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STN Database Summary Sheet

The **Derwent Journal of Synthetic Methods File (DJSMDs)**: subscriber file; **DJSMONLINE**: non-subscriber file) is a structure-searchable chemical reactions database, designed on the principles set out originally by Theilheimer, which provides key references to novel synthetic methods from the worldwide patent and scientific literature. The strict selection criteria ensure that only new or the most synthetically useful modifications of known methods are abstracted. In addition, all references are cross-referenced to relevant prior art and other similar reactions. The database and its associated printed Derwent Journal of Synthetic Methods are an expansion and adaptation of Theilheimer's Synthetic Methods of Organic Chemistry.

The records contain reaction information consisting of structure diagrams for reactants and products, DJSM Registry Numbers for all reactants, products, solvents, and catalysts, yields for many products, and textual reaction information. The reactants 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 DJSM Registry Numbers for reaction participants, their names, supplementary terms, and yields are searchable. The records also contain bibliographic information, classification codes, keywords, and abstracts.

Page images of the printed Derwent Journal of Synthetic Methods are included for all records. Images may be viewed directly when using STN on the Web.

Subject Coverage

Chemical reactions for:

- All new or improved synthetic methods
- Known processes effected by new reagents
- Interesting applications and extensions of known reactions
- Applications of organometallic and metal complexes to organic synthesis

Sources

- Over 180 journals
- Patents from 41 issuing authorities

File Data

- 1975 through June 2003
- More than 100,306 records (7/08)
- More than 79,658 single-step reactions (7/08)
- More than 5,713 multi-step reactions (7/08)
- 14,994 records from 1975 to 1979 do not contain structures
- Automatic current-awareness searches (SDIs) are not available

User Aids

- DJSM Technical Guide (available from the producer)
- DJSM Thesaurus (available from the producer)
- Building and Searching Structures on STN
- Online Helps (HELP DIRECTORY lists all help messages available)
- STNGUIDE

Database Producer/Supplier

Thomson Reuters (Scientific) Ltd.
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614-447-3700 (worldwide)
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E-mail: help@cas.org
Internet: www.cas.org

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Fax: +49-7247-808-259
E-mail: helpdesk@fiz-karlsruhe.de
Internet: www.stn-international.de

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)
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customer@jaici.or.jp (Customer Service)
Internet: www.jaici.or.jp

DJSMONLINE**Search and Display Field Codes**

There are no fields that allow left truncation in this file.

Search Field Name	Search Code	Search Example	Display Codes
Basic Index (contains DJSM Registry Numbers for all reaction participants, and single words from the abstract (AB), classification codes (CC), keywords (KW), notes (NTE), and title (TI) fields)	None (or /BI)	S 1981 S STEREOSPECIFIC MICHAEL ADDITION S A (1W) B S "TEMP=" S 44 (L) 1981 S ACETAL-DERIV S RING OPEN?	AB, CC, KW, NTE, TI, RX formats
Accession Number	/AN	S 75005D/AN S 88:75005/AN S 8875005/AN S 198875005/AN S 1988:75005D/AN	AN
Atmosphere	/ATM	S O3/ATM	RX formats
Author	/AU	S CINQUINI M/AU S CINQUINI, M./AU	AU
Catalyst Chemical Name	/CAT.CN	S TICL3/CAT.CN	RX formats
Catalyst DJSM Registry Number (1)	/CAT	S 404/CAT S ANY/CAT	RX formats
Catalyst Supplementary Term	/CAT.ST	S 68/CAT AND HYDRATE/CAT.ST	RX formats
Classification Code	/CC	S (A AND B)/CC	CC
Document Type	/DT (or /TC)	S DIARYLSULFON?/TI AND P/DT S DIARYLSULFON?/TI AND J/TC	DT
Entry Date (2)	/ED	S L1 AND ED=16961118	ED
International Standard (Document) Number (contains CODEN and ISSN)	/ISN	S TETRAB/ISN S 0040-4020/ISN	ISN, SO
Journal Title	/JT	S TETRAHEDRON/JT	JT, SO
Keyword	/KW	S PROTECTION-NH/KW	KW
Nonproduct	/NPRO	S FERROCENE/NPRO	RX formats
Nonreacting Group Keyword	/NON.KW	S O-SULFONYL/NON.KW	NON.KW
Note	/NTE	S L6 AND VACUUM/NTE	NTE
Number of Steps (2)	/NS	S L5 AND 1/NS	NS
Other Source	/OS	S 85-160803/OS	OS
Patent Assignee (3)	/PA (or /CS)	S BOEHRINGER/PA S DAIICHI KAGAKU/CS	PA
Patent Number	/PN	S EP330058/PN	PI
Pressure (2,4)	/P	S 2/P S 2-3 ATM/P	RX formats
Product DJSM Registry Number (5)	/PRO	S 200/PRO	RX formats
Product Keyword	/PRO.KW	S PURINE/PRO.KW	PRO.KW
Product Supplementary Term	/PRO.ST	S 51498/PRO AND CHIRAL/PRO.ST	RX formats
Publication Year (2)	/PY	S 1990/PY S PY>1985 AND CZECH B P/AU	PY, SO
Reactant DJSM Registry Number (6)	/RCT	S 40/RCT	RX formats
Reactant Keyword	/RCT.KW	S STEROID/RCT.KW S "HYDROXYLAMINE+ "/RCT.KW	RCT.KW
Reactant Supplementary Term	/RCT.ST	S 41468/RCT AND CHIRAL/RCT.ST	RX formats
Reaction Symbol	/SYM	S CC-ELI-O/SYM	SYM
Reagent Keyword	/RGT.KW	S SILANE/RGT.KW S "ACID=7 "/RGT.KW	RGT.KW

