

SPECINFO

Subject Coverage	<ul style="list-style-type: none"> • Identification of substance • Spectroscopic information • 13C-NMR 	<ul style="list-style-type: none"> • 17O-NMR • 19F-NMR • 31P-NMR 	<ul style="list-style-type: none"> • 15N-NMR • IR • MS
-------------------------	---	---	---

File Type Numeric, Structure

Features	Thesaurus	None			
	Alerts (SDIs)	Not available			
	CAS Registry Numbers®	<input checked="" type="checkbox"/>	Page Images	<input type="checkbox"/>	STN AnaVist <input type="checkbox"/>
	Keep & Share	<input type="checkbox"/>	SLART	<input type="checkbox"/>	STN Easy <input type="checkbox"/>
	Learning Database	<input type="checkbox"/>	Structures	<input type="checkbox"/>	STN Viewer <input type="checkbox"/>

Record Content

- Spectral data for a representative section of organic chemistry, including organometallic substances.
- For each compound NMR, IR and/or mass spectra are given. The information includes experimental conditions, e.g., instrument, solvent and temperature, and bibliographic information.
- For NMR spectra coupling constants and relaxation times are included, if available.
- In addition to the spectral data for each compound, the following information on substance identification is given: SPECINFO Registry Number, molecular formula, molecular weight, chemical name. For a part of the records, CAS Registry Numbers are available.
- SPECINFO also contains the following data generation packages, which can be started with the Messenger RUN command.

<u>PROGRAM PACKAGE</u>	<u>FUNCTION</u>
CHESS	Search for chemical structures identical or similar to a query structure (structure code similarity search)
COUPCAL	Estimation of coupling constants from a query structure
EDSPEC	Spectrum editor to modify existing or create new spectra to be searched with GETSPEC
GETSPEC	Search for spectra similar to a query spectrum
SPECIAL	Estimation of NMR-spectroscopic information from a query structure

File Size 152,500 compounds, with 98,500 13C-NMR spectra, 1800 19F-NMR, 1000 15N-NMR, 800 17O-NMR, 2200 31P-NMR, 18500 IR spectra, and 62,200 mass spectra (12/10).

Updates Not updated

Language English

Database Producer / Supplier
 Chemical Concepts GmbH
 Boschstr. 12
 69469 Weinheim,
 Germany
 Phone: 49 6201/606-433
 Fax: +49 6201/606-430
 E-mail: marketing@cc.wiley-vch.de
 Copyright Holder

SPECINFO

User Aids

- Online Helps (HELP DIRECTORY lists all help messages available)
 - STNGUIDE
-

Clusters

- CASRNS
 - NUMERIC
- [STN Database Clusters](#) information (PDF).
-

Pricing

See the [STN Price List](#) or enter HELP COST at an arrow prompt.

Search and Display Field Codes

Substance Identification

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from CN, <X>NMR.NTE, IR.NTE, MS.NTE, as well as molecular formulas, and SPECINFO and CAS Registry Numbers) (1)	None or /BI	S STEREOISOMER#	SRN, CN, MF,<X>NMR, RN,IR.NTE, MS.NTE
Accession Number (SPECINFO Registry Number) Atom Count (2) Chemical Name Chemical Name Segment Element Count (2) Element Count (total) (2) Element Ratio (2,3) Element Symbol Field Availability (4) Molecular Formula Molecular Weight (2) Periodic Group ReaxysFile Accession Number	/SRN /ATC /CN /CNS /Element Symbol /ELC /ELR.XX /ELS /FA /MF (or /FW) /MW (/FW) /PG /RAN	S STCC-10007-945/SRN S 3/ATC S HYDROCYANIC ACID/CN S ACID/CNS S 5/BR S 8/ELC S 2E-1/ELR.NO S C/ELS AND F/ELS S ONMR/FA S C11 H8 F6/MF S 50-55/MW S A1/PG S 1000598/RAN	AN, SRN not displayed CN CN not displayed not displayed not displayed not displayed FA MF MW not displayed RAN

- (1) <X> is C, F, N, O, or P.
 (2) Numeric search field that may be searched with numeric operators or ranges.
 (3) Ratio of elements C, H, N, and O in a molecular formula.
 (4) D FA displays the field codes and their occurrences.

