

# Wiley Registry® 12th Edition/NIST 2020

User Manual

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Installation Manual Copyright © 2022 John Wiley and Sons, Inc., Hoboken, New Jersey. All Rights Reserved.

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# **PUBLISHER'S NOTE**

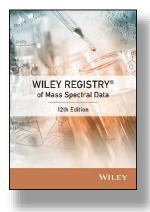
For over 45 years, John Wiley and Sons and Wiley-VCH have worked with the world's leading researchers and practitioners to deliver the spectral libraries scientists have come to rely on.

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 12th Edition and the latest 2020 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 12th Edition/NIST 2020 library contains over 1 million mass spectra collected by the NIST Mass Spectrometry Data Center and Wiley Science Solutions.

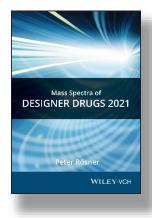
# COMPOUND SEARCH

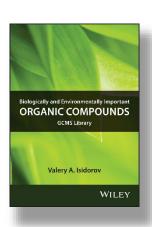
Address: <a href="http://www.compoundsearch.com">http://www.compoundsearch.com</a>

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









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# **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: <a href="mailto:dbinquiry@wiley.com">dbinquiry@wiley.com</a>

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.wilev.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

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# **GETTING STARTED**

# **Hardware and Software Recommendations**

- Operating System: Microsoft Windows (Windows 10 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 <a href="https://support.wiley.com/s/">https://support.wiley.com/s/</a>.

# **Registration Code**

A registration code accompanies the packaging provided with the flash drive. This database may be installed on only <u>one</u> 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 <a href="mailto:dbinquiry@wiley.com">dbinquiry@wiley.com</a>.

Help keep the cost of libraries down by reporting all copyright and license violations to the publisher at <a href="mailto:dbinquiry@wiley.com">dbinquiry@wiley.com</a>.

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# 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	SetupW12N20ChemStation.exe	C:\Database\{libraryname}\{filename}
MassHunter	SetupW12N20MassHunter.exe	C:\MassHunter\Library\{libraryname}\{filename}
MS Search	SetupW12N20MSSearch.exe	C:\NIST20\MSSEARCH\{libraryname}\{filename}
TurboMass	SetupW12N20TurboMass.exe	C:\TurboMass\Idendb\{libraryname}\{filename}
		C:\TurboMass\Idendb\STRUCTDB\{libraryname}\{filename}
GCMSsolution	SetupW12N20GCMS-	C:\GCMSsolution\Library\{libraryname}\{filename}
	Solution.exe	
Xcalibur	SetupW12N20Xcalibur.exe	C:\ProgramFiles\NISTMS\MSSearch\{libraryname}\{filename}
MassLynx	SetupW12N20MassLynx.exe	C:\MassLynx\Idendb\{libraryname}\{filename}
		C:\MassLynx\Idendb\STRUCTDB\{libraryname}\{filename}

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<sup>\*</sup>Installations will include download of a minimum of four {libraryname}: W12N20main, W12N20rep, W12N20leg, W12N20lq

# **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 <a href="https://www.wileyptmediareg.com/Activation">https://www.wileyptmediareg.com/Activation</a> 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 <a href="https://support.wiley.com/s/">https://support.wiley.com/s/</a> 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.

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# 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.



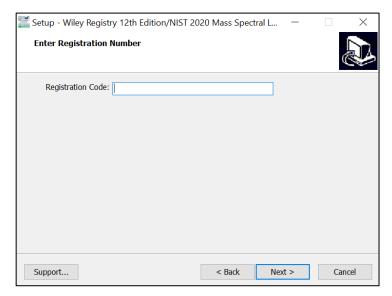
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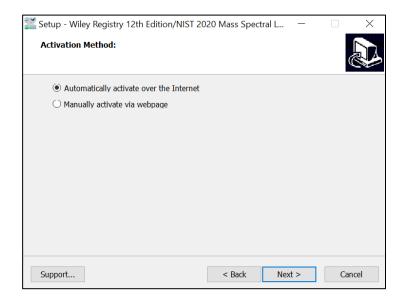
#### 3. Registration Code and Machine ID

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.



