCE

The table below lists the format, installation file, and their default target directory. If two directories are listed, the first directory is for the spectral data files, the second directory is for the structure files. If one directory is listed, all spectra and structure files are installed into that directory. All installations allow a manual override of the default directory path.

Format	Installation File	Default Directory
ChemStation	SetupW23N23ChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupW23N23MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
MS Search	SetupW23N23MSSearch.exe	C:\NIST23\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupW23N23TurboMass.exe	C:\TurboMass\Idendb\{libraryname}\{filename} C:\TurboMass\Idendb\STRUCTDB\{libraryname}\{filename}
GCMSsolution	SetupW23N23GCMS-Solution.exe	C:\GCMSsolution\Library\{libraryname}\{filename}
Xcalibur	SetupW23N23Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearch\{libraryname}\{filename}
MassLynx	SetupW23N23MassLynx.exe	C:\MassLynx\Idendb\{libraryname}\{filename} C:\MassLynx\Idendb\STRUCTDB\{libraryname}\{filename}

*Installations will include download of a minimum of four {libraryname}: W23N23main, W23N23rep, W23N23leg, W23N23lq

QUICK-START

1. **Registration Code:** After reading the EULA, enter the Registration Code found on the Certificate of Authenticity provided and begin installation.
2. **Computer ID:** The installation program will combine the Registration Code with unique information from your computer to generate a unique Computer ID. If the computer is attached to the internet, the installer can automatically register your computer and provide a Registration Code. If the computer is not attached to the internet, follow procedure 2a or 2b below to manually register your installation.
 - a. Computer ID – No direct internet: Note the Computer ID and Registration Code and go to <https://www.wileyptmediareg.com/Activation> and follow the on-screen instructions. Note the resulting Activation Code and use it to complete on-screen installation prompts on the computer.
 - b. Computer ID – No internet: Contact Wiley Customer Support at <https://support.wiley.com/s/> or by telephone at (877) 762-2974.
3. **Installation:** Please note installation requires the Registration Code that accompanied your packaging. Install the formats you wish to use on a single computer, following the on-screen prompts to “run” the installer. N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.

Customer Care Center – Consumer Accounts

10475 Crosspoint Blvd.
Indianapolis, IN 46256 USA

STEP-BY-STEP INSTALLATION

* This installation process mirrors installation on the NIST MS Search software.

1. A Registration Code will accompany the packaging provided with your flash drive. If your provided code does not work or your flash drive is not accompanied by a Registration Code, alert Wiley Customer Service at <https://support.wiley.com/s/>.

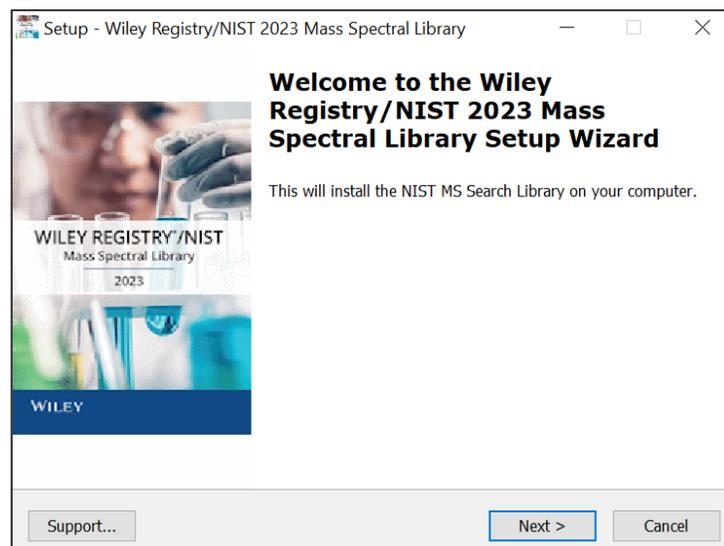
You will be unable to install this library without a Registration Code. Carefully read the End User License Agreement contained on the flash drive or the accompanying packaging before using and/or installing this product.

2. Insert the flash drive for installation. One file "Installation.htm" is included on the drive to simplify installation by using your web browser. Choose the format(s) you wish to install. Choosing to run the installer will bring you to a set-up wizard splash screen. Choose "Next."

N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.

Your license entitles you to install the library on one (1) machine.

Please note that the installation files are unsigned – so a warning may be displayed in Windows. Press run and proceed to the installation. Repeat this process for all of the formats you wish to install on the one computer.



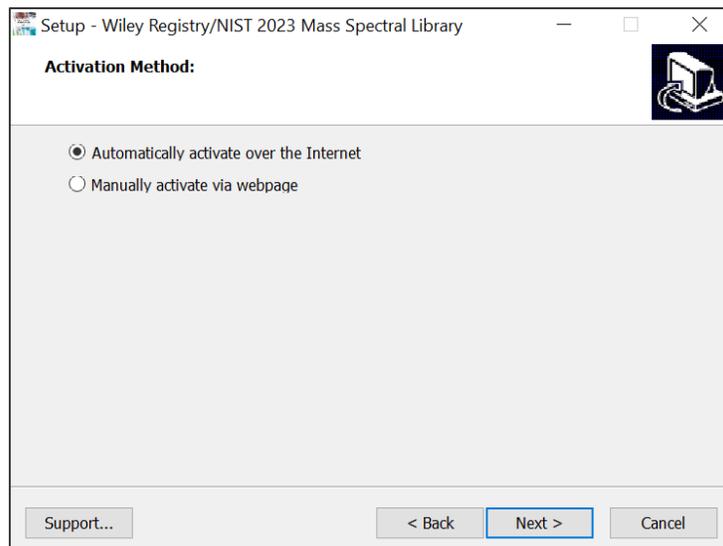
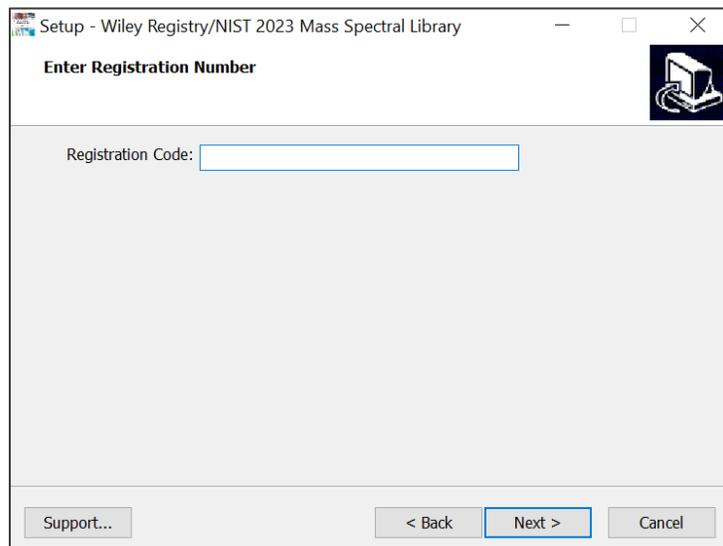
N.B.: Install your spectra/data analysis software prior to installing the format(s) you wish to install.

3. Registration Code and Machine ID

Your Registration Code appears on the Certificate of Authenticity accompanying your packaging.

Enter the Registration Code exactly as it appears to begin the installation and press "Next." If the code is incorrect, an error screen will appear.

