LCASREACT[SM] (Learning CASREACT)

Subject Coverage

- A training reaction database for learning how to use the CASREACT File.
- CAS database of reactions derived from journals covered in CA from 1985 to the present and patents from January 1991 to the present.

File Type

Reactions, Training

Features

Alerts (SDIs)	Unavailable				
CAS Registry Number® Identifiers	☑	Keep & Share	☑	SLART	☑
Learning Database	☑				

Record Content

LCASREACT is a static file that contains 471 documents selected from the CASREACT File, with reaction information derived from journals covered in the Organic Sections of Chemical Abstracts (CA) from 1985 to 1988. The CA Abstract Number is the Accession Number in the file. The document-based file contains both single-step and multistep reactions.

File Size

- 471 records
- Approximately 10,145 single-step reactions
- Approximately 21,477 multistep reactions
- Static file

Coverage

1985 to 1988

Updates

None

Language

English

Database Producer

Chemical Abstracts Service
2540 Olentangy River Road
P.O. Box 3012
Columbus, Ohio 43210-0012 USA
Phone: 800-753-4227 (North America)
Phone: 614-447-3700 (worldwide)
Fax: 614-447-3751
Email: help@cas.org

Sources	Journals covered for CA from 1985 to 1988.
User Aids	• CASREACT User Guide • Getting Started in CASREACT • Search aids are available on the web: http://www.cas.org/training/stn/database-specific • Online HELPs (HELP DIRECTORY lists all HELP messages) • STNGUIDE
Cluster	LEARNING STN Database Cluster information: http://www.stn-international.com/en/customersupport/customer-support#cluster+%7C+subjects+%7C+features
Related Databases	CASREACT

Search and Display Field Codes

The fields that allow left truncation are marked with an asterisk (*).

Reaction Fields

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index* (contains CAS Registry Numbers for all reactants, products, reagents, solvents, and catalysts, and single words from the reaction notes, the title, supplementary terms, abstract, and index terms) **(1)**	None (or /BI or /IA)	S 50-00-0 S CYCLIZATION REACT? S 13129-23-2(L)96695-24-8 S TAUTOMERISM S ?TOXIN?	RX formats, TI, ST, IT, AB, NTE
Catalyst	/CAT	S 104-15-4/CAT S L1 (L) ANY/CAT	RX formats
Functional Group in Product	/FG.PRO	S NITRO/FG.PRO S NITRO/FG.RCT (S) PRIMARY AMINE/FG.PRO S CYCLIC ALC/FG.PRO (L) ALKYNE/FG.RGT S NITRO/FG.PRO (L) ANY/CAT	RX formats
Functional Group in Reactant	/FG.RCT	S TRIHALIDE/FG.RCT S AZIDE/FG.RCT (S) PRIMARY AMINE/FG.PRO S AMIDE/FG.RCT,FG.RGT S ACETAL/FG.RCT (L) ANY/CAT	RX formats
Functional Group in Reactant, Reagent, or Product	/FG	S PRIMARY AMINE/FG	RX formats
Functional Group in Reagent	/FG.RGT	S SULFONATE/FG.RGT S CYCLIC ALC/FG.PRO (L) ALKYNE/FG.RGT S AMIDE/FG.RCT,FG.RGT	RX formats
Functional Group Yield **(2)**	/FG.YD	S FG.YD>=95 S NITRO/FG.PRO (A) FG.YD>=50	RX formats
Functional Group Yield Data	/FG.YDT	S NONE/FG.YDT S (95/FG.YD OR NONE/FG.YDT) S HALIDE/FG.PRO (A) (95/FG.YD OR NONE/FG.YDT)	Not displayed
NonProduct	/NPRO	S 10025-87-3/NPRO	RX formats
Number of Steps **(2)**	/NS	S NS>=2 S 109-99-9 (L) 71-43-2 (L) 1/NS	Not displayed
Product	/PRO	S 2577-41-5/PRO	RX formats
Reactant	/RCT	S 999-97-3/RCT S 928-49-4/RCT (L) 114140-93-1/PRO	RX formats
Reactant or Reagent	/RRT	S 100-07-2/RRT	RX formats
Reaction Notes*	/NTE	S 40 DEGREE/NTE S ?HYDRI?/NTE	RX formats
Reagent	/RGT	S 74-88-4/RGT	RX formats
Solvent	/SOL	S 64-17-5/SOL S 64-17-5/SOL (L) CARBOXYLIC/FG.PRO	RX formats
Yield **(2)**	/YD	S 98/YD S L1 (A) YD>50 S 117638-28-5/PRO (A) 95-100/YD S 2577-41-5/PRO (A) (95-100/YD OR NONE/YDT)	RX formats
Yield Data	/YDT	S NONE/YDT S L5 (A) (95-100/YD OR NONE/YDT) S 2577-41-5/PRO (A) (95-100/YD OR NONE/YDT)	Not displayed

(1) CAS Registry Numbers are from the reaction information, not the IT terms.
(2) Numeric search field that may be searched with numeric operators or ranges.

