



STN is operated in North America
by Chemical Abstracts Service.

STN Database Summary Sheet

ChemInformRX Reaction Search Service is a chemical reaction database that contains reaction information derived from documents covered in ChemInform. The ChemInform Document Number is the Accession Number in ChemInformRX. The document-based database contains both single-step and multistep reactions.

Records contain reaction information consisting of structure diagrams for reactants and products, ChemInform (CI) and CAS Registry Numbers® for all reactants, products, reagents, solvents, and catalysts, yields for many products, and textual reaction information. The reactants, reagents, and products are structure-searchable with a single reaction query. Roles, reaction sites, and mapping of atoms between reactants and products are also structure-searchable. The ChemInform and CAS Registry Numbers for all reaction participants, their roles, textual reaction information, and yields are searchable. Records also contain bibliographic information, in-depth substance and subject indexing, and abstracts.

Subject Coverage

- Single-step and multistep chemical reactions from journals indexed in ChemInform

Sources

- Journals covered by ChemInform

File Data

- 1991 to the present
- More than 136,000 records (7/05)
- More than 872,000 single-step reactions and 451,000 multistep reactions (7/05)
- Updated quarterly with about 5,000 new records
- Automatic current-awareness searches (SDIs) are run quarterly

User Aids

- STN Express User Guide, Chapter 6: Structure Queries
- STN Express User Guide, Chapter 7: Reaction Queries
- STNGUIDE
- Online Helps (HELP DIRECTORY lists all help messages available)

Database Producer/Supplier

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Germany
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614-447-3700 (worldwide)
Fax: 614-447-3751
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CHEMINFORMRX**SEARCH and DISPLAY Field Codes**

There are no fields that allow left truncation.

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains CI and CAS Registry Numbers for all reactants, products, reagents, solvents, and catalysts, and single words from reaction information (RX), title (TI), abstract (AB), and all .CN and .KW fields)	None (or /BI)	S 50-00-0 S 207700 S HYDROGENATION? S 13129-38-9 (L) 16003-05-7 S NEW SYNTHESIS	AB, RX formats, TI
Accession Number Author	/AN /AU	S 200525189/AN S VOSS?/AU S LANGER, P?/ALL	AN AU
Catalyst (includes CI Registry Number, CAS Registry Number, and single words from CAT.CN and CAT.KW) (1)	/CAT	S 498/CAT S 50-21-5/PRO (L) ANY/CAT S 1314-15-4/CAT S PLATINUM/CAT S (PLATINUM (L) OXIDE)/CAT	RX formats
Catalyst, CAS Registry Number	/CAT.RN (or /CAT)	S 1314-15-4/CAT.RN	RX formats
Catalyst, Chemical Name	/CAT.CN	S PLATINUM/CAT.CN S "PLATINUM(II) OXIDE"/CAT.CN S PTO/CAT.CN	Not displayed
Catalyst, Keyword Classification Code (code and text)	/CAT.KW /CC	S ACID BROMIDE/CAT.KW S K2570/CC S AMINO ALCOHOLS/CC S ALKYLATION?/CC	Not displayed CC
Corporate Source (2) Data Entry Date (3) Entry Date (3)	/CS /DED /ED (or /UP)	S BASF/CS S 19970711/DED S L5 AND ED=20050100	CS DED Not displayed
International Standard (Document) Number (contains CODEN and ISSN) Issue (3) Journal Title	/ISN /IS /JT	S 0040-4039/ISN S TELEAY/ISN S TETRAHEDRON/SO AND 10-12/IS S TETRAHEDRON/JT S Z NATURFORSCH/JT	ISN, SO SO JT, SO
Keywords Language (code and text) NonProduct (includes CI Registry Number, CAS Registry Number, and chemical name for reactants, reagents, solvents, and catalysts)	/KW /LA /NPRO	S O-ALKYLATION/KW S EN/LA S 10024-97-2/NPRO S 144/NPRO S NITROGEN DIOXIDE/NPRO S NO2/NPRO	RX formats LA RX formats
Notes Number of Stages (3) Number of Steps (3)	/NTE /NSS /NS	S SEALED TUBE/NTE S 2/NSS S 1/NS S 109-99-9(L)71-43-2(L)1/NS	RX formats Not displayed Not displayed
Page Number (3) Product (includes CI Registry Number, CAS Registry Number, and single words from chemical name and PRO.KW) (1) Product, CAS Registry Number	/PGNO /PRO /PRO.RN (or /PRO)	S 10/PGNO S 96/PRO S 64-18-6/PRO S (FORMIC (L) ACID)/PRO S (ACYL (L) HALIDE)/PRO S 50-00-0/PRO.RN	SO RX formats RX formats
Product, Keyword	/PRO.KW	S ALCOHOL/PRO.KW S ACYL HALIDE/PRO.KW	Not displayed
Publication Year (3)	/PY	S 2004/PY	PY, SO