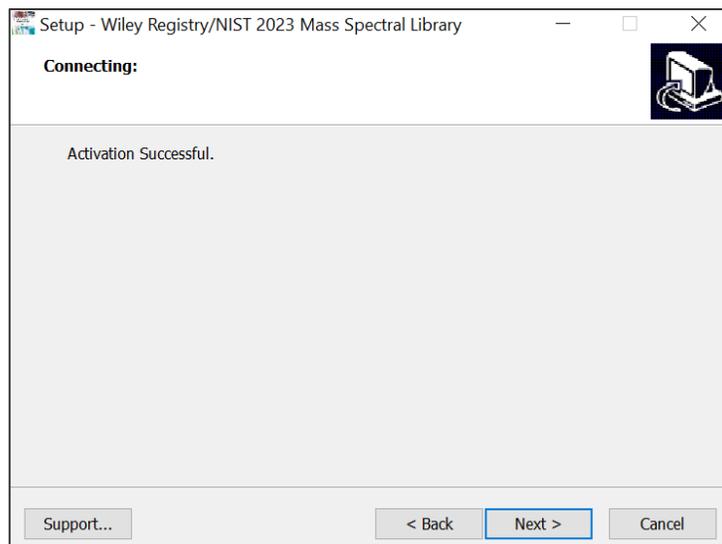
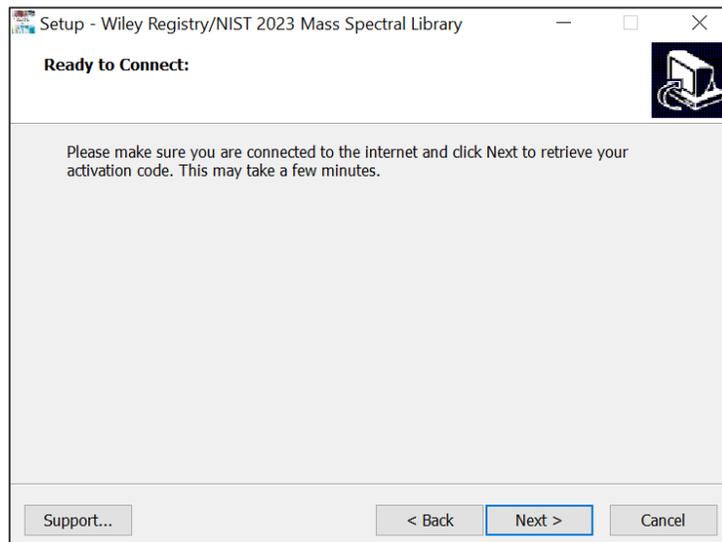
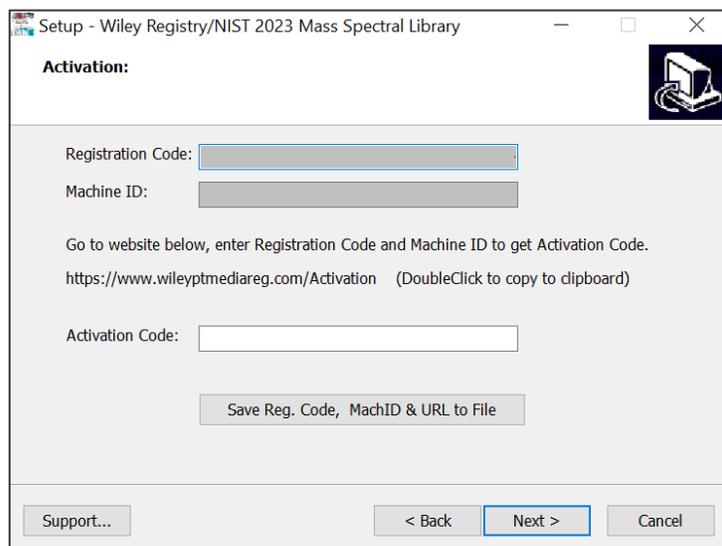
If the Registration Code is correct, you will be brought to the Activation screen. If your machine has internet connectivity, choose to "Automatically activate over the internet" and then click "Next" to begin internet activation.



- If you choose to manually activate, the Registration Code and the Machine ID will be automatically filled in. You may either double click the web address to copy it to your computer's clipboard and paste it in a web browser, or enter the URL as listed in your web browser.

Alternatively, you may save the Registration Code, Machine ID and URL to a text file that will be saved to the root directory.

In the web browser, enter the Registration Code and the Machine ID. The next screen will provide the Activation Code. Copy this code down and save it, entering it into the Activation screen on the computer that you are installing the spectral library on.



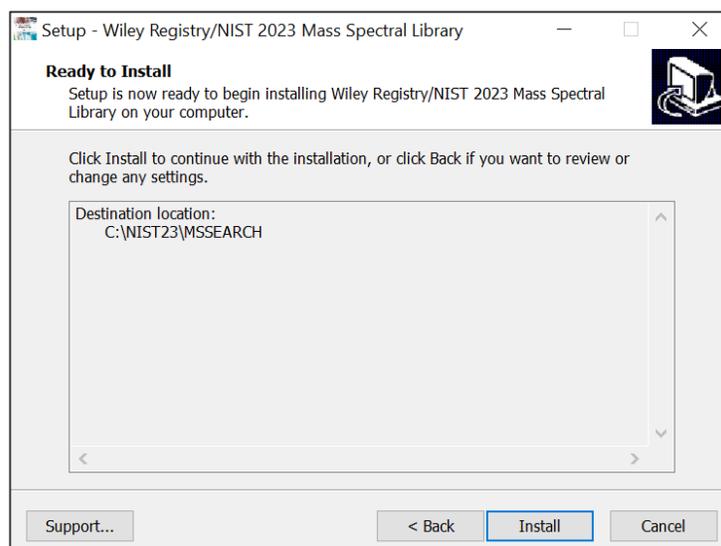
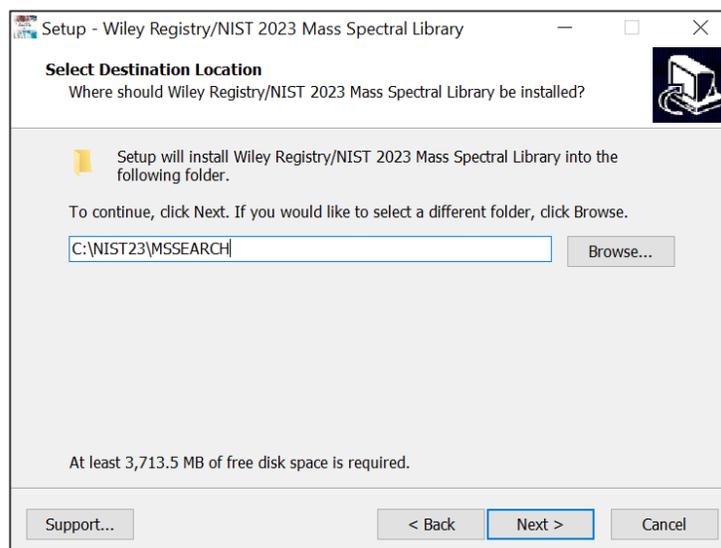
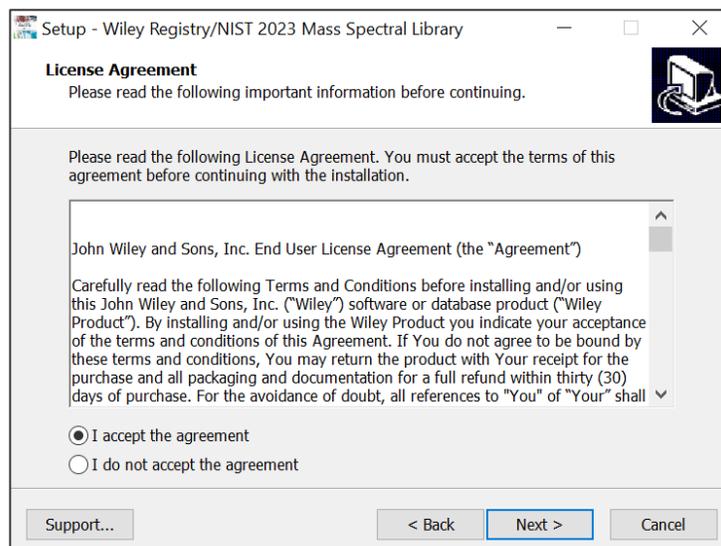
- Once your activation is successful, proceed by pressing "Next." The next screen contains the End User License Agreement (36).

Read the agreement carefully and select the "I accept the agreement" option. Then, choose "Next" to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.

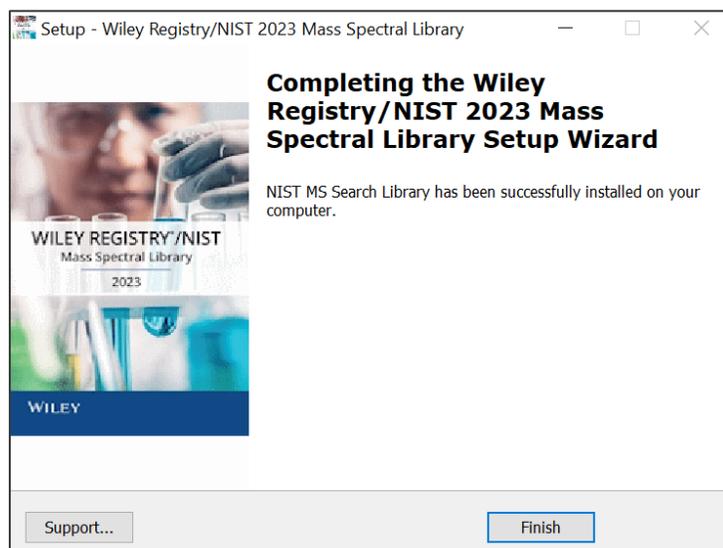
- Press "Next" to proceed to the next step. At this point, the installer will unpack and install the library in the format you have selected. Confirm the target directory and destination location before proceeding.