Document Fields

Search Field Name	Search Code	Search Examples	Display Codes
Abstract	/AB	S PHOTOLY?/AB	AB
Accession Number	/AN	S 109:149648/AN	AN
Author	/AU	S EVANS D?/AU	AU
CA Section Cross-Reference **(1)**	/SX	S 24/CC,SX S CONDENSED BENZENOID/SX	CC
Classification Code **(1)** (contains CA section-subsection number, section title, and section group codes)	/CC	S 24/CC S ALICYCLIC/CC S PHYSICAL ORGANIC/CC	CC
Controlled Term	/CT	S PORPHYRIN#/CT S MICHAEL REACTION/CT	CT, IT
Controlled Word	/CW	S POLYMER/CW	CT, IT
Corporate Source **(1)** (organization name and location)	/CS	S DOW/CS S MERRELL DOW/CS S "DYSON PERRINS"?/CS	CS, PA
Country of Author	/CYA	S USA/CYA	CYA, CS, PA
Document Type (code and text)	/DT	S J/DT S JOURNAL/DT	DT
Entry Date **(2)**	/ED	S ED=930216	Not displayed
Field Availability	/FA	S DIA/FA	Not displayed
File Segment	/FS	S ORG/FS AND L1	FS
Index Term **(3)**	/IT	S REACTION WITH/IT	IT
International Standard (Document) Number (contains CODEN and ISSN)	/ISN	S JACSAT/ISN S 0002-7863/ISN	ISN, SO
Issue Number of Publication **(2)**	/IS	S 1-3/IS	SO
Journal Title	/JT	S J AM CHEM SOC/JT	JT, SO
Language (code and text)	/LA	S L1 AND EN/LA S L1 AND ENGLISH/LA	LA
Publication Date **(2)**	/PD	S PD>870100	PI, SO
Publication Year **(2)**	/PY	S 1987-1988/PY	PY
Source (contains publication title, date, publisher, volume, issue, pagination, CODEN, and ISSN)	/SO	S J AM CHEM/SO S JACSAT/SO S 0002-7863/SO	SO
Supplementary Term	/ST	S (ASYM (S) SYNTHESIS)/ST	ST
Title	/TI	S REDOX AGENT#/TI	TI
Update Date **(2)**	/UP	S 930216/UP	Not displayed
Volume and Issue of CA	/VI	S 107-25/VI	Not displayed
Volume Number of Publication **(2)**	/VL	S 32-33/VL	SO

(1) Search with implied (S) proximity is available in this field.
(2) Numeric search field that may be searched with numeric operators or ranges.
(3) There are no stopwords in this field.

Limiting Search Codes

Only an L-number for an answer set created in CASREACT may be limited.

Search Field Name	Search Code	Search Example
Answers completely iterated	/COMPLETE **(1)**	S L4/COM
Answers incompletely iterated	/INCOMPLETE **(1)**	S L4/INC

(1) The code may be abbreviated to the first three letters.

Structure Search Terms

Terms (1)	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

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

Type of Structure Searching

Type	Search Definition	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

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.

Type	Search Definition	Code	Search Examples
Sample **(1)** (default)	Search a fixed 5% of the file.	SAM	SEARCH L1 SAM SSS
Full Range	Search 100% of the file. Search a user-specified portion of the file.	FUL RAN	S L5 SSS FUL S L4 RAN=(V109)
Subset Sample	Search a fixed sample of an answer set created by a search in LCASREACT.	SUB SAM	S L9 SUB=L8 SAM
Subset Range	Search a user-specified portion of an answer set created by a search in LCASREACT.	SUB RAN	S L12 SUB=L11 RAN=(V107,V108)
Subset Full	Search 100% of an answer set created by a search in LCASREACT.	SUB FUL	S L2 CSS SUB=L1 FUL

(1) EXTEND not valid with SAMPLE.

DISPLAY and PRINT Formats

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

Hit-term highlighting is available in all fields except compressed reaction displays. In reaction fields, highlighting occurs in the Reaction Map and in the Reaction Summary. Highlighting must be ON in order to use the CRD, CRDREF, FHIT, FCRD, FCRDREF, FPATH, FSPATH, HIT, OCC, PATH, RX, RXG, RXL, and SPATH formats.