Search and Display Field Codes (cont'd)

Search Field Name	Search Code	Search Example	Display Codes
Source (contains journal title, collation, ISSN, CODEN)	/SO	S TETRAB/SO S (TETRAHEDRON(L)35)/SO S 0040-4020/SO	SO
Solvent Chemical Name	/SOL.CN	S NH3/SOL.CN	RX formats
Solvent DJSM Registry Number (7)	/SOL	S 12/SOL	RX formats
Solvent Keyword	/SOL.KW	S ESTER/SOL.KW	SOL.KW
Solvent Supplementary Term	/SOL.ST	S 12/SOL AND GAS/SOL.ST	RX formats
Temperature (2,8)	/T	S 200-220/T	RX formats
Time (2,9)	/TIM	S L1 AND TIM<1	RX formats
Title	/TI	S CYCLOPROPYLKETONE?/TI	TI
Update Date (2)	/UP	S UP=19971200	UP
Volume/Issue (printed DJSM)	/VI	S 16-1/VI	VI
Yield Product (2)	/YDP	S L1 AND YDP>95	RX formats
Yield Product Text	/YDPT	S NONE/YDPT	Not displayed

(1) A search in /CAT includes the Catalyst Chemical Name (/CAT.CN) and the Catalyst Supplementary Term (/CAT.ST) fields.

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

(3) Search with implied (S) proximity is possible in this field. Images may be viewed directly when using STN on the Web.

(4) ATM is the default unit for this field.

(5) A search in /PRO includes the Product Supplementary Term (/PRO.ST) field.

(6) A search in /RCT includes the Reactant Supplementary Term (/RCT.ST) field.

(7) A search in /SOL includes the Solvent Chemical Name (/SOL.CN) and Solvent Supplementary Term (/SOL.ST) fields.

(8) C is the default unit for this field.

(9) HR is the default unit for this field.

Structure Search Terms

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
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L3 OR L4
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

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

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances that 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

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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
Full (default)	Search 100% of the file.	FUL	S L5 SSS FUL
Range	Search a user-specified portion of the file.	RAN	S L4 RAN=(1990,1993)
Subset Range	Search a user-specified portion of an answer set created by a search in DJSMDS.	SUB RAN	S L12 SUB=L11 RAN=(77000J,77100J)
Subset Full	Search 100% of an answer set created by a search in DJSMDS.	SUB FUL	S L2 CSS SUB=L1 FUL

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 L1 1-5 TI RX(1). The fields are displayed or printed in the order requested.

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

Format	Content	Examples
RX RX(n) (1) RXG (1) RXG(n) (1) RXS (1) RXS(n) (1)	Reactions (Map, Diagram, Summary for all single-step reactions) Reaction n (Map, Diagram, Summary for reaction n) Reaction Graphics (Map and Diagram for all single-step reactions) Reaction n Graphics (Map and Diagram for 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(1) D RXG, CBIB D RXG(3) D TI AU RXS D RXS(3)
AB AN (2) AU CC (2) DT (TC)(2) ED (1,2) GI (1,3) (PAGE) ISN (1) JT (1) KW (2) NS (2) NTE (2) OS PA (CS) PI (PN) (4) PY (2) SO SYM (2) TI (2) UP (2) VI	Abstract Accession Number Author Classification Code Document Type Entry Date Graphic Image International Standard (Document) Number Journal Title Keyword (includes RCT.KW, RGT.KW, PRO.KW, SOL.KW, and NON.KW) Number of Steps Note Other Source Patent Assignee Patent Information (Patent Number) Publication Year Source Reaction Symbol Title Update Date Volume/Issue (printed DJSM)	D AB D L5 1-10 AN D AU TI D CC D DT D ED D GI D ISN D JT D KW D NS D NTE D OS D PA D PI OS D PY D SO D SYM D TI D UP D VI TI 1-10

