CASREACT®
User Guide

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CAS®
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

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Chapter 1: Overview of CASREACT

Content

Chemical Abstracts Reaction Search Service (CASREACT) is a chemical reaction database that contains chemical synthesis information derived from documents from 1840 to the present.

CASREACT is a structure-searchable, document-based database. The CA Abstract Number is the file accession number. In September 2016, the database contained over 91 million single-step and multistep reactions and synthetic preparations. It is updated daily.

Sources

The information sources for CASREACT are:

- Journals covered for *Chemical Abstracts* from 1984 to the present
- Patents covered for *Chemical Abstracts* from January 1989 to the present
- The reaction collection jointly built by the All-Union Institute of Scientific and Technical Information of the Academy of Sciences of the USSR (VINITI) and German Zentrale Informationsverarbeitung Chemie, Berlin (ZIC) and supplied by the German software company, InfoChem (journals 1974-1999, patents 1982-1999)
- Rxn: Core Reactions database from the French organization, INPI (Institut National de la Propriete Industrielle) (1840-1985)
- Biotransformations database compiled (1971-1997) under the direction of Professor Doctor Klaus Kieslich
- Encyclopedia of Reagents for Organic Synthesis (EROS)
- Wiley reaction collections from John Wiley & Sons, reproduced under license. All Rights Reserved.
- Selected Organic Reaction Database (SORD) (1961-2011)
- Ph.D. dissertations from 1944-1984

Reaction Information

The reaction information in CASREACT document records consists of:

- Structure diagrams with marked reaction sites for reactants and products
- CAS Registry Number® identifiers for reactants, products, reagents, catalysts, and solvents
- Names or line formulas for reagents, solvents, and catalysts
- Yields for many products
- Information on reaction types, safety, conditions, etc.

Document Information

In addition, bibliographic information, in-depth substance and subject indexing, and abstracts prepared for *Chemical Abstracts* are a part of each CASREACT record. All of the information is searchable and displayable.[1]

LCASREACT

A learning database, LCASREACT, is available for practice or training purposes. All of the search and display options available in CASREACT may be used in the learning database without any search or display charges and with a low connect-hour charge. LCASREACT is a static database of approximately 471 records. There are over 10,000 single-step reactions and over 21,000 multistep reactions in LCASREACT. The information contained in this *Guide* is applicable to LCASREACT, as well as CASREACT.

Getting Started in CASREACT

In addition to this *Guide*, you may wish to review *Getting Started in CASREACT*, a useful compendium of what you need to know about CASREACT. It is available at www.cas.org or from CAS Customer Center.

Database Summary Sheet

For a summary of the search and display fields and formats, refer to the *Database Summary Sheet*, available at www.cas.org or from CAS Customer Center.

This information is also available online in STNGUIDE.

Search and Display Fields

To see a list of the search fields, enter HELP SFIELD at an arrow prompt (=>) in CASREACT. Searching is described in detail throughout this *Guide*.

Various display fields and formats are available to let you see the data online or to print it. Enter HELP DFIELD at an arrow prompt for a list of the display fields. Enter HELP FORMAT for descriptions of the display formats available in CASREACT.

[1]CAS Registry Numbers in the IT field indexing are not searchable in CASREACT. Only CAS Registry Numbers in reaction roles are searchable.

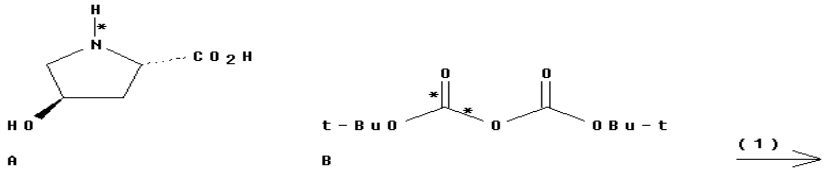
Reaction Information

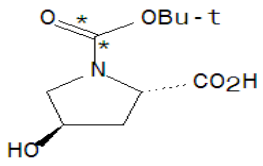
The reaction information for each reaction within a record consists of three parts:

- **Reaction Map** (This example shows one step of a multistep reaction.)

```
RX(1) OF 3     A  +  B  ===>  C...
```

- **Reaction Diagram**





C
YIELD 80%

- **Reaction Summary**

```
RX(1)     RCT  A 51-35-4

        STAGE(1)
           RGT  D 1310-73-2 NaOH
           SOL  7732-18-5 Water
           CON  20 - 25 deg C, pH 5.5 -> 10.5

        STAGE(2)
           RCT  B 24424-99-5
           RGT  D 1310-73-2 NaOH
           SOL  7732-18-5 Water, 67-64-1 Me2CO
           CON  1 - 2 hour, 25 - 28 deg C, pH 10.5

        STAGE(3)
           RGT  E 7647-01-0 HCl
           SOL  7732-18-5 Water
           CON  SUBSTAGE(1) 30 minutes, 25 deg C, pH 2.6
                SUBSTAGE(2) 15 minutes, 25 deg C, pH 2.6
        STAGE(4)
           SOL  108-10-1 i-BuCOMe
           CON  15 - 20 minutes, 35 - 40 deg C

        PRO  C 13726-69-7
```

Reaction Map

The reaction map contains the reaction number, i.e., "RX(1)" in this example, the total number of reactions in the record, i.e., "3", and alphabetic identifiers for the reactants and products, i.e., "A", "B", and "C." All other reaction participants are also labeled and shown in the summary.

Multistep Reaction Map

If the reaction is a multistep reaction, the map states that it is composed of two or more single-step reactions and the reaction numbers of the single-step reactions involved are shown. This example shows a single-step reaction, but the dots following the product "C" indicate that it is the first step of a multistep reaction. If it were a later step in a multistep reaction sequence, there would be dots on both ends of the reaction map, except for the final step.

Reaction Diagram

The reaction diagram contains the structure images of reactants and products. Each has its generic identifier (i.e., "A", "B", "C") from the map.

- Yield (when present) is displayed beneath the product identifier.
- Number of steps is displayed above the arrow.
- Reaction sites (i.e., bonds that are broken, formed, or changed) are indicated by an asterisk (*) on the bond line. Reactions sites are marked in both the reactant and product.