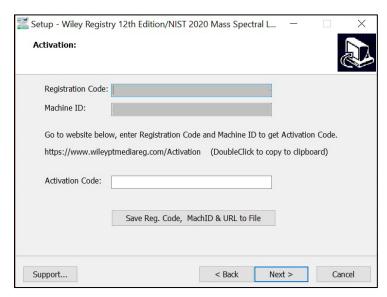


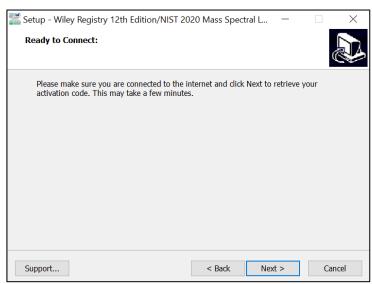
-7- WILEY

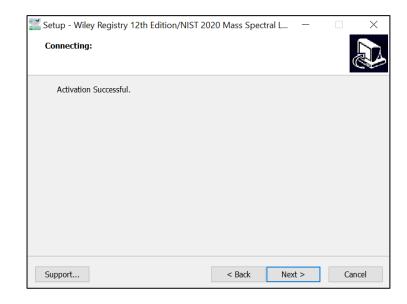
4. If you choose to manually activate, the Registration Code and the Machine ID will be automatically filled in. You may either double click the web address to copy it to your computer's clipboard and paste it in a web browser, or enter the URL as listed in your web browser.

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.







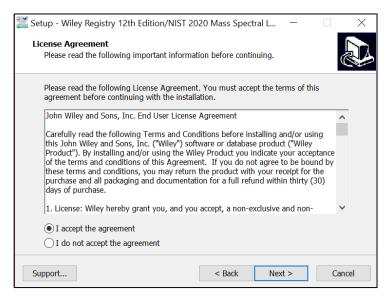
-8- WILEY

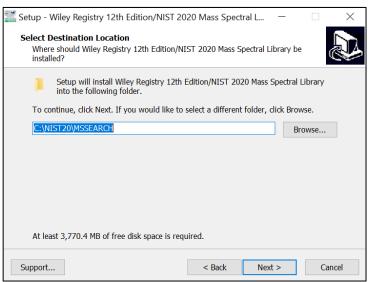
5. Once your activation is successful, proceed by pressing "Next." The next screen contains the End User License Agreement (32).

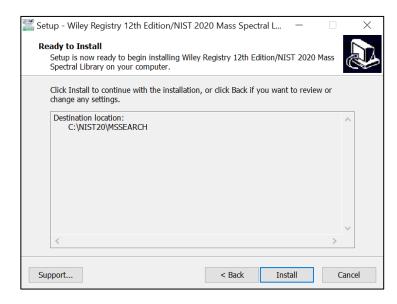
Read the agreement carefully and select the "I accept the agreement" option. Then, choose "Next" to proceed to install the library. Spectral libraries should only be used by qualified individuals who meet the requirements outlined in the agreement.

- 6. 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.
- 7. 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.

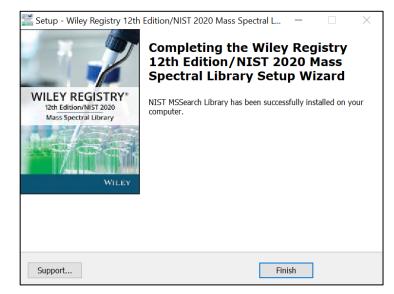






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8. Once installation is complete, press "Finish." Be sure to consult your spectra/data analysis software's instructions for connecting to new libraries – some are automatic, but some require manual connection within the software.