Spectral Data

Fields	Default Units	Search Code	Search Examples	Display Code
NMR Data Conversion Shift (1,2) Coupling Constant (1,2) Coupling Nucleus (1,2) Instrument Intensity (relative) (1,2) Line (1,2,3) Multiplicity (1) Note Peak Position (1,2) Reference (1) Relaxation Time (1,2) Solvent (1) Spectrum Number Standard (1) Temperature (1,2) VCH Number (1)	ppm Hz - - none none - - ppm - s - - - K -	/<X>NMR.CS /<X>NMR.CC /<X>NMR.NUC /<X>NMR.INS /<X>NMRS.IN /<X>NMRS.LIN /<X>NMRS.MUL /<X>NMR.NTE /<X>NMRS.PP /<X>NMR.REF /<X>NMRS.RT /<X>NMR.SOL /<X>NMR.NR /<X>NMR.STD /<X>NMR.T /<X>NMR.VCH	S 1.88/CNMR.CS S 100-102/CNMR.CC S O/CNMR.NUC S BRUKER WP-200/CNMR.INS S 9/CNMRS.IN S 127.0 D 1/CNMRS.LIN S 80-85/CNMRS.PP(S)T/CNMRS.MUL S ABSORPTION/CNMR.NTE S 80-82/CNMRS.PP S DUDDECK/CNMR.REF S 62-63/CNMRS.RT S CD3OD/CNMR.SOL S CNCC-1007-516Q/CNMR.NR S CS2/CNMR.STD S 298/CNMR.T S 100040/CNMR.VCH	<X>NMR COUP<X> COUP<X> <X>NMR <X>NMR <X>NMRS <X>NMRS <X>NMR <X>NMRS <X>NMR <X>NMRS <X>NMR <X>NMR <X>NMR <X>NMR <X>NMR <X>NMR

SPECINFO

Spectral Data (cont'd)

Fields	Default Units	Search Code	Search Examples	Display Code
IR Data				
Band Width (1)	cm** ⁻¹	/IRS.BDW	S L1(S)5-15/IRS.BDW	IRS
Instrument	-	/IR.INS	S BRUKER IFS 112/IR.INS	IR
Intensity (absolute) (1)	none	/IR.IN	S 3-3.2/IR.IN	IR
Intensity (1)	%	/IRS.IN	S 2935-2938/IRS.PP(S)57/IRS.IN	IRS
Note	-	/IR.NTE	S PU/IR.NTE(L)100/IR.NTE	IR
Peak Position (1)	cm** ⁻¹	/IRS.PP	S 2935-2938/IRS.PP	IRS
Reference	-	/IR.REF	S 1990/IR.REF	IR
Sample Form	-	/IR.SPF	S MULL/IR.SPF	IR
Spectrum Number	-	/IR.NR	S MPCC-10033-662Y/IR.NR	IR
VCH Number	-	/IR.VCH	S 500/VCH	IR
MR Data				
Base Peak (1)	m/z	/MS.BS	S 28-30/MS.BS	MS
Base Peak Intensity (1)	none	/MS.BSI	S 99.98/MS.BSI	MS
Intensity (1)		/MSS.IN	S 3.98-4.01/MSS.IN	MSS
Ionization Mode	-	/MS.IOM	S "EI+"/MS.IOM	MS
Nominal Mass (1)	none	/MS.NOM	S 30-40/MS.NOM	MS
Peak Position (1)	m/z	/MSS.PP	S 4-10/MSS.PP	MSS
Spectrum Number	-	/MS.NR	S LMCM-10434-118/MS.NR	MS

(1) <X> is 13C, 19F, 15N, 17O, or 31P.

(2) Numeric search field that may be searched with numeric operators or ranges.

(3) Simplified query input <X>NMRS.PP, <X>NMRS.MUL, <X>NMRS.IN.

DISPLAY and PRINT Formats

Any combination of display fields and formats may be used to display or print answers. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested. The default format in the SPECINFO database is the dynamic display format QRD (Query Related Data) providing information on identification of substance (IDE) plus those display fields in which your search term appears (HIT).

All predefined formats are listed in an hierarchical order, whereby the indented subformats are included in the previous format.

Format	Content	Examples
CN	Chemical Name	D 1,10 CN
MF	Molecular Formula	D 1-5 MF
MW	Molecular Weight	D MW
RAN	ReaxysFile Accession Number	D RAN
RN	CAS Registry Number	D 1 10 RN
SRN	SPECINFO Registry Number	D SRN
STR	Chemical Structure Image	D STR
UP	Update Date	D UP

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
ALL IDE ALL<X> <X>NMR <X>NMRS <X>NMR.GSP COUP<X> ALLIR IR IRS IRS.GSP ALLMS MS MSS MSS.GSP QRD TRIAL	All Data (IDE, ALL<X>, ALLIR, ALLMS) (1) Identification of Substance (SRN, RN, BRN, MF, MW, CN, STR) All information available about <X>NMR (<X>NMR, <X>NMRS, <X>NMRS.GSP, COUP<X>) (1,2) <X>NMR Spectral Data (1) <X>NMR Spectrum (1) <X>NMR Graphical Spectrum (1,2) <X>Coupling Constants (1) All information available about IR (IR, IRS, IRS.GSP) (2) IR Spectral Data IR Spectrum IR Graphical Spectrum (2) All information available about MS (MS, MSS, MSS.GSP) (2) MS Spectral Data Mass Spectrum MS Graphical Spectrum (2) Query related data (default) (IDE HIT) SRN, RN, MF, MW, FA	D ALL D L1 IDE D ALLC D L2 CNMR D ONMRS D ONMRS.GSP D L1 COUPC D ALLIR D L1 IR D IRS D L1 IRS.GSP D ALLMS D MS D MSS D MSS.GSP D QRD L1 D TRI
HIT OCC	Hit term(s) and field(s) Number of occurrences of hit term(s) and field(s) in which they occur	D HIT D OCC

(1) <X> is C, F, N, O, or P.