Reaction Summary

The reaction summary contains all reaction participants. Participants fall into five categories:

- RCT (Reactant: A reactant contributes at least one carbon atom to a reaction product, and may also contribute noncarbon atoms.)
- RGT (Reagent: A reagent can contribute only noncarbon atoms to a reaction product.)
- PRO (Product: A product is the end result of a reaction.)
- CAT (Catalyst: A catalyst initiates or promotes the action of other participants in a reaction.)
- SOL (Solvent: A solvent is the medium in which a reaction occurs.)

In the summary, the role, followed by a generic identifier and the CAS Registry Number for the substance, is listed for each reaction participant.

For multistep reactions, each single-step reaction summary is displayed. Single-step reactions may include two or more stages (see below). Reaction notes and conditions are also included when available.

Reaction Steps

A reaction step in CASREACT shows a single conversion of reactant to product. This conversion is generally bounded by either a yield or single experimental procedure.

Stages and Substages

Single-step reactions may contain multiple stages, where a stage of the reaction reflects a new experimental change, e.g., addition of a new reactant, reagent, catalyst, or quenching solvent.

Stages are not created for changes in conditions. For example, heating and then cooling with no change in reaction participants are not considered to be separate stages.

A substage is defined as any change in the time, temperature, pressure, and/or pH within a specific stage. For example, heating and then cooling without a change in the reaction participants are considered to be separate substages. Thus, several substages can occur within a single stage.

Reagents, Catalysts, and Solvents

Reagents, catalysts, and solvents, i.e., the reaction participants that do not have structures in the reaction diagram, have a CA Index Name, common name, or line formula to help you identify these substances.

Notes (NTE) Field

The notes (NTE) field is used to describe types of reactions, safety information, and other reaction information not shown in the diagram and summary. NTE displays as part of the reaction summary, and the information is searchable. Some examples of the types of notes are:

```
NTE  stereoselective, high pressure, 78% conversion, 21% ee,
     [bmim]BF4 as co-solvent gave lower conversion but higher
     stereoselectivity

NTE  Diels-Alder reaction, high pressure

NTE  failed reaction

NTE  safety - perchlorates are potentially explosive
```

Reaction Conditions

Reaction conditions are shown in the CON field, which is displayed as part of the reaction summary information. The CON field is not searchable. Some examples are:

```
CON  3 days, room temperature

CON  60 hours, 50 deg C

CON  SUBSTAGE(1) 39 hours, 90 deg C
     SUBSTAGE(2) 90 deg C -> room temperature
```

Bibliographic Information

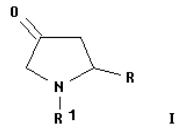
In addition to the reaction information, each record contains bibliographic information for the document that reports the reactions. This information includes the Accession Number (AN) of the record, title (TI), author (AU), source (SO), type of document (DT), and language (LA) of the publication.

```
AN   143:326630  CASREACT
TI   Preparation of N-protected 4-ketoproline derivates via
     ruthenium-catalyzed oxidn. of hydroxyproline
IN   Rossen, Kai; Hoffmann, Rolf; Sarich, Martin
PA   Degussa Ag, Germany
SO   Ger. Offen., 7 pp.
     CODEN: GWXXBX
DT   Patent
LA   German
IC   ICM  C07D207-24
CC   34-2 (Amino Acids, Peptides, and Proteins)
     Section cross-reference(s): 27
FAN.CNT 1
     PATENT NO.       KIND DATE         APPLICATION NO.      DATE
     ---------------  ---- --------     ---------------      --------
PI   DE 102004010943  A1   20050929     DE 2004-102004010943 20040303
     WO 2005095340    A1   20051013     WO 2005-EP1750       20050219
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
            SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM,
            ZW
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
            IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR
PRAI DE 2004-102004010943  20040303
```

Abstract

The abstract (/AB) is included in the CASREACT record. When present, graphic images display in the GI field.

```
GI
```



I

```
AB   The present invention concerns a procedure for the prodn.
     of compds. (I; R = acid, ester, or amide function; R1 =
     carbonyl-contg. N-protecting group) via ruthenium-
     catalyzed oxidn. of the corresponding 4-hydroxyproline.
     These compds. can be used as starting materials for
     further prodn. of bioactive active substances.  Thus, L-
     hydroxyproline was first N-protected using Boc2O,
     followed by oxidn. using RuO2.H2O and NaIO4 in a single-
     phase aq. system to give, after work-up, L-I [R = CO2H;
     R1 = (H3C)3COC(O)].
```

Indexing Information

Indexing information is available with each document record. This information includes Supplementary Terms (/ST), Controlled Terms (/IT) and associated descriptive text, CAS Registry Numbers (/IT, not searchable), and cited references.

```
ST   oxidn hydroxyproline prepn ketoproline ruthenium
     catalysis
IT   Oxidation
        (prepn. of N-protected ketoproline derivates via
        ruthenium-catalyzed oxidn. of hydroxyproline)
IT   Amino acids, preparation
     Heterocyclic compounds
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN
     (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of N-protected ketoproline derivates via
        ruthenium-catalyzed oxidn. of hydroxyproline)
IT   7790-28-5, Sodium periodate   80948-44-3
     RL: CAT (Catalyst use); USES (Uses)
        (prepn. of N-protected ketoproline derivates via
        ruthenium-catalyzed oxidn. of hydroxyproline)
IT   13726-69-7P
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN
     (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of N-protected ketoproline derivates via
         ruthenium-catalyzed oxidn. of hydroxyproline)
```

(continued on next page)

```
IT   84348-37-8P
     RL: IMF (Industrial manufacture); SPN (Synthetic
     preparation); PREP (Preparation)
        (prepn. of N-protected ketoproline derivates via
        ruthenium-catalyzed oxidn. of hydroxyproline)
IT   51-35-4, L-Hydroxyproline
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of N-protected ketoproline derivates via
        ruthenium-catalyzed  oxidn. of hydroxyproline)
RE.CNT  3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
        RECORD
RE
(1) Anon; DD 283626 A5 CAPLUS
(2) Anon; J Org Chem 2001, V66(10), P3593
(3) Anon; Synthesis 1986, 1, P81
```

CAS Registry Numbers

Many of the CAS Registry Numbers indexed for the reaction participants will not also be found in the IT field. The opposite is also true; not all CAS Registry Numbers found in the IT field will be indexed (and searchable) as reaction participants.

Search Options

CASREACT offers an array of search options. You can choose the one that best fits your reaction question.