- Ready to install? After selection of the Destination Folder, choose the "Install" button to begin installation. Allow installation to finish before closing out any applications.

N.B.: For Chrome and Firefox browsers, copy the install file onto a temporary directory. The installer requires RegistrationProcess.dll. Please copy the installer and dll into one directory and activate the installer.



8. Once installation is complete, press "Finish." Be sure to consult your spectra/data analysis software's instructions for connecting to new libraries – some are automatic, but some require manual connection within the software.



Repairing or Uninstalling

Repairing or uninstalling the library should be managed using the "Add/Remove Programs" utility in Windows. If the library is manually moved, removed, or installed using overwrite mode, the Windows utility may not work.

Getting Help

Getting Help – you can choose to go to: <https://support.wiley.com/s/>

GENERAL DATABASE CONTENT

Wiley mass spectrometry libraries have a wide variety of uses. Practitioners and researchers are encouraged to evaluate their own needs and decide what libraries are appropriate for them.

Wiley Registry/NIST 2023 – 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.

- W23N23 main: Use this library for untargeted analysis in everyday scientific work.
- W23N23 replicate: Use this library when further confirmation or results are required.
- W23N23 legacy: Use this library when searching for confirmation on past work.
- W23N23 low quality: Use this library when further confirmation or results are required.

See <https://sciencesolutions.wiley.com/> for other mass spectrometry, NMR, IR, and enterprise spectroscopy software from Wiley-VCH and John Wiley and Sons, Inc.

Basic Functions

The enclosed library can be used as the primary search library or can be searched along with other libraries. We recommend, for mission-critical tasks, that users consult both a general library such as the *Wiley Registry/NIST Mass Spectral Library 2023* and a specialized library such as the *GC-MS Library of Drugs, Poisons, and Their Metabolites, 6th Edition* or *Mass Spectra of Flavors and Fragrances of Natural and Synthetic Compounds 3rd Edition*.

Search Tips

When using parametric searching, many text search programs provide better results when names are begun and ended with wild cards (e.g., "*""). However, in NIST MS Search, this approach will not work.

While every effort has been made to include a broad spectrum of compounds, when trying to match an unknown against the database, bear in mind that some unknowns, especially new variants of designer drugs and steroids established after publication may only be available in our specialized collections.

NIST MS Search:

Comprised of four parts:

- W23N23 MAIN
- W23N23 REP
- W23N23 LQ
- W23N23 LEG

The REP, LQ, and LEG parts are the W23 REP, LQ, and LEG libraries.

The following 'fields' were added to the COMMENT field (tagged comment fields):

- DOI – Literature source reference, resolvable via doi.org
- Exp-RI_Any – Retention Index values – theoretical values for n-alkanes
- Exp-RI_Polar – Retention Index values – Standard Polar column
- Exp-RI_Semi-standard_non-polar – Retention Index values – Standard Semi-Non-Polar column
- Exp-RI_Standard_non-polar – Retention Index values – Standard Non-polar column
- NIST_Seq# - For records from NIST23 mainlib and replib (indicates record number in NIST23 mainlib and replib respectively, leading/prefix letters M and R are used to indicate from which part (mainlib or replib) a record comes). N.B.: The NIST spectrum number (NIST#, NISTNO) – a unique spectrum ID given by NIST (which is preserved through different versions of the NIST library) is given in data field 'NISTNO'.
- Note – Additional comments, mainly from expert review
- QI – Quality Index
- Source – Source of spectrum/contributor/literature reference
- SpectrumID – WileyID (a unique spectrum ID given by Wiley - which is preserved through different versions of the Wiley Registry – and since NIST11 also for the NIST spectra)
- SplashID – Hash value for a spectrum
- The experimental RI (Exp_RI...) values were also added to the Retention Index field – and indexed accordingly to the given type, only for NIST23 records.

For records for which no experimental RI data was available, calculated RI values (where available) were entered in the Retention Index field. These are 'Estimated non-polar retention index (n-alkane scale)' values which are calculated with the algorithm implemented in the NIST MS Search software. These are indexed as 'Unspecified'.

NIST MS Search works by default by calculating Match Factors on only a range of m/z values in the two mass spectra that are compared. The starting value of this range is determined by the lowest m/z value exhibiting ion current in either the sample spectrum or the library spectrum, whichever is higher. In the case where a library spectrum contains no peaks below m/z 256, all the peaks below m/z 256 in the sample spectrum are disregarded in calculating the Match Factor if the library spectrum has only ion current at m/z 256 and above. This gives that library spectrum an artificially high Match Factor. By specifying a lower m/z value, rather than letting the program determine it, the MF in the above example will be much lower because it is being penalized based on the fact that the library spectrum has no peaks at m/z values where the sample does.

Library Search Options

Search MS/MS Libraries Automation Limits Constraints RI (GC)

Apply Limits

Minimum Off 1

Minimum m/z equals to 10

Maximum m/z Off 2000

Set Default

Agilent ChemStation/MassHunter:

Comprised of four parts:

- W23N23 MAIN
- W23N23 REP
- W23N23 LQ
- W23N23 LEG

COMMENTS (Miscellaneous Information) field:

- For all records, the WileyID is given as 'SpectrumID: '.
- For NIST records, the NIST spectrum number (NISTNO/NIST#) and the Sequential NIST record number is given as 'NIST MS#' and 'Seq#' respectively. The Seq# has M or R to indicate from which NIST library part the NIST spectrum comes.
- 'Molform' – given if the molecular formula differs from the molecular formula given with the spectrum
- 'Orig. form.' – given for compounds which have non-standard isotopes, except for deuterium (which is given as 'D')
- Additional comments, mainly from expert review (no data field name given for these)

Semi-Standard Non-polar experimental RI values added to the Retention Index field (for n-alkanes the theoretical/definition values are given). 'Estimated non-polar retention index (n-alkane scale)' values are added to the User Index field.

Pseudo CASNOs were used to point to the structures in the structure add-on files.

Shimadzu GCMSolution:

Comprised of seven parts:

- The W23N23 main part split into four parts:
 - MAIN 1: 250,000 records
 - MAIN 2: 250,000 records
 - MAIN 3: 250,000 records
 - MAIN 4: 160,115 records
- W23N23 REP
- W23N23 LQ
- W23N23 LEG

COMMENTS field – no such field available

'Estimated non-polar retention index (n-alkane scale)' values are added to the 'Retention Index' field.

PerkinElmer TurboMass/Waters MassLynx:

Comprised of four parts:

- W23N23 MAIN
- W23N23 REP
- W23N23 LQ
- W23N23 LEG

COMMENTS field:

- For records from NIST23 (mainlib/replib), the NISTNO is given as 'NIST#' - '(M)' or '(R)' indicate from which part (mainlib or replib) a spectrum comes from.
- For Wiley spectra, the WileyID is given – as 'WID: '.

Semi-Standard Non-polar experimental RI values added to the 'Value 1' field (for n-alkanes the theoretical/definition values are given). 'Estimated non-polar retention index (n-alkane scale)' values are added to the 'Value 2' field.

Pseudo CASNOs were used to point to the structures in the structure add-on files.

Source Codes

If code stands for a literature reference, the meaning of the four items are for: 'source-volume-page number-compound label'

E.g. The source information 'K-108-2070-19' decodes to:

- K - Journal Chem. Ber. (Chemische Berichte)
- 108- Volume 108 of the journal
- 2070 - Page number on which the spectrum or compound is given
- 19 - Label of the compound in the article

If the source points to anything other than a scientific publication, 'volume-page number-compound label' have varying information (usually year and/or ID number).