# **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: <a href="https://support.wiley.com/s/">https://support.wiley.com/s/</a>

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# 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 12th/NIST 2020 – 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.

- W12N20 main: Use this library for untargeted analysis in everyday scientific work.
- W12N20 replicate: Use this library when further confirmation or results are required.
- W12N20 legacy: Use this library when searching for confirmation on past work.
- W12N20 low quality: Use this library when further confirmation or results are required.

See <a href="https://sciencesolutions.wiley.com/">https://sciencesolutions.wiley.com/</a> 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 Wiley Registry 12th Edition/NIST 2020 Mass Spectral Library and a specialized library such as MS and GC Data of Drugs, Poisons, Pesticides, Pollutants, and Their Metabolites 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:**

Main part split into 3 parts (for compatibility reasons):

- MAIN 1: 366,144 records (records with nominal mass up to 250)
- MAIN 2: 338,518 records (records with nominal mass from 251 to 350)
- MAIN 3: 292,493 records (records with nominal mass above 350) records for which no molecular formula and thus no nominal mass is available are also included here.

The REP, LQ, and LEG parts are the W12 REP, LQ, and LEG libraries.

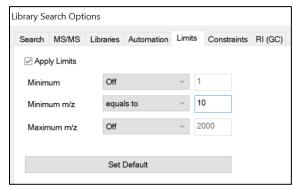
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The following 'fields' were added to the COMMENT field (tagged comment fields):

- Classification Compound classification information
- DOI Literature source reference, resolvable via doi.org
- Exp-RI\_Any Retention Index values theoretical values for n-alkanes (for 137 records)
- Exp-RI\_Polar Retention Index values Standard Polar column (for 15,904 records)
- Exp-RI\_Semi-standard\_non-polar Retention Index values Standard Semi-Non-Polar column (for 128,266 records)
- Exp-RI\_Standard\_non-polar Retention Index values Standard Non-polar column (for 30,335 records)
- NIST\_Seq# For records from NIST20 mainlib and replib (indicates record number in NIST20 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 NIST20 records. For the Wiley part, no experimental RI values are given.

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.



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#### **Agilent ChemStation/MassHunter:**

Comprised of four parts:

- W12N20 MAIN
- W12 RFP
- W12 LQ
- W12 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.
- Classification info is given as 'Class: '.
- 'Molform' given if the molecular formula differs from the molecular formula given with the spectrum
- 'Orig. form.' given for compounds with 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) – for 128,400 records (experimental RI only for NIST records). 'Estimated non-polar retention index (n-alkane scale)' values are added to the User Index field (MAIN: 871,934; REP: 26,922; LQ: 46878; LEG: 1,239).

Pseudo CASNOs were used to point to the structures in the structure add-on files. These pseudo CASNOs are 9-digit numbers (in CASRN format) starting with '990' (i.e. are of form: '990...-..-').

#### **Shimadzu GCMSsolution:**

#### Comprised of seven parts:

- The W12N20 main part split into four parts:
  - MAIN 1: 250,000 records
  - MAIN 2: 250,000 records
  - MAIN 3: 250,000 records
  - MAIN 4: 247,155 records
- W12 REP
- W12 LQ
- W12 LEG

#### COMMENTS field - no such field available

'Estimated non-polar retention index (n-alkane scale)' values are added to the 'Retention Index' field (MAIN: 871,934; REP: 26,922; LQ: 46878; LEG: 1,239).

#### PerkinElmer TurboMass/Waters MassLynx:

Comprised of four parts:

- W12N20 MAIN
- W12 REP
- W12 LQ
- W12 LEG

#### COMMENTS field:

- For records from NIST20 (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: '.
- For 10-digit CASRNs (which are removed/replaced see below), an 'OCAS' entry with the original 10-digit CASNO is made.