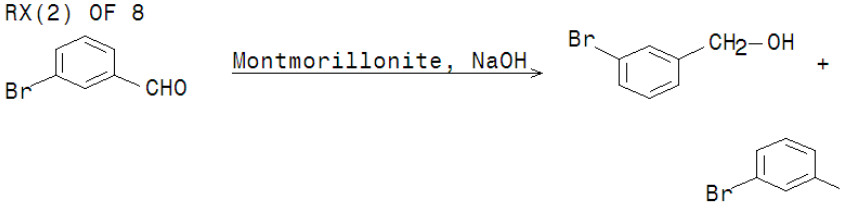
- Structure searching for reactants, reagents, and/or products using reaction roles, reaction sites, and atom-atom mapping between reactants and products (usually the best approach)
- Searching using CAS Registry Numbers or a REGISTRY L-number answer set to find reactants, reagents, products, solvents, and/or catalysts
- Functional group searching for more generic reactions
- Using text terms to refine a previous reaction search
- Text searching in the Basic Index or other text and numeric fields

---

Default Display Format

Substances that are reactants and products display as structures in the compact default display. Reagents, solvents, and catalysts display over the reaction arrow. The reference, notes, and conditions display below the reaction.

```
=> D

L1   ANSWER 1 OF 13  CASREACT  COPYRIGHT 2006 ACS on STN
RX(2) OF 8
```




```
REF:  Prace Naukowe - Wyzsza Szkola Pedagogiczna Czestochowa, Chemia i
      Ochrona Srodowiska, 7,, 59-62;  2003
NOTE: microwave irradiation, no solvent, solid state, Cannizzaro
      reaction, 4 drops of water added, overall yield 60%
CON:  15 seconds
```

Further HELP

For further assistance, contact your STN Service Center. Enter HELP STN at an arrow prompt for contact information.

Chapter 2: Structure Searching in CASREACT

Structure Searching

A reaction query may consist of the structure(s) for one or more reactants, reagents, and/or products. Usually, the query includes one or more reactant structures and one or more product structures in a single L-number.

Within one structure query, you can build a total of four structures. You can also:

- Specify the role of each reaction participant
- Designate the bonds that are reaction sites
- Map atoms in a reactant to atoms in a product

This *Guide* covers the use of structure queries in conjunction with the other searchable information in the database and use of the nonstructural information to create subsets of the database for the structure searches.

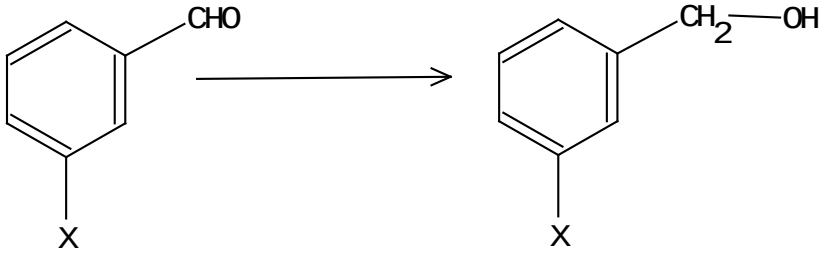
Structure queries may be built with:

- STN Express® software
- STN® on the Web℠ structure plug-in
- Online STRUCTURE command

This *Guide* does not cover the building of structure queries. Information can be found in Chapter 7 of the *STN Express User Guide,* available at www.cas.org or from CAS Customer Center.

Search Example

Find reactions that convert *m*-halobenzaldehydes into *m*-halobenzyl alcohols.



Reactant/Reagent Product

Upload the reaction query and run a SAMPLE SEARCH. After verifying the query and the results, run a FULL FILE search.

```
=> S L1 FULL
FULL SEARCH INITIATED 15:18:56
SCREENING COMPLETE - 62382 REACTIONS TO VERIFY FROM   7193 DOCUMENTS

100.0% DONE   62382 VERIFIED   176 HIT RXNS   92 DOCS
SEARCH TIME: 00.00.06

L3           92 SEA SSS FUL L1 (   176 REACTIONS)
```

Structure Search Precision

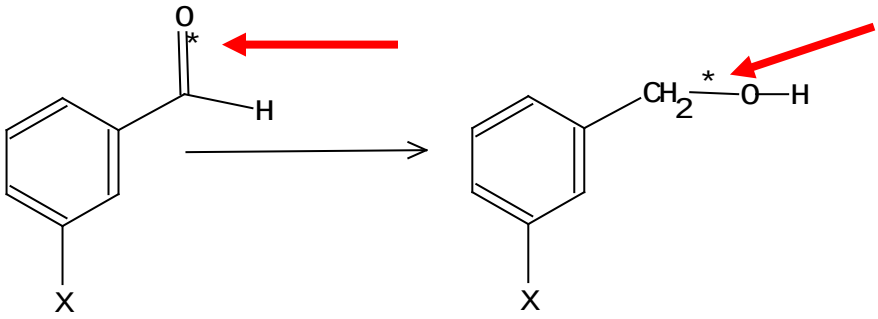
Structure queries are the most precise type of reaction search. You can retrieve good results with just the structure(s). For added precision, you can mark reaction sites and map atoms from a reactant to a product.

It is not necessary to mark every reaction site or map every atom from the reactant to the product. A good guideline is to indicate one or two reaction sites and map one or two atoms.

Precision Example

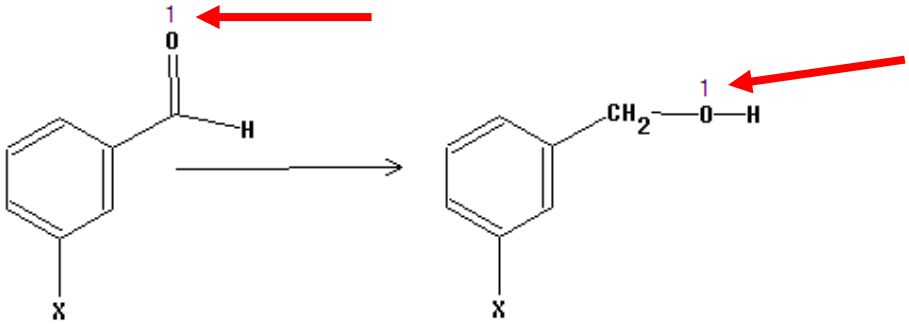
More precision may be obtained by specifying reaction sites and/or atom mapping. For this example, adding reaction sites results in 88 answers instead of 92.