Source Code	Source
A	Archives of Mass Spectral Data
A1	Organic Letters
A1	JN Ronson, SJRowland, Nature, 561-563
A2	Mendeleev Communications
A2	Jeanne Ayache, profil reactionnel des reactions de fragmentatin des ethylene-acetals des cyclanones substituees en spectrometrie de masse par impact electronique, These, University of Paris, 1978
A3	Organic Preparations and Proceedings
A3	Dr. Allenmark, Univ. Hosp., Linkoping, Sweden
A4	Organometallics
A4	F. Arcamone, G. Cassinelli, G. Franceschi, S. Penco, C. Pol, S. Redaelli and A. Selva, Structure and Physical Properties of Adriamycin, Springer-Verlag, Berlin, 1972
A5	Organic Process Research and Development
A5	Yoshiro Masada, Analysis of Essential Oils by Gas Chromatography and Mass Spectrometry
A6	Journal of Chemical Technology and Biotechnology
A6	Vlada Hanus, The J. Heyrovsky Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Czechoslovakia
A7	Journal of the American Society for Mass Spectrometry
A7	Parmar, V. S., University of Delhi, Delhi-110 007
A8	International Journal for Mass Spectrometry
A8	Gustav Graff, The Hormel Institute, University of Minnesota, Austin, Minn., 55912
A9	European Journal for Mass Spectrometry
A9	Muramatsu, T., University of Minnesota, The Hormel Institute, Austin, Minn., 55912
AA	Atlas of Mass Spectral Data (Wiley)

AB	Biochimica et Biophysica Acta
AC	Bulletin Societe Chimique de France
ACI	Angewandte Chemie International Edition
ACR	Analytical Chemistry Research
ACS	ACS Comb. Sci.
AD	Mass Spectrometry Data Centre, AWRE, Aldermaston, Berks., England
AE	Journal of Biological Chemistry
AF	Journal of Medicinal Chemistry
AG	Journal of Organometallic Chemistry
AH	Monatshefte fur Chemie
AI	Archiv der Pharmazie
AJ	Bulletin of the Chemical Society of Japan (Nippon Kagakukai)
AJC	Arabian Journal of Chemistry
AJO	Asian J. Org. Chem.
AK	The Biochemical Journal
AL	Biochimie (Bull. Soc., Chim. Biol. Fr.)
AM	S. P. Markey, University of Colorado Medical Center, Denver, CO
AN	Bulletin Societe Chimique de Belges
AO	Environ. Health Perspec.
AOC	Appl. Organometal. Chem.
AP	Amer. Petroleum Inst., Res. Project 44
APC	Arch. Pharm. Chem. Life Sci.
AQ	Pure Appl. Chem.
AR	Pest. Biochem. Physiol.
ARK	Arkivoc: A Platinum OA Journal of Organic Chemistry
AS	J. G. Lawless, NASA, Moffett Field, CA
ASC	Adv. Synth. Catal.
AT	Tetrahedron Letters
AU	Carbohydrate Research
AV	Analytical Biochemistry
AW	Inorganic Chemistry
AX	Amer. Petroleum Inst., Res. Project 44
AY	Journal of Lipid Research
AZ	Chemistry and Industry, London
B	Australian Journal of Chemistry
B1	Synthetic Communications
B2	The Metropolitan Museum of Art
B2	A. P. Bruins, Intramolecular Functional Group Interactions and Ion Molecule Reactions of Gaseous Ions from Some Benzylamino and Benzyloxy Compounds, Amsterdam, 1976
B3	Journal of Synthetic Organic Chemistry

B3	Advances in Prostaglandin, Thromboxane, and Leukotriene Research, vol. 18, Mass Spectra of Prostaglandins and Related Products, New York 1989
B4	Journal of Chemical Research
B4	HP Particle Beam LC/MS Book of Spectra, Dr. Alex Apffel, Hewlett-Packard Company, Palo Alto, California 94304
B5	Chemical Science
B5	Mervyn Lewis, University of Bristol
B6	Russian Chemical Review
B6	Yao-Zu Chen, Department of Chemistry, Lanzhou University, Lanzhou, PRC
B7	Journal of the Chemical Society - Dalton Transactions
B7	Polycyclic Aromatic Compounds
B8	Biochemica, Biophysica Acta
B8	William T. Miller, Department of Chemistry, Cornell University, Ithaca, NY 14850
B9	Carbohydrates Research
B9	Chrys Wesdemiotis, Department of Chemistry, University of Akron, Akron, OH 44325-3601
BA	D. J. Harvey and M. G. Horning, Baylor College of Medicine, Houston, TX, W. R. Sherman and M. Zinbo, Washington University School of Medicine, St. Louis, MO, C. J. W. Brooks and B. S. Middleditch, University of Glasgow, Glasgow, Scotland
BB	Dibenzoacridine, R. Depaus, CES Joint Research Center, Netherlands
BC	J. L. Aubagnac (see MA)
BD	A. T. Balaban, Comitetul de State Pentru Energia Nucleara, Institutul de Fizica Atomica, Bucharest, Romania
BJO	Beilstein J. Org. Chem
BK	Bruce Kennett, CSIRO, Australia (see XW)
BL	BLR Drug Spectra, Subcommittee 6, Amer. Soc. Mass Spectrom.
BM	Quantitative Mass Spectrometry, B. J. Millard
BR	Mass Spectra of Paraffins with 10-24 Carbon Atoms, V.A. Herlan
BS	Biomedical Mass Spectrometry, Indexing Reference Forms
BU	Buchert, Arne, Ministry of the Environment, National Food Institute, Denmark (obtained 1981)
BW	Bruce Wilkes
C	J. Amer. Chem. Soc.
C1	Revue Roumaine de Chimie

C1	Kiyotaka Kobayashi, Department of Chemistry, Gakushuin University, Toshima-ku, Tokyo, Japan
C2	Bio Organic & Medicinal Letters
C2	Richard Caprioli, The Analytical Chemistry Center, University of Texas Medical School (obtained 1981)
C3	New Journal of Chemistry
C3	Takeshi Kinoshita, Central Research Laboratories, Sankyo Co., Ltd., Hiromachi Shinagawa-ku, Tokyo 140
C4	Chemistry Letters
C4	Akio Kinumaki, Microbiloligical Department, Biological and Chemical Research laboratories, Tanabe Seiyaku Co., Ltd., Toda, Saitama, Japan
C5	Chimia
C5	Tamio Ueno, Pesticide Research Institute, College of Agriculture, Kyoto University, Kyoto
C6	E. Brachen
C7	Lu Xiang-Jun, Central laboratory, Nankai University, Tianjin, PRC
C8	Firmenich
C9	Quaderni di laboratorio di spettrometria di massa, No.2 1991
CA	Archives of Mass Spectral Data, 3, 536-514 (1972)
CAJ	Chem. Asian J.
CAY	Cayman Chemical Company
CB	A. L. Burlingame, ed., Advances in Analytical Chemistry and Instrumentation, Vol. 8, Wiley-Interscience, New York, NY, 1970
CBC	ChemBioChem (Wiley journal)
CBD	CHEMISTRY & BIODIVERSITY
CC	Callery Chem. Co., Callery, PA
CCA	Croat. Chem. Acta
CCC	ChemCatChem (Wiley journal)
CCL	Chinese Chemical Letters
CD	P. Z. Chong, Y. E. Peng, Q. N. Fang; Mass Spectra of Natural Organic Compounds, Chinese Academy of Medical Science: Institute for Pharmacological Studies, 1983
CE	Catherine E. Costello, MIT, Dept. of Chem., Cambridge, MA 02139
CG	G. Spiteller, Massenspektromische Strukturanalyse Organischer Verbindungen, Verlag Chemie, GmbH, Weinheim, Germany, 1966
CH	M. T. Cheng, Polyandrocarpidines: Antimicrobial and Cytotoxic Compounds from the Marine Tunicate Polyandrocarpa SP. (Thesis), U. of Ill. at Urbana-Champaign, 1978