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
ABS ALL (4)	AN, AB Journal: AN, TI, AU, SO, DT, VI, AB, CC, SYM, KW, RCT.KW, PRO.KW, RGT.KW, SOL.KW, NON.KW, NTE, NS, RX Patent: AN, TI, PA, PI, DT, VI, OS, AB, CC, SYM, KW, RCT.KW, PRO.KW, RGT.KW, SOL.KW, NON.KW, NTE, NS, RX	D ABS D ALL
BIB (4)	Journal: AN, TI, AU, SO, DT, VI Patent: AN, TI, PA, PI, DT, VI, OS (BIB is the default)	D 1-5 BIB
CBIB IABS	Compressed bibliographic information ABS, indented with text labels	D CBIB 1-5 D IABS
IALL (4)	ALL, indented with text labels	D IALL
IBIB (4)	BIB, indented with text labels	D IBIB 1-5
IIND (2)	IND, indented with text labels	D IIND
IND (2)	CC, SYM, KW, RCT.KW, PRO.KW, RGT.KW, SOL.KW, NON.KW, NTE, NS	D IND
SCAN (2,5)	AN, TI (random display with no answer number)	D SCAN
FHIT HIT OCC (2)	First hit Reaction Map, Diagram, and Summary Reaction Map, Diagram, Summary for all hit reactions and fields containing hit terms All hit fields and the number of occurrences of the hit terms in each HIT reaction. Labels reactions that have incomplete verifications.	D FHIT D CBIB HIT DIS 1-10 OCC

- (1) Custom display only.
- (2) No online display charge for this format.
- (3) You can use the GI format in the DISPLAY command for the page images of the printed Derwent Journal of Synthetic Methods. Any program that handles Tiff images compressed in Group 4 fax format, e.g., STN Express, may be used to capture the graphic images.
- (4) By default, patent numbers are displayed in STN format. To display them in Derwent format, enter SET PATENT DERWENT at an arrow prompt. To reset display to STN format, enter SET PATENT STN.
- (5) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

SELECT and SORT Fields

The SELECT command is used to create E-numbers or 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	SELECT	SORT
Abstract	AB	Y (2)	N
Accession Number	AN	Y	N
Author	AU	Y	Y
Catalyst Chemical Name	CAT.CN	Y (3)	N
Catalyst DJSM Registry Number	CAT	Y	N
Catalyst Supplementary Term	CAT.ST	Y (3)	N
Classification Code	CC	Y	Y
CODEN	CODEN	N	Y
Document Type	DT	Y	Y
International Standard (Document) Number	ISN	Y (4)	N
International Standard Serial Number	ISSN	N	Y
Journal Title	JT	Y	Y
Keyword	KW	Y (5)	Y
Non-reacting Group Keyword	NON.KW	Y	N
Note	NTE	Y	Y
Other Source	OS	Y	Y
Patent Assignee	PA	Y	Y

DJSMONLINE**SELECT and SORT Fields (cont'd)**

Field Name	Field Code	SELECT	SORT
Patent Information	PI	Y (6,7)	Y
Patent Number	PN	Y (7)	Y
Product DJSM Registry Number	PRO	Y	N
Product Keyword	PRO.KW	Y	N
Product Supplementary Term	PRO.ST	Y (3)	N
Publication Year	PY	Y	Y
Reactant DJSM Registry Number	RCT	Y	N
Reactant Keyword	RCT.KW	Y	N
Reactant Supplementary Term	RCT.ST	Y (3)	N
Reaction n	RX(n)	Y (8)	N
Reaction Symbol	SYM	Y	Y
Reactions	RX	Y (9)	N
Source	SO	Y (10)	N
Solvent Chemical Name	SOL.CN	Y (3)	N
Solvent DJSM Registry Number	SOL	Y	N
Solvent Keyword	SOL.KW	Y	N
Solvent Supplementary Term	SOL.ST	Y (3)	N
Title	TI	Y (default)	Y