Reaction Sites (marked with asterisks)



Reactant/Reagent Product

Atom Mapping (indicated with numbers next to the mapped atom)



Reactant/Reagent Product

Note: Reaction sites or atom mapping may not be used with structure shortcuts.

CASREACT Screen Number 2082

A structure search in REGISTRY may be limited to only substances that are found in CASREACT by using screen 2082. To do so, search the screen L-number with your structure query L-number in REGISTRY (e.g., L1).

```
=> FIL REGISTRY
=> SCREEN 2082
L2    SCREEN CREATED

=> S L1 AND L2 FUL
L3       28 SEA SSS FUL L1 AND L2
```

The answer set is then ready for crossover to CASREACT to be searched in the desired reaction role.

Chapter 3: Searching Reactions with CAS Registry Numbers

Introduction

The CAS Registry Number of each reaction participant may be used a search term. You may enter the CAS Registry Number directly or search the L-number of REGISTRY answer set. The CAS Registry Numbers contained in that answer set are searched.

CAS Registry Numbers in the IT Field

The reaction participant CAS Registry Numbers listed in the reaction summaries are the only CAS Registry Numbers that are searchable in CASREACT. Those found in the IT field of the indexing are not searchable.

To verify that a CAS Registry Number is indexed in CASREACT, use the EXPAND command.

```
=> E 26159-35-3 5
E1           1     26159-23-9/BI
E2           2     26159-34-2/BI
E3          20 --> 26159-35-3/BI
E4           6     26159-36-4/BI
E5           4     26159-40-0/BI
```

CAS Registry Numbers and Reaction Roles

You may either search the CAS Registry Numbers in the Basic Index by entering them directly or by using a REGISTRY L-number answer set as a search term.[2]

For more precise results, you may search with a reaction search field appended. These search fields are:

/RCT - reactant
/RGT - reagent
/PRO - product
/SOL - solvent
/CAT - catalyst

There are two search fields that allow you to search for the substance in more than one role:

/RRT - reactant or reagent
/NPRO - nonproduct, i.e., reactant, reagent, solvent, or catalyst

Combinations of roles are allowed, e.g., /RRT,PRO, if the CAS Registry Numbers are searched directly, but may not be used with REGISTRY L-number answer sets.

Reaction Role Search Examples

The table illustrates examples of the various role searches:

If you want to find a substance as a:	Then:
Reactant	=> **S 50-00-0/RCT**
Reagent	=> **S 50-00-0/RGT**
Reactant or Reagent	=> **S 50-00-0/RRT**
Solvent	=> **S 50-00-0/SOL**
Catalyst	=> **S 50-00-0/CAT**
Anything but a product	=> **S 50-00-0/NPRO**
Product	=> **S 50-00-0/PRO**
Solvent or Catalyst	=> **S 50-00-0/SOL,CAT**

[2]The search uses the CAS Registry Numbers from the REGISTRY L-number answer set as the actual search terms.

REGISTRY L-Number Search Example

Find all reactions that use a non-ferrous metallocene catalyst.

Upload the metallocene structure query and find all metallocenes in REGISTRY.

```
=> FIL REGISTRY
L1      STRUCTURE UPLOADED

=> S L1 FUL
L2       115273 SEA SSS FUL L1
```

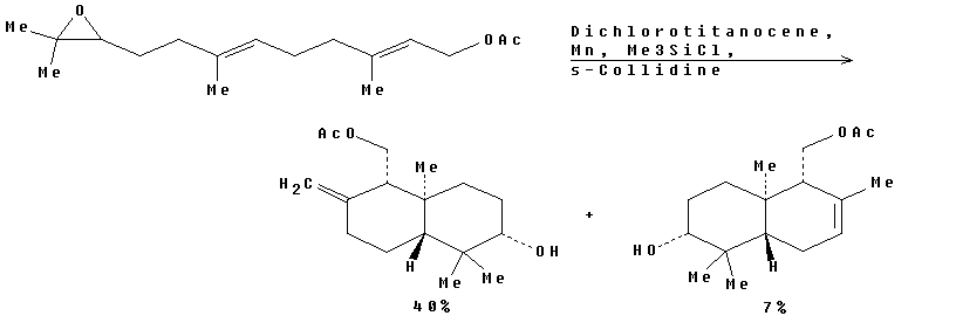
Limit the results to those in CASREACT and remove the ferrocenes.

```
=> S L2 AND CASREACT/LC
L3       34150 L2 AND CASREACT/LC

=> S L3 NOT FE>0
L4       15691 L3 NOT FE>0
```

Cross the result (L4) into CASREACT[3] and find the non-ferrous metallocene catalyzed reactions.

```
=> FIL CASREACT;S L4/CAT
L5        1064 L4/CAT

=> D SCAN
L5   1064 ANSWERS   CASREACT  COPYRIGHT 2006 ACS on STN

TI   Total synthesis of 3-hydroxydrimanes mediated by
     titanocene(III) -  evaluation of their antifeedant
     activity
```

RX(1) OF 68



NOTE: key step, regioselective, stereoselective, major product is key intermediate

The catalyst is indicated over the reaction arrow.

[3]There is a limit of 300,000 CAS Registry Numbers allowed in the REGISTRY L-number that is searched in CASREACT. For details, see HELP RNCROSSOVER at an arrow prompt in CASREACT.

CAS Registry Numbers vs. Structure

If you are searching for a specific reactant, reagent, and/or product, it is less costly to use the CAS Registry Numbers (when known) in the role search fields instead of a structure query. The search fields may be linked with (L) proximity to require that the various participants must occur in the same reaction.

(L) Proximity Example

Find the conversion of *m*-bromobenzaldehyde (3132-99-8) to *m*-bromobenzyl alcohol (15852-73-0). Here, /RRT is used to allow for the possibility that the substance is either a reactant or reagent.

```
=> S 3132-99-8/RRT (L) 15852-73-0/PRO
           550 3132-99-8/RRT
            20 15852-73-0/PRO
L1          13 3132-99-8/RRT (L) 15852-73-0/PRO
```

Other proximity operators cannot be used to link reaction participants.

Combining Results Example

You may also combine the results of a structure search with a CAS Registry Number search using (L) proximity.