CHO	ChemistryOpen
CI	M. T. Cheng, Chevron Research & Technology Company, 100 Chevron Way, Richmond, CA 94802-0627
CIZ	Chemie in unserer Zeit
CJ	Claus Koppel - Free Univ. of Berlin
CJC	Chin. J. Chem.
CK	J. H. Beynon, R. A. Saunders and A. E. Williams, The Mass Spectra of Organic Molecules, Elsevier Publishing Co., Amsterdam, The Netherlands, 1968
CL	W. H. McFadden, Techniques of Combined Gas Chromatography/Mass Spectrometry: Applications in Organic Analysis, Wiley-Interscience, New York, NY, 1973
CM	Chemical Concepts GmbH, Tel. +49(0)6201-606433, P.O. Box 100202, D-69442 Weinheim, Federal Republic of Germany
CMC	ChemMedChem
CO	Continental Oil Co., Ponca City, OK
CP	Wan-Kai Chu, Painting Industry Research Institute of Chemical Industry, Lanzhou, China
CPC	ChemPlusChem (Wiley journal)
CR	CRC Handbook of Mass Spectra of Drugs, 1981
CR	Chem Research in Toxicology
CRT	Chemical Research in Toxicology
CRY	Cryst. Res. Technol.
CS	J. Seibl, Massenspektrometrie, Akademische Verlagsgesellschaft, Frankfurt am Main, Germany, 1970
CSC	ChemSusChem (Wiley journal)
CSS	Chem. Sci. - Chemical Science RSC
CST	Catal. Sci. Technol.
CT	Journal of Toxicology: Clinical Toxicology
CU	Arch. Mass Spec. Data, 3, 510-524 (1972)
CW	D. H. Williams and I. Howe, Principles of Organic Mass Spectrometry, McGraw-Hill Book Co. (UK), 1972
CY	Arch. Mass Spec. Data, 3, 388-402 (1972)
D	Biochemistry (USA)
D1	Synletter
D2	E. G. DeJong, Mass Spectrometry of Permethylated Disaccharides and some Related Compounds, Rotterdam, 1980
D3	Waller-Dermer, Biomedical Applications of Mass Spectrometry, Wiley-Interscience, 1980
D4	Dragoco Inc., Gordon Dr., POB 261, Totowa, NJ 07512

D5	McGuire, J.M., United States Environmental Protection Agency, Environmental Research Laboratory, Athens, Georgia, 30613-7799
D6	Comptes rendus des (Seances de l'Academie Francaise Series ?)
D7	Comptes rendus des Seances de l'Academie Francaise Series D
D8	Archiv der Pharmazie
D9	Journal of the Brazilian Chemical Society
DA	Chemosphere
DB	H. Budzikiewicz, C. Djerassi, and D. H. Williams, Structural Elucidation of Natural Products by Mass Spectrometry, Vols. 1 and 2, Holden-Day, San Francisco, 1964
DC	Ibid., Mass Spectrometry of Organic Compounds, 1967
DD	Int. J. Environ. Anal. Chem.
DE	C. Djerassi, Stanford University, Palo Alto, CA
DF	Zhurnal Organicheskoi Khimiia
DG	Khimiya Geterotsiklicheskih Soedinenii
DH	Zhurnal Obshchei Khimii
DI	Akademia nauk SSSR, Doklady, Seria Khimiia
DJ	Recueil Des Travaux Chimiques Des Pays-Bas
DK	C. R. Acad. Sci., Paris, Ser. C. Sciences Chimiques
DL	Bulletin de la Societe Royale des Sciences de Leige
DM	F. W. McLafferty, Interpretation of Mass Spectra, 2nd ed. 1973
DN	O. A. Mamer, W. J. Mitchell and C.R. Scriver, Eds. Application of GC/MS to the Investigation of Human Disease
DO	A. Frigerio and N. Castagnoli, Jr., Eds. Mass Spectrometry in Biochemistry and Medicine, Raven Press, New York, 1974
DP	Spectroscopy Letters
DQ	Z. Phys. Chem. (Frankfurt)
DR	Bulletin de l'Academie Royale de Belgique (Classe des Sciences)
DS	Safe and Hutzinger, Mass Spectrometry of Pesticides and Pollutants
DT	R. Hague and F. J. Biros, Eds. Mass Spectrometry and NMR Spectroscopy in Pesticide Chemistry, Plenum Press, New York, 1974
DU	Drug Metabolism and Disposition
DV	Svensk Kemisk Tidskrift
DW	Brennstoff-Chemie
DX	J. Chem. Soc. Japan (Nippon Kagaku Zasshi)
DY	Antimicrob. Agents Chemother
DZ	Zeitschrift fur Anorganische und Allgemeine Chemie

E	Anal Chem
E1	Chemical & Pharmaceutical Bulletin
E1	Edgewood Arsenal Technical Report EC-TR-76059, June, 1976 Samuel Sass, Theodore W. Dolzine, and Timothy L. Fisher
E2	Chemia Switzerland
E2	Edgewood Arsenal Technical Report EC-TR-76111, July, 1977 Timothy L. Fisher and Samuel Sass
E3	Edgewood Arsenal, private communication
EA	Walter Shackelford, USEPA, ERL, Athens, GA 30605, Pollutant Collection
EB	Ella Baranofsky
EC	Chem. Div., Air Pollution Control Directorate, Ottawa, Canada
ED	E. F. Domino, Department of Pharmacology, University of Michigan
EK	James Little, Eastman Chemical Co., Kingsport, TN
EL	Eli Lilly, J. Occolowitz, MAT 731
EM	European Journal of Mass Spectrometry
EMC	European Journal of Medicinal Chemistry
EN	Proceedings of the International Conference on Environmental Pollution, September 1981, Thessaloniki, Greece, Editor, A. Anagnostopoulos
EP	J. McGuire, Environmental Protection Agency, Athens, GA
ES	Environmental Science and Technology
ET	Misc Spectra
EU	R. Depaus, Commission of the European Communities Joint Research Center, Holland
F	Tetrahedron
F1	Doklady Chemistry
F2	Acta Chimica Hungarica
F2	Edwin H. Flynn, Cephalosporins and Penicillins, Academic Press, New York, NY, 1972
F2	Journal of Medicinal Chemistry
F3	Israel Journal of Chemistry
F4	Synthesis
F5	Organic and Biomolecular Chemistry
F6	Angewandte Chemie
F7	Chemical Society of Pakistan Journal
F8	Oriental Journal of Chemistry
FA	Analytical News, Finnigan MAT
FAC	Field Analyt. Chem. Technol.
FCX	Food Chemistry: X
FF	Flavour Fragr. J.
FI	Application Tips, Finnigan Corp., Sunnyvale, CA
FL	Finnigan Spectra, Finnigan Corp.
FM	Oliver Fiehn, UC Davies

FT	F. Turecek, J. Heyrovsky, Inst. of Phys. Chem. and Electrochem. Czechoslovakia
FV	V. Hanus, F. Turecek, Contribution To The Registry of Mass Spectral Data, Czechoslovak Academy of Sciences, The J. Heyrovsky Inst. of Phys. Chem. and Electrochem., July, 1982
FY	Kexure Tongbao
G	Collection of Czechoslovak Chemical Communications
G1	Prof. Pirjo Vainiotalo, Department of Chemistry, University of Joensuu, Joensuu, Finland
G2	Bioorganic & Medicinal Chemistry
G2L	Bioorg. Med. Chem. Lett.
G3	Bulletin of the Chemical Society of Japan
G4	Journal of Natural Products
G5	Journal of Labelled Cpds and Radiopharmaceuticals
GA	Walter Shackelford, USEPA, Athens, GA (see EA)
GC	GC-MS News
GCH	Green Chem.
GM	G. W. A. Milne, Lab. of Chem., National Heart, Lung and Blood Inst., NIH, Bethesda, MD 20014
GT	L. Abbey, Georgia Tech
H	Helv Chim Acta
H	Helv. Chim. Acta
H1	Heterocycles
H2	H. J. Hofman, On the Mass Spectrometry of Some Cyclopropyl Compounds, Amsterdam, 1966
H3	C. S. Hsu, Exxon Research and Engineering Co. Analytical and Information Division, POB 121, Linden, NJ 07036 (obtained 1980)
HAC	Heteroatom Chemistry
HB	W. Haddon and Buttery, Western USDA Lab.
HC	Chemistry of Heterocyclic Compounds (Chem Hetero Comp)
HE	Dieter Henneberg, Max Planck Inst. fur Kohlenforschung, Mulheim, West Germany, Magnetic Tape Collection
HO	Arch. Mass Spec. Data, 3, 172-188 (1973)
HU	Huang Yaozeng and et al., A Novel Acetylenic Ester-Vinyl Ether Rearrangement, Shanghai Inst. of Org. Chem., Academia Sinica, Shanghai, China
HY	C. H. Huang and Y. M. Yang, Inst. Maateria Medica, Shanghai, China
I	Canadian J. Chem. (Can. J. Chem.)
IC	Industrial Chemical Industries PLC, Eight Peak Index
IT	Ion Trap Newsletter
IV	Ivan Vidan