Semi-Standard Non-polar experimental RI values added to the 'Value 1' field (for n-alkanes the theoretical/definition values are given) – for 128,400 records (experimental RI only for NIST records). 'Estimated non-polar retention index (n-alkane scale)' values are added to the 'Value 2' field (MAIN: 871,934; REP: 26,922; LQ: 46878; LEG: 1,239).

Pseudo CASNOs were used to point to the structures in the structure add-on files. These pseudo CASNOs are 9-digit numbers (in CASRN format) starting with '990' (i.e. are of form: '990...-..-.'). Since Masslynx/Turbomass can't handle 10-digit CASRNs, these were also replaced with 9-digit numbers (in CASRN format) to differentiate them from the records which have fake CASRNs. Because no real CASRN is available, the pseudo CASRNs created start with '991' (i.e. are of form: '991...-..-.'). The original 10-digit CASRNs are added to the Comment field of a record. A pseudo CASRN is only assigned for records which have a structure.

#### **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

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	electronique, These, University of Paris, 1978
A3	Organic Preparations and Proceedings
A3	Dr. Allenmark, Univ. Hosp., Linkoping, Sweden
A4	Organometallics
A4 A4	F. Arcamone, G. Cassinelli, G. Franceschi, S. Penco, C. Pol,
A4	S. Redaelli and A. Selva, Structure and Physical Properties
	of Adriamycin, Springe-Verlag, Berlin, 1972
A5	Organic Process Research and Development
A5	Yoshiro Masada, Analysis of Essential Oils by Gas
AS	Chromatography and Mass Spectrometry
A6	Journal of Chemical Technology and Biotechnology
A6	Vlada Hanus, The J. Heyrovsky Institute of Physical
Ab	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
<b>A</b> O	Minnesota, Austin, Minn., 55912
A9 A9	European Journal for Mass Spectrometry
A9	Muramatsu, T., University of Minnesota, The Hormel
ΛΛ	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  ACS Comb. Sci.
ACS	
AD	Mass Spectrometry Data Centre, AWRE, Aldermaston,
٨٢	Berks., England
AE	Journal of Biological Chemistry
AF	Journal of Medicinal Chemistry
AG	Journal of Organometallic Chemistry
AH	Monatshefte fur Chemie  Archiv der Pharmazie
Al	
AJ	Bulletin of the Chemical Society of Japan (Nippon
AIO	Kagakukai)
AJO	Asian J. Org. Chem.
AK AL	The Biochemical Journal
	Biochimie (Bull. Soc., Chim. Biol. Fr.)
AM	S. P. Markey, University of Colorado Medical Center, Denver, CO
ANI	
AN	Bulletin Societe Chimique de Belges
AOC	Environ. Health Perspec.
AOC	Appl. Organometal. Chem.
APC	Amer. Petroleum Inst., Res. Project 44
APC	Arch. Pharm. Chem. Life Sci.
AQ	Pure Appl. Chem.
AR	Pest. Biochem. Physiol.
AS	J. G. Lawless, NASA, Moffett Field, CA

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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
В	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	Polycylic 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
ВВ	Dibenzoacridine, R. Depaus, CES Joint Reseearch Center,
	Netherlands
BC	J. L. Aubagnac (see MA)
BD	A. T. Balaban, Comitetul de State Pentru Energia
	Nulleara, Institutal de Fizica Atomica, Bucharest,
	Romania
ВК	Bruce Kennett, CSIRO, Australia (see XW)
BL	BLR Drug Spectra, Subcommittee 6, Amer. Soc. Mass
	Spectrom.