The PRINT command is not valid in LCASREACT.

Reaction Formats

Format	Content	Examples
CRD(n) CRDREF(n) RX(n) RXG(n) RXL(n) RXS(n) SSRX(n)	Compact Display of Reaction n Compact Display of Reaction n and SO, PY for Reference Reaction n (Map, Diagram, Summary for reaction n) Reaction n Graphics (Map and Diagram for reaction n) Reaction n Long (Map, Diagram, Summary for all steps of reactions n) Reaction n Summary (Map and Summary for reaction n) Single-Step Reaction n (Map, Diagram, and Summary for single-step reaction n)	D CRD**(1)** D CRDREF**(2)** D RX**(3)**, RX**(5)** D RXG**(5)** D RXL**(8)**, RXL**(13)** D RXS**(13)** D SSRX(n)
ALL **(1)** DALL **(1)** IALL **(1)** MAX SSRX	BIB, ABS, IND, SSRX ALL, delimited for post-processing ALL, indented with text labels Same as ALL Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)	DISPLAY L2 1-7 ALL DIS L1 DALL 1-3 D IALL D MAX D SSRX
CRD CRDREF FCRD FCRDREF FHIT FPATH FSPATH HIT OCC PATH RX RXG RXL RXS SCAN **(2)** SPATH	Compact Display of All HIT Reactions Compact Reaction Display and SO, PY for Reference First Hit Reaction in Compact Format First Hit Reaction in Compact Format and SO, PY for Reference (FCRDREF is the default) First HIT Reaction Map, Diagram, and Summary Full PATH - PATH plus Reaction Summary Full SPATH - SPATH plus Reaction 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 field. Includes total number of HIT, PATH, 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. Hit Reactions (Map, Diagram, Summary for all hit reactions) Hit Reaction Graphics (Map and Diagram for all hit reactions) Hit Reaction Long (Map, Diagram, Summary for all hit reactions) Hit Reaction Summaries (Map and Summary for all hit reactions) TI and FCRD (random display, no answer number 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	D CRD D CRDREF 1-2 D FCRD 3-5 D FCRDREF 5 D FHIT D BIB FPATH D FSPATH D CBIB HIT DIS 1-10 OCC D PATH D TI RX D RXG CBIB DIS RXL D TI AU RXS D SCAN D SPATH

(1) Structure diagrams in abstracts in the GI (Graphics Image) field are available only on graphics terminals and in offline prints
(2) No online display charge for this option. SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

Document Formats

Format	Content	Examples
AB	Abstract Text	D AB
AN	Accession Number	DISPLAY L2 1-10 AN
AU	Author	D AU TI
CC	Classification Code	D CC
CS	Corporate Source	D AU CS
CT	Controlled Term	D CT
CYA	Country Name of Author	D CYA
DT	Document Type	D 1,5,10 DT
FS	File Segment	D FS
GI **(1)**	Graphic Image or Availability Information	D GI
ISN	International Standard (Document) Number	D ISN
IT	Index Term	D ST IT
JT	Journal Title	D JT
LA	Language	D LA
PY	Publication Year	D PY
SO	Source (Name of journal, volume, issue, pages)	D TI AU SO
ST	Supplementary Term	D ST
SX **(2)**	CA Section Cross-Reference Code	D SX
TI	Title of Document	D TI RX
ABS **(1)**	GI, AB	DIS 2,4,6 CBIB ABS
ALL **(1)**	BIB, ABS, IND, SSRX	DISPLAY L2 1-7 ALL
BIB	AN, TI, AU, CS, SO, DT, LA	D 1-3 BIB
CAN	List of CA abstract numbers, no L-number header	
CBIB	AN, plus Compressed Bibliographic Data	DISPLAY L1 1 CBIB
DALL **(1)**	ALL, delimited for post-processing	DIS L1 DALL 1-3
IND	ST,IT	D IND
SCAN	TI, FHIT (random display, no answer number) **(3)**	D SCAN
MAX	ALL	D MAX
IABS **(1)**	ABS, with text labels	D IABS
IALL	ALL, indented with text labels	D IALL
IBIB	BIB, indented with text labels	D IBIB

(1) Structure diagrams in abstracts in the GI (Graphics Issue) field are available only on graphics terminals.
(2) SX displays all information in the CC field, i.e., CA section and section cross-references.
(3) SCAN must be entered on the same line as the command, e.g., D 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).