SEARCH and DISPLAY Field Codes (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Reactant (includes CI Registry Number, CAS Registry Number, and single words from the chemical name and RCT.KW) (1)	/RCT	S 95/RCT S 27437/RCT(L)293006/PRO S 139-13-9/RCT(L)24553-06-8/PRO S (ACETIC (L) ACID)/RCT S ACID/RCT S 75-09-2/RCT.RN	RX formats
Reactant, CAS Registry Number	/RCT.RN (or /RCT)		RX formats
Reactant, Keyword	/RCT.KW	S HETEROCYCLE/RCT.KW S HYDROXAMIC ACID/RCT.KW	Not displayed
Reagent (includes CI Registry Number, CAS Registry Number, and single words from RGT.CN and RGT.KW) (1)	/RGT	S 18/RGT S 80-15-9/RGT S (BROMINE (L) CYANIDE)/RGT	RX formats
Reagent, CAS Registry Number	/RGT.RN (or /RGT)	S 80-15-9/RGT.RN	RX formats
Reagent, Chemical Name	/RGT.CN	S BR2/RGT.CN S BROMINE CYANIDE/RGT.CN	RX formats
Reagent, Keyword	/RGT.KW	S AMINE OXIDE/RGT.KW	Not displayed
Reactant or Reagent (includes CI Registry Number, CAS Registry Number, and chemical names) (1)	/RRT	S 45799/RRT S 109-99-9/RRT S THIOBENZOIC ACID/RRT	RX formats
Solvent (includes CI Registry Number, CAS Registry Number, and single words from SOL.CN and SOL.KW) (1)	/SOL	S 123/SOL S 67-56-1/SOL S (METHYL(L)ACETATE)/SOL	RX formats
Solvent, CAS Registry Number	/SOL.RN (or /SOL)	S 60-29-7/SOL.RN	RX formats
Solvent, Chemical Name	/SOL.CN (or /SOL)	S MEOH/SOL.CN S METHYL ACETATE/SOL.CN	RX formats
Solvent, Keyword	/SOL.KW (or /SOL)	S ALCOHOL/SOL.KW	Not displayed
Source (contains journal title, CODEN and ISSN, collation, and pagination)	/SO	S (TETRAB AND 53 AND 7)/SO S 0040-4020/SO	SO
Temperature, Keyword	/T.KW	S REFLUX/T.KW	RX formats
Title	/TI	S CATALY?/TI S BECKMANN REARRANG?/TI	TI
Volume (3)	/VL	S ANGEW CHEM/JT AND 109-110/VL	SO
Yield Product (3)	/YDP	S 90-100/YDP S 502-49-8/PRO(A)94-100/YDP	RX formats
Yield Product Text	/YDPT	S NONE/YDPT S 502-49-8/PRO(A)(95-100/YDP OR NONE/YDPT)	Not displayed
Yield Stage (3)	/YDS	S 90<YDS S 502-49-8/PRO(L)94-100/YDS(L)1/NS	RX formats
Yield Stage Text	/YDST	S NONE/YDST S 502-49-8/PRO(L)(95-100/YDS OR NONE/YDST) (L) 1/NS	Not displayed

(1) ChemInform Registry Numbers for all substances renumbered in 08/93.

(2) Implied (S) proximity is available in this field.

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

Property SEARCH and DISPLAY Field Codes

Search Field Name	Default Units	Search Code	Search Examples	Display Codes
Pressure Temperature	atm Cel	/P /T	S P1 S 100-110/T	RX formats RX formats

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Structure Search Terms

The L-number answer set from a structure search may be combined with text terms, e.g., S L6 (L) ANY/CAT.

Terms	Search Examples
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express (Boolean logic allowed between the L-numbers)	SEARCH L1 CSS FUL S L1 NOT L2 S L3 OR L4
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L1 NOT L3

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances that at match the query. Substitution is allowed at all open positions.	SSS	SEARCH L1 SSS FUL S L2
Closed Substructure	Search for substances that match the query exactly. Substitution is allowed at positions opened by CONNECT.	CSS	SEARCH L1 CSS FUL SEA L4 CSS

Scopes of Structure Searches

To create an L-number answer set containing candidate structures that have passed the screening step of your structure search, enter EXTEND on the search command line or enter SET EXTEND ON or SET EXTEND ON PERM at an arrow prompt (=>). For details, enter HELP SET EXTEND at an arrow prompt.