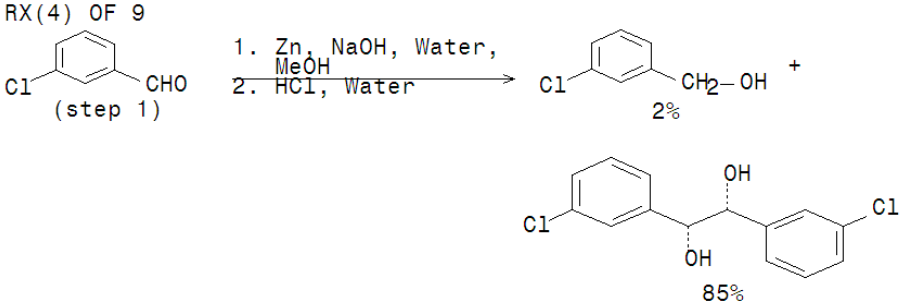
In the structure search results for the conversion of benzaldehydes, find reactions that have sodium-containing reactants or reagents:

1. Search REGISTRY for all substances that contain one or more sodiums and are also in CASREACT.
2. Then search CASREACT to see if any of these participate in the conversion reactions already found.

```
L1      STRUCTURE UPLOADED

=> S L1 FULL
L2           92 SEA SSS FUL L1 (   176 REACTIONS)

=> FIL REG
=> S NA>0 AND CASREACT/LC
         298516 NA>0
        4018188 CASREACT/LC
L3        19732 NA>0 AND CASREACT/LC

=> FIL CASREACT
=> S L2 (L) L3/RRT
         162897 L3/RRT
L4           44 L2 (L) L3/RRT
```

(continued on next page)

```
=> D

L4   ANSWER 1 OF 44  CASREACT  COPYRIGHT 2006 ACS on STN
RX(4) OF 9
```




```
REF:  Hecheng Huaxue, 12(5), 429-431;  2004
NOTE: stereoselective (55:45 dL:meso), chemoselective, ultrasound 1st
      stage
CON:  STAGE(1) 30 minutes, room temperature
```

Nonproduct Role

If you are looking for reaction information for a single substance or a group of substances where the role may be anything but a product, use the /NPRO search field.

Answers retrieved have the specified reaction participants as reactants, reagents, solvents, or catalysts. Reactions that contain the substances as products are not retrieved.

Nonproduct Example

Find the various uses of *tert*-butyl alcohol (75-65-0).

```
=> S 75-65-0/NPRO
L1       11040 75-65-0/NPRO
```

The NPRO role cannot be assigned to a structure query. To search in this multiple-use field, you must use CAS Registry Numbers or an L-number answer set from REGISTRY.

Chapter 4: Searching for Solvents and Catalysts

Introduction

Searches for solvents and catalysts can only be done with CAS Registry Numbers or L-number answer sets from REGISTRY.

Solvents

CASREACT gives you access to solvent information not found in other databases. Solvents are usually known compounds and are not usually the novel information in the document. Therefore, they are often not indexed in the nonreaction databases. However, solvents are often a critical part of the reaction information and are indexed in CASREACT whenever they are shown in the original document.

You can find information on the solvents in reactions by searching in the /SOL search field. Use CAS Registry Numbers or REGISTRY L-numbers as the search terms in the field.

Solvent Display

The solvents are displayed in the reaction summary. The CAS Registry Number and a name or line formula are shown. In the default display, they appear over the reaction arrow.

Searching for Solvents: Examples

Solvents may be combined with other reaction participants in the other role indexes or with reaction search results by using the (L) operator.

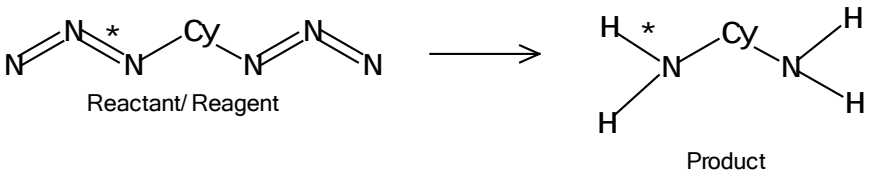
```
=> S 71-43-2/SOL (L) 1333-74-0/RRT
         52024 71-43-2/SOL
         41928 1333-74-0/RRT
L1        5635 71-43-2/SOL (L) 1333-74-0/RRT
```

Substances may be combined with OR logic in the /SOL field as well.

```
=> S (71-43-2 OR 108-88-3)/SOL
         52024 71-43-2/SOL
         60607 108-88-3/SOL
L2      102645 (71-43-2 OR 108-88-3)/SOL
```

Combining Solvents and Reaction Structure Results

Search terms in the /SOL field may be combined with the results of a structure search with the (L) operator. Because the solvent may not be included in the structure query, this is the strategy to use when the solvent is one participant in the search requirements.




```
L1      STRUCTURE UPLOADED

=> S L1 FULL
L2           90 SEA SSS FUL L1 (  1508 REACTIONS)

=> S L2 (L) 67-56-1/SOL
         98201 67-56-1/SOL
L3          56 L2 (L) 67-56-1/SOL
```

(NOTL) Proximity

If you are looking for one substance in the /SOL and not another, use the (NOTL) operator to remain within the same reaction.

```
=> S (71-43-2 (NOTL) 108-88-3)/SOL
         52024 71-43-2/SOL
         60607 108-88-3/SOL
L3       51566 (71-43-2 (NOTL) 108-88-3)/SOL
```

Catalysts

Finding information on catalysts is often a critical part of a reaction search. Whenever a catalyst is given in the original document, it is indexed in CASREACT.

You can search for catalysts in the /CAT search field by using either CAS Registry Numbers or REGISTRY L-numbers as the search terms.

Catalyst Display

The catalysts are displayed over the reaction arrow in the default display or in the reaction summary with a CAS Registry Number and a name or line formula.