J	J Org Chem
JA	JASMS
JB	J. Biochem., Tokyo
JC	J Chromatography (J. Chromatog.)
JCR	J. Chem. Research
JCS	J. Chem. Sci.
JD	J. Chromatog. Sci.
JE	J. Chromatography A
JF	J. Prakt. Chem.
JFC	Journal of Fluorine Chemistry
JH	J. D. Henion and et al., Equine Drug Testing & Research Program MS Data Base, NYS Coll. of Vet. Med. 1st Ed. 1982
JL	J. Labelled Compounds
JM	Jim Shoemaker, Metabolic Screening Lab, Cardinal Glennon Children's Hospital, St Louis Univ Medical Center
JN	JEOL News
JOC	J. Org. Chem.
JS	Cornell University, Department of Chemistry
JZ	Dr. Jiri Zamecnik, Defence & Civil Institute of Environmental Medicine, Biosciences Div, North York, Ontario
K	Chemische Berichte
K1	Eur J Org Chem
KA	J. Chem. Soc., Phys. (A) (1969-1971), Dalton Trans. (1972-)
KB	J. Chem. Soc. (B) (1969-1971), Faraday Transactions I & II, (1972-)
KC	J. Chem. Soc. (C) (1969-1971), Perkin Transactions I & II, (1972-)
KD	Chemical Communications (J. Chem. Soc., Chemical Communications)
KE	Experientia
KF	Int. J. Mass Spectrom. Ion Phys.
KG	La Gazzetta Chimica Italiana
KH	J. Phys. Chem.
KI	G. S. King, Queen Charlotte's Maternity Hospital, London
KK	J. Chem. Soc., London
KL	J. Chem. Phys.
KM	J. Bacteriol.
KN	Can. J. Biochem.
KO	Biomedical Mass Spectrometry (Biomedical Mass Spec)
KP	Biochem. Biophys. Res. Comm.
KQ	Fortschritte der Chemischen Forschung
KR	Anal. Chim. Acta
KS	Svensk Papperstidning

KT	J. Chem. Eng. Data
KU	Chimia
KV	Prostaglandins
KW	A. Naturforsch. B.
KY	New Zealand J. Sci.
KZ	Z. Anal. Chem.
L	J. Assoc. Offic. Anal. Chem.
L2	P. A. Leclercq, Some Applications of Mass Spectrometry in Biochemistry, The Netherlands, 1975
L3	Ingo Luderwald, Abbaureaktionen Monomerer, Oligomerer und Polymerer Carbonsaureamide im Massenspektrometer (Thesis), Marburg/Lahn, 1972
L4	W. C. M. M. Luijten, Mass Spectrometry of some Nitrodiazoles (Thesis), 1981
LA	J. Lieberman, M. Alexander, Cornell University
LOC	Letters in Organic Chemistry
LQ	Dr. J. L. LeQuere, Institut National de la Recherche Agronomique, Dijon, France
LS	Robert E. Carter, Chemical Center, Lund, Sweden
LU	J. Hogg, Lucta SA Fabrica de Esencias y Productos Aromaticos, 1983
M	Mass Spectros. (M.S. Soc. of Japan)
MA	J. L. Aubagnac, Universite des Sciences et Techniques du Languedoc, 34060 Montpellier Cedex, France
MB	G. Raspe, Ed. Advances in the Biosciences, Vol. 2, Pergamon Press Vieweg
MC	MFG Chem. Assoc. (see TR)
MCS	ACS Med. Chem. Lett.
ME	Mellor's Comprehensive Treatise on Inorganic and Physical Chemistry
MF	Cornell University, 1978
MG	J. K. Grant, Ed. Memoirs of the Society for Endocrinology, No. 16, Cambridge University Press, London
MI	K. Biemann, MIT, Cambridge, MA
MK	C. R. Acad. Sci. Ser. D
ML	Lipids
MM	Charles Merritt, Jr. and Charles N. McEwen, Eds. Mass Spectrometry, Part B, Practical Spectroscopy Series, Vol. 3, Marcel Dekker, New York, 1980
MO	O. A. Mamer, Montreal Childrens Hosp. (see OM)
MP	E. Kendrick, Ed. Advances in Mass Spectrometry, Vol. 4, 1968
MQ	A. Quayle, ed. Advances in Mass Spectrometry, Vol. 5, The Institute of Petroleum, London, 1970

MR	A. R. West, Ed. <i>Advances in Mass Spectrometry</i> , Vol. 6, Applied Science Publishers LTD, Barking, Essex, England, 1974
MS	K. Ogata and T. Hayakawa, Eds. <i>Recent Developments in Mass Spectroscopy</i> , University Park Press, Baltimore, USA, 1970
MSJ	Mass Spectrometry Society Japan
MT	<i>Advances in Mass Spectrometry</i> , Vol. 3, The Institute of Petroleum, London
MU	Robert C. Murphy, University of Colorado Health Sciences Ctr., School of Medicine, Dept. of Pharmacology, Denver, CO 80262
MV	M. V. Buchanan, Oak Ridge National Laboratory, Oak Ridge, TN
MX	J. Fernando Jaureguy-Calzada legaria #608 Mexio D.F.11500-Mexico
MY	Laurence Dusold, DHEW, PHS, FDA, Washington, D.C. 20204 FDA Mycotoxin Collection, obtained 1981
N	Chemica Scripta (Arkiv fur Kemi)
N2	R. Neeter, <i>Electron Impact Induced Decompositions of Some Alkylpyridines, Pyridine Carboxylic Acids and Esters</i> , Rotterdam, the Netherlands, 1973
N3	Ritsuo Nishida, <i>Cockroach Pheromones</i> , 1977
N4	N. M. M. Nibbering, <i>Mass Spectrometry of Some Aralkyl Compounds with a Functional Group in the Side Chain</i> , 1968
N5	N. Nicolaidis, <i>Dermatology</i> , University of Southern California School of Medicine, 2025 Zonal Ave., Los Angeles, CA 90033, 1980
NA	Nature
NB	K. Biemann, MIT, Cambridge, Mass.
NI	Nicolet Instruments, R. B. Cody
NO	J. L. Laseter and R. Kloepfer, Univ. of New Orleans (NO-59)
NP	commonly shared spectrum with NIST. Isotope corrected
NS	National Bureau of Standards
NW	Bruce Wilkes, Union Carbide Corp.
O	J Mass Spectrometry
O	Organic Mass Spectrometry (Org. Mass. Spec.)
O1	J. Org. Chem USSR
O2	J Mass Spectrometry
OCF	Organic Chemistry Frontiers (RSC)
OD	G. Odham, L. Larsson, P.-A. Mardh, <i>Gas Chromatography-Mass Spectrometry: Applications in Microbiology</i> , Plenum Press, New York, 1984

OH	Mass Spectra of Oxygen Heterocycles, University of Manchester
OM	O. A. Mamer, MS Unit, McGill University, 1130 Pine Ave. W., Montreal, Canada H3A 1A3, Metabolic Library collection
ON	Old NIST spectrum
OR	W. T. Rainey, Oak Ridge National Laboratory
OS	Organic Mass Spectrometry, Indexing Reference Forms
P	Phytochemistry
PA	Phytochemical Analysis (Wiley journal)
PC	Department of Pathology, College of Physicians and Surgeons of Columbia University
PG	P. Groll, ERC Project 64b, Karlsruhe
PJ	Pakistan Journal of Scientific and Industrial Research
PL	Pierre Longevialle, Centre National de la Recherche Scientifique Institut de Chimie des Substances Naturelles, Paris, France, added March, 1982
PM	Pharmaceutical Mass Spectra, CRE Aldermaston, England
PO	Cong Pu-Zhu, Mass Spectrometry of Tropine Ester Alkaloids, Acta Chimica Sinica 39(1), Feb. 1981
PR	W. Noel Einolf, Philip Morris Research Center, PO Box 26583, Richmond, VA 23261
PS	Pakistani Collection
PU	Cong Pu-Zhu, Study on the Mass Spectrometry of Cephalotaxine Alkaloids, Inst. of Materia Medica, Chinese Academy of Medical Sciences, Beijing, Later published in Acta Chimica Sinica, added Feb, 1982
Q	Bull. Envir. Contamin. Toxicol.
QA	Chinese Chemical Society, J.
QB	Bulletin of the Korean Chemical Society
QC	Tetrahedron-Asymmetry
QD	Chemical research in Chinese Universities
QE	Chemistry-A European Journal
QF	Russian Chemical Bulletin
R	Europ. J. Biochem.
R2	Dr. W. T. Rainey, Oak Ridge National Laboratory, obtained 1981
R3	Thomas N. Riley, University of Mississippi, Sch. of Pharm., University, Miss 38677
R4	Riber, Nermag, Santa Clara, CA and the Dow Chemical Company
RA	M. W. Couch and C. M. Williams, Coll. of Medicine, Univ. of Florida, Gainesville, FL