Scope	Definition	Search Code	Search Examples
Sample (default) (1)	Search a fixed 5% of the file.	SAM	SEARCH L1 SAM SSS
Full	Search 100% of the file.	FUL	S L5 SSS FUL
Range	Search a user-specified portion of the file.	RAN	S L4 RAN=(V112) S L1 RAN=(RCR) S L9 SUB=L8 SAM
Subset Sample	Search a fixed sample of an answer set created by a search in CHEMINFORMRX.	SUB SAM	
Subset Range	Search a user-specified portion of an answer set created by a search in CHEMINFORMRX.	SUB RAN	S L12 SUB=L11 RAN=(200401000,200407000) S L3 SUB=L2 RAN=(20040100,20050100)
Subset Full	Search 100% of an answer set created by a search in CHEMINFORMRX.	SUB FUL	S L2 CSS SUB=L1 FUL

(1) EXTEND not valid with SAMPLE.

DISPLAY and PRINT Formats

Any combination of formats may be used to display or print answers. Multiple Codes must be separated by commas or spaces, e.g., D TI FHIT. The fields are displayed or printed in the order requested.

Hit-term highlighting is available in all fields except CC and NTE. In the RX fields, highlighting occurs in the Reaction Map and Reaction Summary. Highlighting must be ON in order to use the HIT, FHIT, OCC, PATH, FPATH, SPATH, and FSPATH formats. The default display format is a combination of two formats: FHIT CBIB.

Reaction Formats

Format	Content	Examples
RX RX(n) (1) RXF (1) RXF(n) (1) RXG (1) RXG(n) (1) RXL (1) RXL(n) (1) RXS (1) RXS(n) (1)	Reactions (Map, Diagram, and Summary for all single-step reactions) Reaction n (Map, Diagram, and Summary for reaction n) Reactions Full(Map, Diagram, and Summary for all single-step reactions plus all substance keywords and chemical names in the reaction summary) Reaction Full n (Map, Diagram, and Summary for reaction n plus all substance keywords and chemical names in the reaction summary) Reaction Graphics (Map and Diagram for all single-step reactions) Reaction n Graphics (Map and Diagram for reaction n) Reaction Long (Map, Diagram, and Summary for all single-step reactions) Reaction n Long (Map, Diagram, and Summary for all steps of reaction n) Reaction Summary (Map and Summary for all single-step reactions) Reaction n Summary (Map and Summary for reaction n)	D TI RX D RX(3),RX(5) D RXF D BIB,RXF(1) D RXG CBIB D RXG(5) DIS RXL D RXL(8) RXL(13) D TI AU RXS D RXS(13)
ALL SCAN (2,3)	AN, TI, AU, CS, SO, LA, CC, AB, RX TI, FHIT (random display with no answer number)	D L2 1-7 ALL D SCAN
FHIT FHITCBIB FPATH FSPATH HIT OCC (2) PATH SPATH	First HIT Reaction Map, Diagram, and Summary CBIB FHIT (FHITCBIB is the default) Full PATH - PATH plus Reaction Summary Full SPATH - SPATH plus Reaction Summary Fields containing hit terms and the Reaction Map, Diagram, and Summary for all hit reactions. Number of occurrences of hit terms and fields in which they occur. Includes total number of HIT, PATH, and SPATH reactions. Labels reactions that have incomplete verifications. Reaction Map(s) and Diagram(s) of longest PATH(s). Displays all hit reactions except those whose steps are totally included within another hit reaction. Reaction Map(s) and Diagram(s) for short PATH(s). Displays reactions having a hit substance in the first and last step except for those whose steps are totally included within another SPATH reaction.	D FHIT D L4 2,4 FHITCBIB D BIB FPATH D FSPATH D CBIB HIT DIS 1-10 OCC D PATH D SPATH

(1) Custom display only.

(2) No online display fee for this option.