Reaction Fields

Field Name	Field Code	SELECT(1)	SORT
All Registry Numbers from Hit Reactions	RX	Y	N
All Registry Numbers from Reaction n	RX(n)	Y	N
All Registry Numbers from Single-Step Reactions	SSRX	Y	N
All Registry Numbers from Single-Step Reaction n	SSRX(n)	Y	N
Catalyst Registry Numbers from HIT Reactions	CAT	Y	N
Catalyst Registry Numbers from Reaction n	CAT(n)	Y	N
Product Registry Numbers from Hit Reactions	PRO	Y	N
Product Registry Numbers from Reaction n	PRO(n)	Y	N
Reactant Registry Numbers from Hit Reactions	RCT	Y	N
Reactant Registry Numbers from Reaction n	RCT(n)	Y	N
Reagent Registry Numbers from Hit Reactions	RGT	Y	N
Reagent Registry Numbers from Reaction n	RGT(n)	Y	N
Solvent Registry Numbers from Hit Reactions	SOL	Y	N
Solvent Registry Numbers from Reaction n	SOL(n)	Y	N

Document Fields

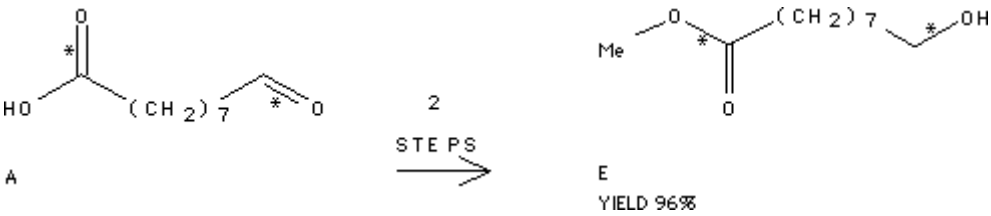
Field Name	Field Code	SELECT	SORT
Abstract Text	AB	Y	N
Accession Number	AN	Y	N
Author	AU	Y	Y
CA Classification Code	CC	Y	Y
CA Section Cross-Reference Code	SX	Y	Y
CODEN	CODEN	Y **(2)**	Y
Controlled Term	CT	Y	N
Corporate Source	CS	Y	Y
Corporate Source, Division	CS.DIV	Y	N
Corporate Source, Organization	CS.ORG	Y	N
Country of Author	CYA	Y	Y
Document Type	DT	Y	Y
File Segment	FS	Y	Y
Index Term	IT	Y	N
International Standard (Document) Number	ISN	Y **(3)**	N
International Standard Serial Number	ISSN	Y **(4)**	Y
Journal Title	JT	Y	Y
Language	LA	Y	Y
Occurrence Count of Hit Terms	OCC	N	Y
Publication Date	PD	Y	Y
Publication Year	PY	Y	Y
Source of Document	SO	Y	N
Supplementary Term	ST	Y	N
Title of Document	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) Selects CODEN and appends /ISN.
(3) Selects CODEN and ISSN and appends /ISN.
(4) Selects ISSN and appends /ISN.
(5) CAS Registry Numbers selected with /RX appended.
(6) CAS Registry Numbers selected with /SSRX appended.

Sample Records

DISPLAY FHIT CBIB

```
RX(13) OF 42 COMPOSED OF RX(1), RX(2)
RX(13)      ***A***    ===>    ***E***
```



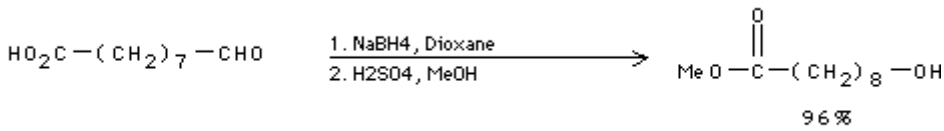

```
RX(1)      RCT  A   ***2553-17-5***
                       RGT  C 16940-66-2 NaBH4
                       PRO  B 3788-56-5
                       SOL  123-91-1 Dioxane

RX(2)      RCT  B 3788-56-5
                       RGT  F 67-56-1 MeOH
                       PRO  E   ***34957-73-8***
                       CAT    ***7664-93-9***   H2SO4
```

CA107(25):237159z Synthesis of phospholipids suitable for covalent binding to surfaces. Kallury, R. Krishnamohanrao; Krull, Ulrich J.; Thompson, Michael (Dep. Chem., Univ. Toronto, Toronto, ON M5S 1A1, Can.). J. Org. Chem., 52(24), 5478-80 (Eng) 1987. CODEN: JOCEAH. ISSN: 0022-3263.

DISPLAY FCRDREF

RX(13) OF 42 - 2 STEPS



REF: J. Org. Chem., 52(24), 5478-80; 1987

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