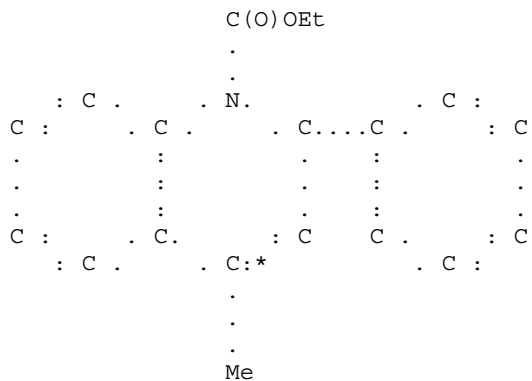
- (1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT KW.
- (2) Appends /BI.
- (3) SELECT HIT is not valid with this field.
- (4) Selects CODEN and ISSN with /ISN appended.
- (5) Selects terms from KW, RCT.KW, PRO.KW, RGT.KW, SOL.KW, and NON.KW and appends /KW.
- (6) Selects the patent number with /PN appended.
- (7) Enter SET PATENT DERWENT at an arrow prompt (=>) to SELECT patent numbers in Derwent format.
- (8) Selects DJSM Registry Numbers from RCT, SOL, CAT, and PRO in Reaction n and appends /RX.
- (9) Selects DJSM Registry Numbers from RCT, SOL, CAT, and PRO in each reaction and appends /RX.
- (10) Selects CODEN and ISSN with /SO appended.

Sample Records

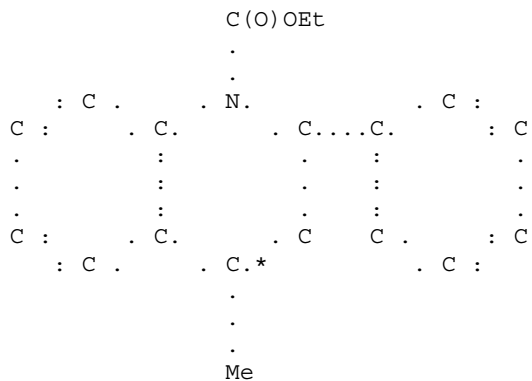
DISPLAY ALL

AN 1990:77763F DJSMONLINE
TI TRANSFER-HYDROGENATION OF QUINOLINE RING . 1,2,3,4-
TETRAHYDROQUINOLINES . ALSO 9,10-DIHYDROACRIDINES
AU Baiczewski, P.; Joule, J. A.
SO Synth Commun, 20(18), p.2815-9 (1990)
CODEN: SYNCAV ISSN: 0039-7911
DT J
VI 16-12
AB Chloro and nitro groups were also reduced. 2-Amino- and
4-methyl-6-methoxy-quinoline were not reduced, and isoquinolines
were reduced less efficiently (14%, 23%). For further examples,
(two; 65%) from quinolines, also 9,10-dihydroacridines (72%),
see litref(1).
CC R Reduction
Y Selective, preferential and partial reactions
SYM HC-Add-CC
KW ORG-REDN
RCT.KW DIHYDRO; UNSATD; HETEROARENE-6
PRO.KW TETRAHYDRO
RGT.KW PD; PT-GROUP,ELEMENT; C-ACID-SALT; AMMONIUM,NH4; FORMIC;
PALLADIUM-CARBON; AMMONIUM-FORMATE
SOL.KW ALCOHOL
NON.KW FUNCT; URETHAN; QUINOLINE; ACRIDINE
NTE TEMP=5 (40-110 degC)
NS 1

RX(1) OF 1 A ==> B



A



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DISPLAY ALL (cont'd)

B

YIELD 95.0%

RX(1) RCT A, 59064; Suspension
SOL 15, MeOH
CAT 73, Pd(m); 10%, on Carbon
952, NH4-Formate; 25 Eq.
PRO B, 59065
TIM 2.5 hr
ATM Ar
CMT Reflux

DISPLAY IIND

CLASSIFICATION CODE:

H Heterocyclic ring closure
X Stereochemistry
G Heterocyclic ring opening

REACTION SYMBOL: CC-Add-CC; CC-Eli-C

KEYWORD: CYCLOADDN,DIPOLAR; RING-LOSS

REACTANT KEYWORD: DIAZO; UNSATD; ISOTHIAZOLE; FUNCT; S-DIOXIDE,CYCLIC;
PYRAZOLE; COND-C; DIHYDRO; UNFUNCT; AMIDINE,CYCLIC

PRODUCT KEYWORD: PYRAZOLE; ISOL; HETEROARENE-5; UNSATD; C-FUNCT;
COND-C; DIHYDRO

SOLVENT KEYWORD: ETHER

NON-REACTING GROUPS KEYWORD:
C-ESTER; PYRAZOLE; ISOTHIAZOLE; S-DIOXIDE,CYCLIC;
AMIDINE,CYCLIC

NOTE TEMP=4 (10-40 degC); TEMP=5 (40-110 degC)

NUMBER OF STEPS: 2