ANY/CAT Search Term

ANY/CAT is a special catalyst search term. The term by itself finds all catalyzed reactions. The term combined with other reaction search results using (L) proximity retrieves only records with the desired catalyzed reactions.

```
=> S 486-25-9/RRT (L) ANY/CAT
           438 486-25-9/RRT
        188126 ANY/CAT
L3         116 486-25-9/RRT (L) ANY/CAT
```

Searching for Catalysts: Examples

Catalysts may be combined with other reaction participants in the other role indexes using the (L) operator.

```
=> S 20816-12-0/CAT (L) 75-65-0/SOL
L2         650 20816-12-0/CAT (L) 75-65-0/SOL
```

When searching for reactions containing two or more substances in the /CAT field, combine the terms with (L) proximity.

```
=> S (104-15-4 (L) 14221-01-3)/CAT
L3         203 (104-15-4 (L) 14221-01-3)/CAT
```

Substances may be combined with OR logic in the /CAT field as well.

```
=> S (104-15-4 OR 14221-01-3)/CAT
L4       16162 (104-15-4 OR 14221-01-3)/CAT
```

If you are looking for one substance in the /CAT field and not another, use the (NOTL) operator.

```
=> S (104-15-4 (NOTL) 14221-01-3)/CAT
L5        8472 (104-15-4 (NOTL) 14221-01-3)/CAT
```

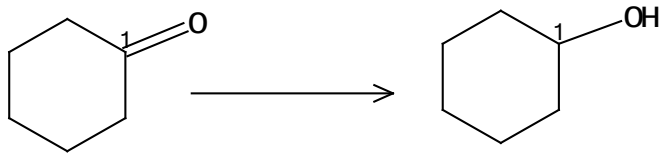
Search terms in the /CAT field may be combined with the results of a structure search with the (L) operator.

```
=> S L1 FULL
L2   30175 SEA SSS FUL L1 (374882 REACTIONS)

=> S L2 (L) 99646-28-3/CAT
            40 99646-28-3/CAT
L18         10 L16 (L) 99646-28-3/CAT
```

Using REGISTRY L-Numbers

Find all reactions that involve nickel-containing catalysts. Begin in REGISTRY to retrieve all CASREACT substances that contain nickel.

```
=> FIL REG
=> S NI>=1 AND CASREACT/LC
        491951 NI>=1
       4018188 CASREACT/LC
L1       14993 NI>=1 AND CASREACT/LC

=> FIL CASREACT
=> S L1/CAT
L2        8750 L1/CAT
```



Reactant/Reagent Product

```
L3      STRUCTURE UPLOADED

=> S L3 SUB=L2 FUL
FULL  SEARCH INITIATED 15:14:36
SCREENING COMPLETE - 41030 REACTIONS TO VERIFY FROM  2891 DOCUMENTS

L4          133 SEA SUB=L2 SSS FUL L3 (   560 REACTIONS)
```

For more details, refer to the section on subset searching.

Catalysts without CAS Registry Numbers

Some catalysts do not have CAS Registry Numbers and are not searchable in the /CAT field. They are, however, mentioned in the NTE field. To look for this type of catalyst, search the Basic Index or the NTE field.

```
RX(10)    RCT  F 870119-73-6
          RGT  C 7803-57-8 N2H4-H2O
          PRO  V 870119-80-5
          CAT  7440-02-0 Ni
          SOL  67-56-1 MeOH, 109-99-9 THF
          CON  1 hour, reflux
          NTE  Raney Ni used as catalyst
```

Chapter 5: Reaction Steps, Yields, and Range Search

Number of Steps

CASREACT contains both single-step and multistep reactions, and as mentioned in Chapter 1, reaction steps may contain stages and substages. When you search within the reaction information, you retrieve all types of reactions. For example, if you search for a reactant linked to a product, you retrieve both single-step and multistep reactions.

The Number of Steps (/NS) search field gives you the ability to limit the search results to:

- Single-step reactions
- Multistep reactions
- Multistep reactions with a specific number (or range) of steps

The /NS field may be searched with any of the numeric operators (i.e., <, <=, >, >=, =, -).

The /NS field is usually combined with terms in other reaction information fields or with a REGISTRY L-number, using the (L) operator.

Number of Steps: Examples

Search for methanol as a solvent and palladium as a catalyst.

```
=> S 67-56-1/SOL (L) 7440-05-3/CAT
          98499 67-56-1/SOL
          29259 7440-05-3/CAT
L1        16490 67-56-1/SOL (L) 7440-05-3/CAT
```

To limit the search to single-step reactions:

```
=> S L1 (L) 1/NS
         541538 1/NS
L2        11132 L1 (L) 1/NS
```

To limit the search to multistep reactions:

```
=> S L1 (L) NS>=2
         254191 NS>=2
L3        15494 L1 (L) NS>=2
```

To search for records including 3-5 step reactions:

```
=> S L1 (L) 3-5/NS
         147705 3-5/NS
L4        13662 L1 (L) 3-5/NS
```

Yield Information

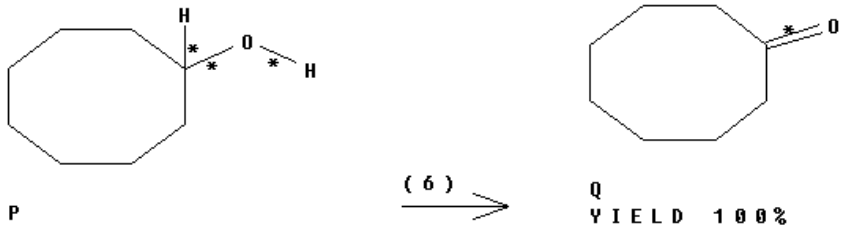
Specific yield information for products has been indexed in CASREACT from October 1986 to the present. The yields are searchable in the Yield (/YD) field, which may be searched with numeric operators.

The /YD field contains whole numbers from 1 to 100 that represent the yields given in the original document.

Yields are usually combined with the product by using the (A) operator.

The yield displays in the reaction diagram below the structure of the product it describes. It is not highlighted.

```
=> S 502-49-8/PRO (A) YD>=90
           225 502-49-8/PRO
        198659 YD>=90
L1          39 502-49-8/PRO (A) YD>=90

=> D HIT

L1   ANSWER 1 OF 39  CASREACT  COPYRIGHT 2006 ACS on STN

RX(6) OF 17     P  ===>  Q
```




```
 P                                   Q
                                     YIELD 100%
RX(6)     RCT  P 696-71-9

            STAGE(1)
               CAT  32503-27-8 Bu4N.HSO4, 13472-45-2 Na2WO4
               SOL  75-65-0 t-BuOH
               CON  room temperature -> 90 deg C

            STAGE(2)
               RGT  C 7722-84-1 H2O2
               SOL  7732-18-5 Water
               CON  SUBSTAGE(1) 90 deg C
                    SUBSTAGE(2) 30 minutes, 90 deg C

          PRO  Q 502-49-8
          NTE  green chemistry-reagent
```

Yield Proximity Operators

The use of the (A) operator ensures that yield information refers to a specific product (as above).