RB	Haddon, W., Jarboe, C. H.: Purdue University or Riber Data Systems
RC	K. Biemann, Proceedings, Robert A. Welch Foundation, 11/63 pp. 199-232
RCM	Rapid Commun. Mass Spectrom.
RD	Nature, 228, 923 (1970)
RE	Brohult and et al., Mass Spectrometric Studies of Hop Bitter Substances, Eur. Brewery Convention, 1960, pp. 121-127
RF	Anal. Biochem 44, 473
RG	F. W. McLafferty, Interpretation of MS
RH	V. Hanus, Heyrovsky Inst., Prague, Czechoslovakia
RI	J. Am. Chem. Soc. 95, 1433 (1973)
RJ	G. L. Cook and G. U. Dineen, Mass spectra of Organic Sulfur Compoundssss, U.S. Department of the Interior, Bureau of Mines, RI 6698
RK	D. G. I. Kingston, Virginia Polytechnic
RL	Amer. Labor. 3(2), 27 (1971)
RM	B. J. Millard, Advances in Drug Research, Ch. 6, Vol. 6, Harper and Simmonds, Eds. 1971
RN	AEI 9th Users Conference, January 1973, Manchester, UK.
RO	C. Djerassi, H. Budzikiewicz and J. M. Wilson, Proceedings First Int. Congress Hormonal Steroids, Vol. 2, Academic Press, NY, 1965
RP	A. Frigerio, Ed. Proc. Int. Symp. Gas Chromatography/Mass Spectrometry, Tamburini Editore, Milano, 1972
RQ	F. E. Saalfeld and M. V. McDowell, Naval Res. Laboratory, Washington, D.C. 20390, NBL Report 6639
RR	N. M. M. Nibbering, Mass Spectrometry of Some Aralkyl Compounds with a Functional Group in the Side Chain (Thesis), University of Amsterdam, 1968
RS	J. N. Anderson and R. O. Martin
RSA	RSC Adv.
RT	S. Facchetti, A. Copet and W. Beyrich, EUR 2713.e, 1966
RU	A. L. Jennings, Jr. A Mass Spectroscopic Study of Selected Heterocycles (M.A. Thesis), University of Texas, Austin, 1963
RV	J. L. Cotter and R. A. Dinehart, Royal Aircraft Establishment, TR 66254
RW	R. H. Wiley, unpublished Archives Spectrum
RX	H. W. Brown, Hewlett-Packard

RY	Beckey and et al., Advances in Experimental Techniques, Applications, and Theory of Field Ionization Mass Spectrometry
RZ	K. Biemann, Detection and Identification of Biologically Significant Compounds by Mass Spectrometry
S	Acta Chem. Scand.
S2	W. Sonneveld, Mass Spectrometry of Fatty Acid Methyl Esters, Delft, the Netherlands, 1967
S3	Robert Smakman, Mass Spectrometry of Some Saturated Heterocycles, Amsterdam, the Netherlands, 1970
S4	J. Seibl, Swiss Federal Techn. Inst., Zurich
SA	Y. D. Cho and R. O. Martin, University of Saskatchewan, Canada
SB	Acta Chem. Scand. Ser. B, Denmark
SC	Commercial Solvent Corporation, Terre Haute, Indiana
SCS	Journal of Saudi Chemical Society
SD	Stanford magnetic tape collection, D. Smith, obtained 1981
SE	Ng Dinh-Nguyen, Ragnar Ryhage, Stina Stallberg-Stenhagen and Einar Stenhagen, Information regarding the fragmentation of long chain compounds obtained from the mass spectra of heavy isotope-labelled molecules
SEP	J. Sep. Sci.
SF	K. Lindstrom, Swedish Forest Products Research Laboratory, Stockholm, Sweden
SFA	Journal of the Science of Food and Agriculture
SG	Stanley P. Griff, Dart and Kraft, Inc.
SH	C. Shackelton, UC-Berkeley
SI	Acta Chimica Sinica
SJ	Scientific Instruments Service - calibration compounds
SK	Synthetic Communications
SL	Adv. Org. Chem. Vol. 3, 1963
SM	S. Abrahamsson, Goteborg University, Sweden
SO	Synthesis
SP	Spectroscopy: An International Journal
SRH	Steve R. Heller
SS	Atlas of Mass Spectra, Novosibirsk, USSR
ST	Swedish Tobacco Co., Stockholm, Sweden
SW	C. C. Sweeley, Selected C-19 and C-20 Steroids, Michigan State University
SWG	SWGDRUG Mass Spectral Library
T	A. Tatematsu and T. Tsuchiya, Structure Indexed Literature of Organic Mass Spectra, Academic Press of Japan, Tokyo, 1966-8

T2	Lucia Tyler, PhD Thesis, Professor T. Acree (Supervisor), 1978, Cornell Univ.
T3	TRC Current Data News, Thermodynamics Research Center, Texas Engineering Experiment Station, Texas A&M University
TA	A. Tatematsu and T. Tsuchiya, Structure Indexed Literature of Organic Mass Spectra, Academic Press of Japan, Tokyo, 1966-8
TB	Industrie Chimie Belge
TC	Mass Spec. Applications, C.V.C. Products, Inc.
TD	American Doc. Inst. 4817
TE	Thomas Cairns, Dept of Health & Human Services, FDA, Office of Regulatory Affairs, LA District Lab, Mass Spec Service Center, 1521 West Pico Blvd, LA, CA 90015
TG	Angewandte Chemie (Angew. Chem.)
TI	Israel J. Chemistry
TIPS	Russian Academy of Sciences: The Institute of Petroleum Sciences
TJ	J. Inorg. Nucl. Chem.
TK	Makromol. Chem.
TL	J. Larsen and R. A. Sneen, Purdue Univ.
TM	M. M. Kochar, Auburn University
TN	J. Res. Natl. Bureau Standards
TP	Appl. Spectrosc.
TQ	Die Pharmazie
TR	Thermodynamic Research Center, College Station, TX
TS	Indian J. Chem.
TU	H.-J. Bultemann and L. Delgmann, Atlas Mess-und Analysentechnik GmbH, Bremen
TV	Colloquium Spectroscopicum Internationale
TX	TRC Spectra (Matrix Format) (see TR)
TY	Yakugaku Zasshi (J. Pharm. Soc. Japan)
TZ	Nord. Kemikermode Aarhus
U	Justus Liebigs Annalen der Chemie
U1	European J Org Chem
U2	European J Inorg Chem
UB	USDA, Beltsville, MD, USA
UE	White, Welch and Hertz, (USEPA) Mass Spectra and Isotopic Purity of Compounds Proposed for Use in the "Master Analytical Scheme for the Analysis of Organic Compounds in Water" N.B.S. Dept. of Commerce
UJ	Lubo Baczynsky, Physical and Analytical Chemistry Research, The UpJohn Co., 1978
UM	Universal Monitor Corp., Pasadena, CA
UN	Unknown Source