(3) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

CHEMINFORMRX**Bibliographic Formats**

Format	Content	Examples
AB AN (1) AU CC (1) CS DED (1) ISN (2) JT (2) LA (1) PY (1,2) SO TI (1)	Abstract Accession Number Author Classification Code Corporate Source Data Entry Date International Standard (Document) Number Journal Title Language Publication Year Source Title	D AB DISPLAY L2 1-10 AN D AU TI D CC TI D AU CS D DED D ISN D JT D LA D PY D TI AU SO D TI RX
ABS ALL BIB CBIB SCAN (1,3)	AN, AB AN, TI, AU, CS, SO, LA, AB, CC, DED, RX AN, TI, AU, CS, SO, LA AN, compressed bibliographic data TI, FHIT (random display with no answer number)	DIS 2,4,6 CBIB ABS D L2 1-7 ALL D 1-3 BIB DISPLAY L1 1 CBIB D SCAN
FHITCBIB HIT OCC (1)	CBIB FHIT (FHITCBIB is the default) Fields containing hit terms and the Reaction Map, Diagram, and Summary for all hit reactions. Number of occurrences of hit terms and fields in which they occur. Includes total number of HIT, PATH, and SPATH reactions. Labels reactions that have incomplete verifications.	D L4 2,4 FHITCBIB D CBIB HIT DIS 1-10 OCC

(1) No online display fee for this option.

(2) Custom display only.

(3) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

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
Abstract	AB	Y	N
Accession Number	AN	Y	N
Author	AU	Y (default)	Y
Catalyst, CAS Registry Number	CAT.RN	Y (2)	N
Catalyst, Chemical Name	CAT.CN	Y (2)	N
Catalyst, Keyword	CAT.KW	Y (2)	N
Catalyst CI Registry Number	CAT	Y (2)	N
Classification Code	CC	Y (2)	Y
CODEN	CODEN	N	Y
Corporate Source	CS	Y	Y
Data Entry Date	DED	Y	Y
International Standard (Document) Number	ISN	Y (3)	N
International Standard Serial Number	ISSN	N	Y
Journal Title	JT	Y	Y
Keywords	KW	Y (2)	N
Language	LA	Y	Y
Non Product CI Registry Number	NPRO	Y (2)	N
Product, CAS Registry Number	PRO.RN	Y (2)	N
Product, Keyword	PRO.KW	Y (2)	N
Product CI Registry Number	PRO	Y (2)	N
Publication Year	PY	Y	Y
Reactant, CAS Registry Number	RCT.RN	Y (2)	N
Reactant, Keyword	RCT.KW	Y (2)	N
Reactant CI Registry Number	RCT	Y (2)	N
Reactant-Reagent CI Registry Number	RRT	Y (2)	N
Reaction Note	NTE	Y (2)	N
Reaction n	RX(n)	Y (2,4,5)	N
Reactions	RX	Y (2,4)	N
Reagent, CAS Registry Number	RGT.RN	Y (2)	N
Reagent, Chemical Name	RGT.CN	Y (2)	N
Reagent, Keyword	RGT.KW	Y (2)	N
Reagent CI Registry Number	RGT	Y (2)	N
Solvent, CAS Registry Number	SOL.RN	Y (2)	N
Solvent, Chemical Name	SOL.CN	Y (2)	N
Solvent, Keyword	SOL.KW	Y (2)	N
Solvent CI Registry Number	SOL	Y (2)	N
Source	SO	Y (6)	N
Title	TI	Y	Y

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

(2) SELECT HIT and ANALYZE HIT are not valid with this field.

(3) Selects or analyzes the CODEN and ISSN with /ISN appended to the terms created by SELECT.

(4) Selects or analyzes ChemInform Registry Numbers. The CI RNs for all substances were renumbered in 08/93.

(5) Appends /RX to the terms created by SELECT.

(6) Selects or analyzes the CODEN and ISSN with /SO appended to the terms created by SELECT.

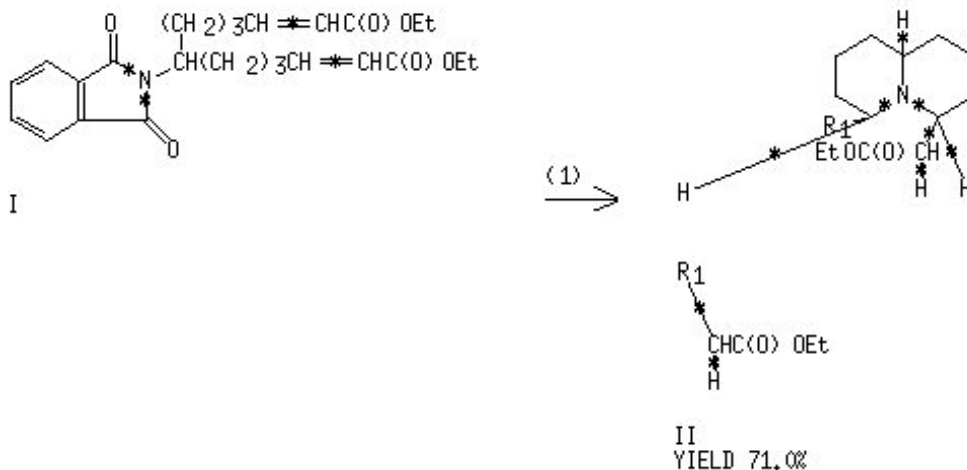
8
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Sample Record