If the (L) operator were used, retrievals would include all of those found with (A) as well as those that have the yield and the product in the same reaction but with the yield associated with a different product.

For example, if (L) were used in the previous example, the search would retrieve two additional answers in which the yield refers to a different product.

Products without Yields

There are many products in the database that do not have a yield value, either because the author did not specify a value or because the paper was added to the database prior to October 1986.

For these products, a yield of NONE is posted to the Yield Data (/YDT) search field.

To do a comprehensive search on yield information, it is best to include NONE/YDT in the search query. There is no display of NONE in the record. The products do not have any yield displayed with them in the reaction diagram.

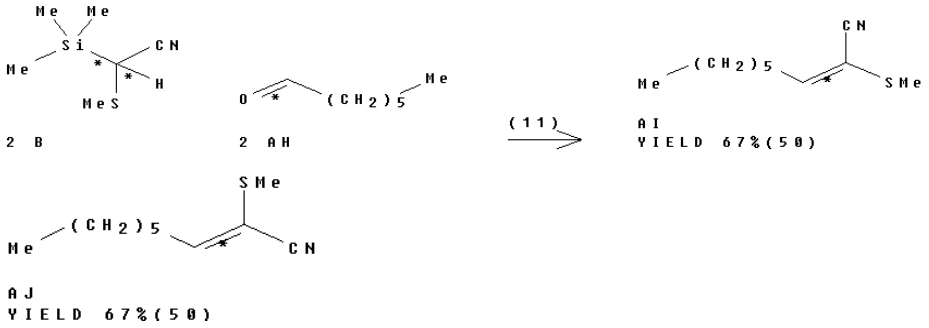
```
=> S 502-49-8/PRO (A) (YD>=90 OR NONE/YDT)
           225 502-49-8/PRO
        198659 YD>=90
        279657 NONE/YDT
L3         114 502-49-8/PRO (A) (YD>=90 OR NONE/YDT)
```

Yields for Multiple Products

If more than one product is formed in a reaction, the yield information may be cited in several ways. A specific yield may be given for each product. These yields are searched as explained previously, with the product combined with the required yield by using (A) proximity.

In some instances, the original document shows the yield distributed among multiple products and the ratio of distribution is given. For example, there might be two products formed with a yield of 67% in a ratio of 48:52. For these, the overall yield is posted with each product and the ratio is ignored. The ratio displays after the yield value in parentheses in the reaction diagram. It is not searchable, only displayable.

```
RX(11) OF 31    ...2 B  +  2 AH  ===>  AI  +  AJ
```




```
RX(11)    RCT  B 121221-45-2

            STAGE(1)
               RGT  I 4111-54-0 LiN(Pr-i)2
               SOL  109-99-9 THF

            STAGE(2)
               RCT  AH 111-71-7
               SOL  109-99-9 THF

           PRO  AI 121221-57-6, AJ 121221-58-7
```

The reaction summary of the answer lists THF as the solvent in each stage in the SOL field. This is an indication of a “pot” reaction. The reaction takes place in stages, but the stages are not represented as individual steps because no intermediate products are produced in the various stages.

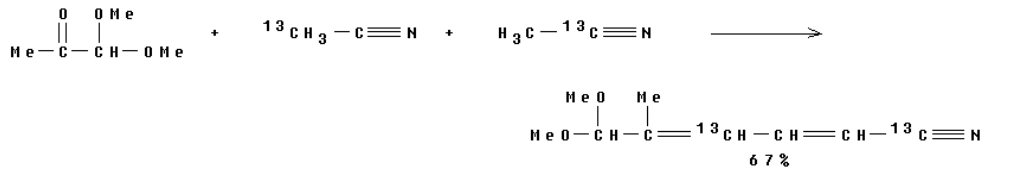
AH was introduced in the second stage of the reaction. However, because no intermediate product is isolated or identified, the only indication in CASREACT of the stages is in the reaction summary. Pot reactions are considered to be single-step reactions in CASREACT. Refer to the section on the /NS field for more information on limiting a search to single-step reactions.

Yield in the NTE Field

The original document may give an overall yield for the reaction and not give the ratio of distribution between products. The yield cannot be associated with any of the products. The yield information is then placed in the NTE field, and NONE/YDT is indexed with each product.

To find this information, the product must be combined with the word YIELD by using (L) proximity.

```
=> S L3 (L) YIELD
         116291 YIELD
          69283 YIELDS
         165533 YIELD
                  (YIELD OR YIELDS)
L6            1 L3 (L) YIELD

=> D

L6   ANSWER 1 OF 1  CASREACT  COPYRIGHT 2006 ACS on STN
RX(122) OF 386 - 3 STEPS
```



```
REF:  Recueil des Travaux Chimiques des Pays-Bas, 113(12), 552-62;
      1994
NOTE: 2) silica gel used in second stage, 86% overall yield, 3)
      stereoselective
```

RCR Range Searches

Reaction searches may be limited to the most recent two volumes of *Chemical Abstracts* by using the Recent Chemical Reactions (RCR) range setting.

```
=> S L2 RANGE=RCR
           6161 HETEROCYCLES/FG.RCT
L3           26 L1 AND HETEROCYCLES/FG.RCT

=> D 1 26 CBIB

L3   ANSWER 1 OF 26  CASREACT  COPYRIGHT 2006 ACS on STN
143:78317  Development of Aliphatic Alcohols as Nucleophiles
for Palladium-Catalyzed DYKAT Reactions: Total Synthesis of
(+)-Hippospongic Acid A.  Trost, Barry M.; Machacek, Michelle
R.; Tsui, Hong C. (Department of Chemistry, Stanford
University, Stanford, CA, 94305, USA).  Journal of the
American Chemical Society, 127(19), 7014-7024 (English) 2005.
CODEN: JACSAT.  ISSN: 0002-7863.  Publisher: American Chemical
Society.
```

(continued on next page)