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BM	Quantitative Mass Spectrometry, B. J. Millard
BR	Mass Spectra of Paraffins with 10-24 Carbon Atoms, V.A.
DK	Herlan
BS	Biomedical Mass Spectrometry, Indexing Reference
	Forms
BU	Buchert, Arne, Ministry of the Environment, National
	Food Institute, Denmark (obtained 1981)
BW	Bruce Wilkes
С	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, Microbilolgical 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
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CA	Archives of Mass Spectral Data, 3, 536-514 (1972)
CAJ	Chem. Asian J.
СВ	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,
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CE	Catherine E. Costello, MIT, Dept. of Chem., Cambridge,
	MA 02139
CG	G. Spiteller, Massenspektromische Strukturanalyse

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	M. T. Cheng, Chevron Research & Technology Company,
	100 Chevron Way, Richmond, CA 94802-0627
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	Chemical Concepts GmbH, Tel. +49(0)6201-606433, P.O.
	Box 100202, D-69442 Weinheim, Federal Republic of
	Germany
С	ChemMedChem
	Continental Oil Co., Ponca City, OK
	Wan-Kai Chu, Painting Industry Research Institute of
_	Chemical Industry, Lanzhou, China
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_	Chem Research in Toxicology
Г	Chemical Research in Toxicology
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	McGuire,J.M.,United States Envirnmental Protection
	Agency, Envirnmental Research Laboratory, Athens,

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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,
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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 Geterotsiklicheskikh Soedinenii
DH	Zhurnal Obshchei Khimii
DI	Akademia nauk SSSR, Doklady, Seria Khimiia
DJ	Recueil Des Traveaux 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.
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DN	O. A. Mamer, W. J. Mitchell and C.R. Scriver, Eds.
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	Disease
DO	A. Frigerio and N. Castagnoli, Jr., Eds. Mass Spectrometry
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	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
DT	Pollutants
DT	R. Hague and F. J. Biros, Eds. Mass Spectrometry and
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DII	New York, 1974
DU	Drug Metabolism and Disposition
DV	Svensk Kemisk Tidskrift  Brennstoff-Chemie
DV	
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,
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E2	Chemia Switzerland
E2	
EZ	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,
EA	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 Chemsitry
FA	Analytical News, Finnigan MAT
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
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FV	V. Hanus, F. Turecek, Contribution To The Registry of
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	The J. Heyrovsky Inst. of Phys. Chem. and Electrochem.,
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FY	Kexure Tongbao
G	Collection of Czechoslovak Chemical Communications
G1	Prof. Pirjo Vainiotalo, Department of Chemistry,

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	Liniversity of Leansur, Leansur, Finland
	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
Н	Helv Chim Acta
Н	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
НВ	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
НО	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
1	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
J⊓	Program MS Data Base, NYS Coll. of Vet. Med. 1st Ed.
	1982
	1302

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JL	J. Labelled Compounds
JM	Jim Shoemaker, Metabolic Screening Lab, Cardinal
<b>5</b>	Glennon Children's Hospital, St Louis Univ Medical
	Center
JN	IEOL News
JS	Cornell University, Department of Chemistry
JZ	Dr. Jiri Zamecnik, Defence & Civil Institute of
	Environmental Medicine, Biosciences Div, North York,
	Ontario
К	Chemische Berichte
K1	Eur J Org Chem
KA	J. Chem. Soc., Phys. (A) (1969-1971), Dalton Trans. (1972-)
КВ	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.
КО	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	I. Assoc. Offic. Anal. Chem.
L2	P. A. Leclercq, Some Applications of Mass Spectrometry
<del></del>	in Biochemistry, The Netherlands, 1975
L3	Ingo Luderwald, Abbaureaktionen Monomerer,
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L4	W. C. M. M. Luijten, Mass Spectrometry of some
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LA	J. Lieberman, M. Alexander, Cornell University
LOC	Letters in Organic Chemistry
LQ	Dr. J. L. LeQuere, Institut National de la Recherche
	2.1.J. Li Legaer ej modeat Hadional de la Recherche