UT	Arthur Tucker, Dept of Agriculture and Natural Resources, Delaware State College, Dover, DE
UW	C.E.C.A. Hop and D. Snyder, University of Wisconsin-Madison, Chemistry Department, Madison, WI 53706
UY	UORSY
V	Steroids
V2	B. VandeGraaf, Studies on Overcrowding in Organic Molecules, Delft University, the Netherlands, 1978
V3	A. Venema, Mass Spectrometry of Aralkyl Compounds and 7-Substituted Cycloheptatrienes, Amsterdam, the Netherlands, 1975
VC	Volatile Compounds in Foods, Central Institute for Nutrition and Food Research TNO, Netherlands
VF	Complete spectra from JCS Perkins Trans. 1981 - P. Vata-Finzi, University of Pavia, Bulgaria
VK	M. C. T. N. deBrauw, Volatile Compounds in Foods, Central Inst. for Nutrition and Food Research - TNO, Utrechtseweg 48, 3704 HE Zeist, The Netherlands
W	G. R. Waller, Ed. Biochemical Applications of Mass Spectrometry, Wiley-Interscience, New York, NY, 1972
W2	Johann Winkler, Elektronenstoss-Induzierte Reaktionen Offenkettiger und Monocyclischer Polymethoxyalkane, Hamburg, 1970
WA	Wang Guang-Hui, Zhang Wen-Xin and Chai Wen-Gang, Adv. Mass Spectrom, 8, pp. 1369-74
WB	Qipong Hong, Bangrong Zhou and Shueihai Chen, Study on Mass Spectra of Metal(II,III) N,N-dialkyl-amino-dithioformate, Institute of Petrochemistry and Engineering, Beijing College of Chemical Engineering
WC	Markesy, Wells College
WH	Walter Hyde, Iowa State Univ.
WS	Walter Shackelford, U.S. EPA, Athens, Georgia
WT	Walter Jennings, Takayuki Shibamoto, Qualitative Analysis of Flavor and Fragrance Volatiles by Glass Capillary Gas Chromatography, ACAD Press, New York
WX	Lu & Wang Xieqing, Research Inst. for Petroleum Processing, Beijing
X	Q. N. Porter and J. Baldas, Mass Spectrometry of Heterocyclic Compounds, Wiley-Interscience, New York, 1971
X2	Chromatographia
X3	Chemistry of Natural Compounds
X4	Izvestiya Akademii Nauk Rsfsr

XD	D. Cooper, US Drug Enforcement Admin.
XW	CSIRO Mass Spectra of Organic Compounds (1-600), 8 vols., Australia
XX-1	Michigan State Univ., n-hydroxyacetaminophene
XX-2	Hewlett Packard, 4,4'-dibromooctafluorobiphenyl
XX-3	Tyler (Thesis), 1978 (see T2)
XX-4	Cornell MS Facility
XX-5	D. Pritchard, Univ. of Alabama
XX-6	J.-L. Aubagnac, P. Champion, and P. Guenot, Spectrometrie de Masse D'Heterocycles Azotes VII Phenyl-1 Triazole-1,2,3. (Aubagnac - Laboratoire de Synthese et d'etude physico-chimique des heterocycles azotes - Universite des Sciences et Techniques du Languedoc - Place E. Bataillon - 34060 Montpellier Cedex France)
XX0	F. Arcamone, G. Cassinelli, G. Franceschi, S. Penco, C. Pol, S. Redaelli and A. Selva, Structure and Physical Properties of Adriamycin, Springe-Verlag, Berlin, 1972
XX7	JN Ronson, SJRowland, Nature, 561-563
XX8	Jeanne Ayache, profil reactionnel des reactions de fragmentatin des ethylene-acetals des cyclanones substituees en spectrometrie de masse par impact electronique, These, University of Paris, 1978
XX9	Dr. Allenmark, Univ. Hosp., Linkoping, Sweden
XY	Yoshiro Masada, Analysis of Essential Oils by Gas Chromatography and Mass Spectrometry
XY0	Polycyclic Aromatic Compounds
XY1	Vlada Hanus, The J. Heyrovsky Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Czechoslovakia
XY2	Parmar, V. S., University of Delhi, Delhi-110 007
XY3	Gustav Graff, The Hormel Institute, University of Minnesota, Austin, Minn., 55912
XY4	Muramatsu, T., University of Minnesota, The Hormel Institute, Austin, Minn., 55912
XY5	A. P. Bruins, Intramolecular Functional Group Interactions and Ion Molecule Reactions of Gaseous Ions from Some Benzylamino and Benzyloxy Compounds, Amsterdam, 1976
XY6	Advances in Prostaglandin, Thromboxane, and Leukotriene Research, vol. 18, Mass Spectra of Prostaglandins and Related Products, New York 1989
XY7	HP Particle Beam LC/MS Book of Spectra, Dr. Alex Apffel, Hewlett-Packard Company, Palo Alto, California 94304
XY8	Mervyn Lewis, University of Bristol

XY9	Yao-Zu Chen, Department of Chemistry, Lanzhou University, Lanzhou, PRC
XZ	William T. Miller, Department of Chemistry, Cornell University, Ithaca, NY 14850
XZ1	Revue Roumaine de Chimie
XZ2	Bio Organic & Medicinal Letters
XZ3	New Journal of Chemistry
XZ4	Chemistry Letters
XZ5	Chimia
XZ6	CRC Handbook of Mass Spectra of Drugs, 1981
XZ7	Edgewood Arsenal Technical Report EC-TR-76059, June, 1976 Samuel Sass, Theodore W. Dolzine, and Timothy L. Fisher
XZ8	Edgewood Arsenal Technical Report EC-TR-76111, July, 1977 Timothy L. Fisher and Samuel Sass
XZ9	Edwin H. Flynn, Cephalosporins and Penicillins, Academic Press, New York, NY, 1972
Y	Journal of Heterocyclic Chemistry (J. Hetero. Chem.)
Y0	Indian Journal of Chemistry - Section A
Y1	Indian Journal of Chemistry - Section B
Y2	Nouveau Journal de Chimie / New Journal of Chemistry
Y3	Bulletin of the Division of Chemical Sciences - USSR / Russian Chemical Bulletin
Y4	Anales de Quimica - Spain
Y5	Journal of the Serbian Chemical Society
YA	Yamagishi, Akiyama & Miyazaki, Application of GC/MS to Bio-Monitoring of Environmental Pollution (JEOL NEWS)
Z	Dr. Uwe Zahorszky, Inst. f. Org. Chemie. Universitat Karlsruhe, D-7500, Karlsruhe, West Germany
ZH	Zhou Yunli and et al., Isolation and Characterization of Maytansine and Maytanprine, Two Anticancer Agents from Maytenus Hookeri Loes, Kexue Tongbao, 25(7), 1980, pp. 612-15

CAS-RN Field

Some mass spectrometry software programs rely on a field labeled "CAS-RN" to link spectral records with corresponding structure record. As many of the compounds found within the Wiley Registry and other libraries do not have an assigned CAS-RN, this engineering decision would result in those spectra not being linked to their unique structure. To solve this problem, Wiley has created unique identifiers for the sole purpose of linking the spectrum and its structure using this field. To differentiate these numbers from actual CAS-RNs, each is either a 9-digit number prefixed by 999, 991, 998, or 981 for Agilent ChemStation/MassHunter and PerkinElmer TurboMass/Waters MassLynx.

Please note that 9-digit IDs prefixed with the numbers 999, 991, 998, or 981 respectively do not in any way represent CAS Registry Numbers, nor are they used for anything other than referring to the structure record in the separate structure database as a workaround to accommodate engineering decisions made by other software publishers.

The IDs used below were created as 9-digit numbers with a leading '999', '991', '998', or '981' to make them distinguishable to real CAS Registry numbers.

CAS Registry Number like identifiers created (pseudo CASRNs) - created as 9-digit CASRN-like numbers:

For records for which a structure is given (and need to be pointed to) and no real CASRN is available:

- 590,024 starting with 999 are those for records with Record IDs below 1,000,000 and
- 132,242 starting with 991 are those for records with Record IDs above 999,999

For records for which a 10-digit real CASRN is replaced by a 9-digit CASRN-like number (not necessarily pointing to a structure):

- 6,576 starting with 998 are those for records with Record IDs below 1,000,000 and
- 392 starting with 981 are those for records with Record IDs above 999,999

Below are given the lists detailing the 'CAS Registry Numbers'-like IDs used in the W23N23 Collection created to point to the chemical structure records.

Appended at the very end is also a list of the 'real' 10-digit CAS Registry Numbers (with corresponding pseudo CASRN used to replace the 10-digit real CASRNs, WileyIDs, NIST#, and name of the compound).

[CASRN ChemStation TurboMass readme.txt](#)

DATA SUBMISSION

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- Tandem MS (MS_n)
- MS-TOF exact mass
- C-NMR, H-NMR, P-NMR, Si-NMR, X-NMR
- FT-IR, Raman, UV-Vis, Near-Infrared, Diamond-ATR

Data proposals, sample data, or inquiries are best sent to dbinquiry@wiley.com.

You might send the original TIC file (Xcalibur (*.raw), ChemStation (.D data folder)) by an e-mail attachment directly to: dbinquiry@wiley.com. The data will be evaluated. If you have questions or if you need assistance, please contact us. We are always willing to help.

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