(2) The .GSP formats only display on graphics terminals (type 2).

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
CAS Registry Number	RN	Y	N
Chemical Name	CN	Y	N
Molecular Formula	MF	Y (default)	N
Molecular Weight	MW	Y	N
ReaxysFile Accession Number	RAN	Y	N
SPECINFO Registry Number	SRN	Y	N
Update Date	UP	Y	N

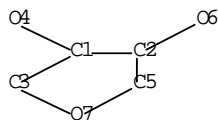
(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answers set, e.g., SEL HIT CT.

SPECINFO

Sample Record

DISPLAY ALL

SpecInfo Reg. No. (SRN) : STCC-92844-623
 CAS Registry No. (RN) : 22554-74-1
 Molecular Formula (MF) : C4 H8 O3
 Molecular Weight (MW) : 104.05
 Chemical Name (CN) : 3,4-Furandiol, tetrahydro-, trans-



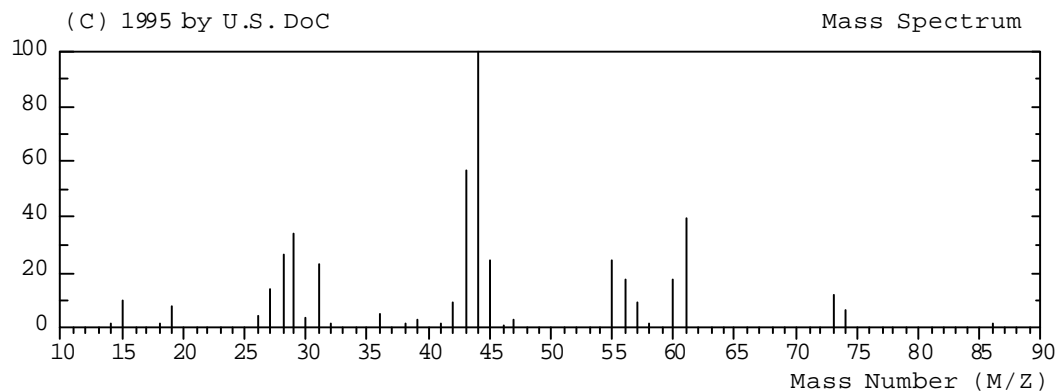
Mass Data :

 Spectrum Number (.NR) : LMCN-86840-389
 Instrument (.INS) : VG QUATTRO
 Base Peak (.BS) : 44
 Base Peak Int. (.BSI) : 99.9
 Nominal Mass (.NOM) : 104
 Ion. Mode (.IOM) : EI+
 Note (.NTE) : EI(70EV)

Mass Spectrum : (C) 1995 by U.S. DoC

Mass Num. .PP (M/Z)	Intensity .IN (rel. Abund.)
14	1.8
15	9.7
18	1.5
19	8.3
26	4.3
27	14.3
28	26.5
29	33.9
30	4.0
31	23.4
32	1.9
36	4.9
38	2.4
39	2.8
41	2.0
42	8.9
43	57.0
44	99.9
45	24.4
46	1.2
47	3.2
55	24.4
56	17.3
57	9.4

58		1.6
60		17.9
61		39.8
73		11.9
74		6.4
86		1.5



In North America
CAS
STN North America
P.O. Box 3012
Columbus, Ohio 43210-0012 U.S.A.

CAS Customer Center:
Phone: 800-753-4227 (North America)
614-447-3700 (worldwide)
Fax: 614-447-3751
E-mail: help@cas.org
Internet: www.cas.org

In Europe
FIZ Karlsruhe
STN Europe
P.O. Box 2465
76012 Karlsruhe
Germany
Phone: +49-7247-808-555
Fax: +49-7247-808-259
E-mail: helpdesk@fiz-karlsruhe.de
Internet: www.stn-international.com

In Japan
JAICI (Japan Association for
International Chemical Information)
STN Japan
Nakai Building
6-25-4 Honkomagome, Bunkyo-ku
Tokyo 113-0021, Japan
Phone: +81-3-5978-3601 (Technical Service)
+81-3-5978-3621 (Customer Service)
Fax: +81-3-5978-3600
E-mail: support@jaici.or.jp (Technical Service)
customer@jaici.or.jp (Customer Service)
Internet: www.jaici.or.jp