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	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
TVI/ C	Languedoc, 34060 Montpellier Cedes, France
MB	G. Raspe, Ed. Advances in the Biosciences, Vol. 2,
WE	Pergamon Press Vieweg
MC	MFG Chem. Assoc. (see TR)
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. Advances in Mass Spectrometry, Vol. 6,
	Applied Science Publishers LTD, Barking, Essex, England, 1974
MC	
MS	K. Ogata and T. Hayakawa, Eds. Recent Developments in Mass Spectroscopy, University Park Press, Baltimore,
	USA, 1970
MSJ	Mass Spectrometry Society Japan
MT	Advances in Mass Spectrometry, Vol. 3, The Institute of
1411	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, Electron Impact Induced Decompositions of
	Some Alkylpyridines, Pyridine Carboxylic Acids and
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N3	Ritsuo Nishida, Cockroach Pheromones, 1977

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N4	N. M. M. Nibbering, Mass Spectrometry of Some Aralkyl Compounds with a Functional Group in the Side Chain, 1968
N5	N. Nicolaides, Dermatology, 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.
0	J Mass Spectrometry
0	Organic Mass Spectrometry (Org. Mass. Spec.)
01	J. Org. Chem USSR
02	J Mass Spectrometry
OCF	Organic Chemistry Frontiers (RSC)
OD	G. Odham, L. Larsson, PA. Mardh, Gas
	Chromatography-Mass Spectrometry: Applications in Microbiology, Plenum Press, New York, 1984
ОН	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
РО	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

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QA       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 Mississispipi, Sch. of Puniversity, Miss 38677         R4       Riber, Nermag, Santa Clara, CA and the Dow Chem Company         RA       M. W. Couch and C. M. Williamas, Coll. of Medicine of Florida, Gainesville, FL         RB       Haddon, W., Jarboe, C. H.: Purdue University or Rib Data Systems         RC       K. Biemann, Proceedings, Robert A. Welch Foundat 11/63 pp. 199-232         RCM       Rapid Commun. Mass Spectrom.         RD       Nature, 228, 923 (1970)         RE       Brohult and et al., Mass Spectrometric Studies of Headen.	
QBBulletin of the Korean Chemical SocietyQCTetrahedron-AsymmetryQDChemical research in Chinese UniversitiesQEChemistry-A European JournalQFRussian Chemical BulletinREurop. J. Biochem.R2Dr. W. T. Rainey, Oak Ridge National Laboratory, obtained 1981R3Thomas N. Riley, University of Mississippi, Sch. of Puniversity, Miss 38677R4Riber, Nermag, Santa Clara, CA and the Dow Chemicomy CompanyRAM. W. Couch and C. M. Williamas, Coll. of Medicine, of Florida, Gainesville, FLRBHaddon, W., Jarboe, C. H.: Purdue University or Ribical Data SystemsRCK. Biemann, Proceedings, Robert A. Welch Foundat 11/63 pp. 199-232RCMRapid Commun. Mass Spectrom.RDNature, 228, 923 (1970)REBrohult and et al., Mass Spectrometric Studies of Headen.	
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Russian Chemical Bulletin REurop. J. Biochem. R2 Dr. W. T. Rainey, Oak Ridge National Laboratory, obtained 1981 R3 Thomas N. Riley, University of Mississippi, Sch. of Puniversity, Miss 38677 R4 Riber, Nermag, Santa Clara, CA and the Dow Cheme Company RA M. W. Couch and C. M. Williamas, Coll. of Medicine of Florida, Gainesville, FL RB Haddon, W., Jarboe, C. H.: Purdue University or Rib Data Systems RC K. Biemann, Proceedings, Robert A. Welch Foundate 11/63 pp. 199-232 RCM Rapid Commun. Mass Spectrom. RD Nature, 228, 923 (1970) RE Brohult and et al., Mass Spectrometric Studies of Heads 1981	
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TE	Thomas Cairns, Dept of Health & Human Services, FDA,
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TL	J. Larsen and R. A. Sneen, Purdue Univ.
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TR	Thermodynamic Research Center, College Station, TX
TS	Indian J. Chem.
TU	HJ. Bultemann and L. Delgmann, Atlas Mess-und
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TV	Colloquium Spectroscopicum Internationale
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