DISPLAY ALL

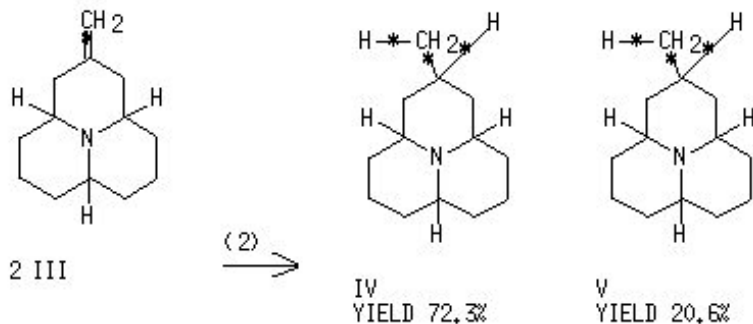
AN 200524184 CHEMINFORMRX Full-text
 TI Combining Two-Directional Synthesis and Tandem Reactions. Part 5. An Efficient Strategy for the Total Syntheses of (+/-)-Hippodamine and (+/-)-epi-Hippodamine.
 AU REJZEK, M.; STOCKMAN, R. A.; HUGHES, D. L.
 CS Sch. Chem. Sci., Univ. East Anglia, Norwich, Norfolk NR4 7TJ, UK
 SO Org. Biomol. Chem., 3(1), 73-83 (2005)
 CODEN: OBCRAK ISSN: 1477-0520
 LA English
 AB The construction of the tricyclic skeleton and control of stereochemistry in the alkaloids (IV) and (V) is accomplished via quinolizine derivative (II). The third ring of target alkaloids is formed by Dieckmann condensation and decarboxylation to give olefin (III). Optimal conditions are developed to convert (III) either into hippodamine (IV) or epi-hippodamine (V).
 CC U0600 Alkaloids

RX(1) OF 3 A == B



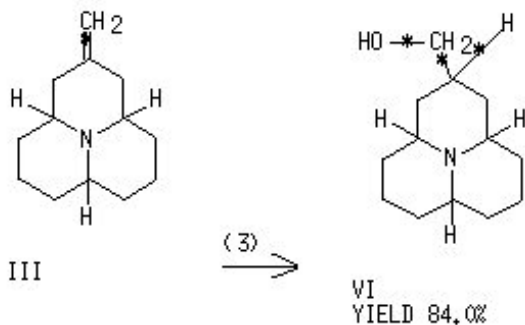
RX(1) RCT I, 916283
 STAGE(1)
 RGT 1156 (16940-66-2), NaBH4
 SOL 115 (67-63-0), iPrOH
 222 (7732-18-5), H2O
 T 25.0 Cel
 STAGE(2)
 RGT 5 (67-64-1), acetone
 STAGE(3)
 RGT 3 (64-19-7), AcOH
 T 0.0 - 80.0 Cel
 STAGE(4)
 RGT 768 (584-08-7), K2CO3
 SOL 14 (71-43-2), benzene
 PRO II, 916284
 YDS 71.0 %
 KW alkylation; N-alkylation
 NTE reaction:I - II

RX(2) OF 3 2 J === K + L



RX(2) RCT III, 1085920
 STAGE(1)
 RGT 1084774, Mst-SO3H
 SOL 206 (109-99-9), THF
 T 25.0 Cel
 STAGE(2)
 RGT 107 (1333-74-0), H2
 SOL 206 (109-99-9), THF
 CAT 1237 (71717-87-8), Pd-C
 T 25.0 Cel
 PRO IV, 1071003
 V, 1085921
 YDS 93.0 %
 KW addition; hydrogenation
 NTE reaction:III - (+/-)-IV and (+/-)-V

RX(3) OF 3 J === Q



RX(3) RCT III, 1085920
 STAGE(1)
 RGT 1084775, 9-BBN.THF
 SOL 206 (109-99-9), THF
 T -78.0
 T.KW REFLUX Cel
 STAGE(2)
 RGT 1158 (7722-84-1), H2O2
 1159 (1310-73-2), NaOH
 SOL 222 (7732-18-5), H2O
 123 (67-56-1), MeOH
 T 0.0 Cel
 PRO VI, 1085922
 YDS 84.0 %
 KW addition; hydration; alkylation; O-alkylation
 NTE reaction:III - VI