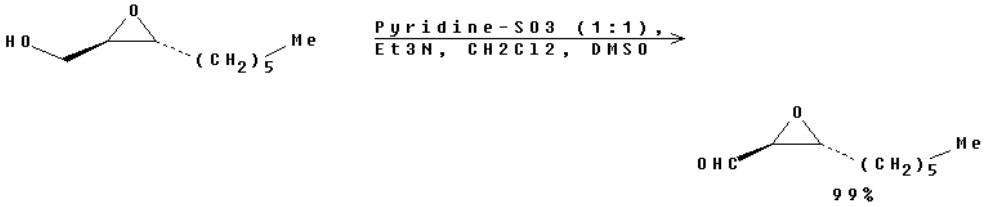
L3 ANSWER 26 OF 26 CASREACT COPYRIGHT 2006 ACS on STN
142:38036 A Straightforward Synthesis of (-)-Phaseolinic Acid. Amador, Marta; Ariza, Xavier; Garcia, Jordi; Ortiz, Jordi (Departament de Quimica Organica, Universitat de Barcelona, Barcelona, E-08028, Spain). Journal of Organic Chemistry, 69(23), 8172-8175 (English) 2004. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

=> **D SCAN**

L3 26 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI An efficient stereoselective synthesis of substituted 1,3-dienes

RX(4) OF 248



NOTE: Parikh-Doering oxidn.

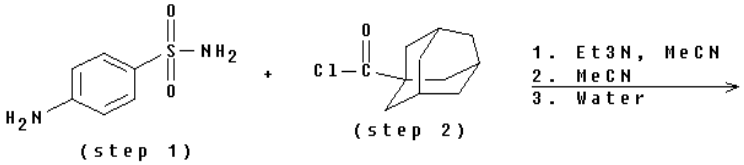
Chapter 6: Looking at Answers in CASREACT

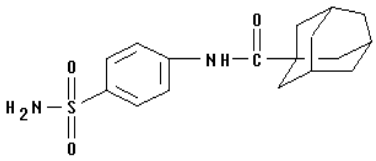
Default Display Format

The information contained in a single record in CASREACT is extensive. For example, a record may have hundreds or even thousands of reactions, each having a map, diagram, and summary. Many display formats are available for looking at all or part of a record.

The default display format is usually the most helpful. It displays the compressed reaction information and the reference for the document (FHIT CRD).

RX(1) OF 29





90%

REF: Bioorganic & Medicinal Chemistry, 12(10), 2717-2726; 2004
CON: STAGE(1) room temperature -> 5 deg C
STAGE(2) .25 hours, 0 deg C; 3 hours, room temperature
STAGE(3) room temperature

A complete list of the display fields and formats is given in the Database Summary Sheet, available at www.cas.org or from CAS Customer Center.

Display information is also available by entering HELP DFIELD or HELP FORMAT at an arrow prompt in CASREACT.

You may define your own display format and make it the default format with the SET command. For information, enter HELP SET FORMAT and HELP SET DFORMAT at an arrow prompt in CASREACT.

DISPLAY BROWSE

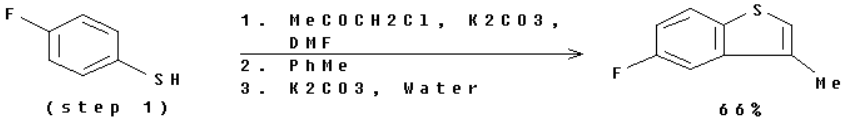
Using DISPLAY BROWSE is an effective way of looking at answers. You may look at the information in one format and then move on to another format for the same answer.

DISPLAY SCAN

You may scan (by using D SCAN) through answers in an answer set to see if the search is retrieving the kinds of reactions you expected. Random answers, without the answer numbers, are displayed, showing the first hit reaction, title (TI) of the document, and notes (NTE). There is no display fee for scanned answers.

```
L3   17 ANSWERS   CASREACT  COPYRIGHT 2006 ACS on STN

TI   C17,20-Lyase inhibitors I.  Structure-based de novo
design
     and SAR study of C17,20-lyase inhibitors
```

RX(45) OF 351



NOTE: polyphosphoric acid used second stage

Hit-Term Highlighting

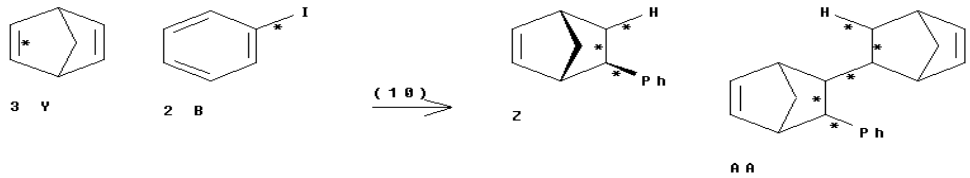
Looking at search results in online displays is made easier by hit-term highlighting. This feature is available in all fields in CASREACT except for compressed reaction displays. The terms that are highlighted in reactions are the hit CAS Registry Numbers in the reaction summary and the generic identifiers in the reaction map that correspond to the CAS Registry Numbers.

Reaction Coefficients

In many reactions, the same participant is used multiple times. This is indicated in the reaction map with coefficients.

```
RX(10) OF 18    3 Y  +  2 B  ===>  Z  + AA
```

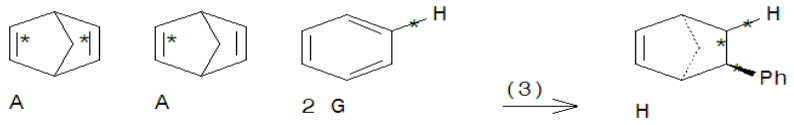
If the reaction sites are alike or no reaction sites are indicated, then coefficients are also used in the reaction diagram.



Coefficients are not indicated in the reaction summary.

```
RX(10)     RCT  Y 121-46-0, B 591-50-4
           RGT  D 1112-67-0 Bu4NCl, O 590-29-4 HCO2K
           PRO  Z 26280-24-0, AA 125382-65-2
           CAT  3375-31-3 Pd(OAc)2
           SOL  68-12-2 DMF
           NTE  20% overall
```

When the same participant occurs with different reaction sites, then it is displayed multiple times.



Multistep Indicator

When a reaction is the first step of a multistep reaction, the map contains dots after the product, indicating that the reaction continues beyond that step. If the displayed reaction is a middle step, dots precede the first identifier and follow the last participant in the map, e.g., RX(2) shown here.

```
RX(2) of 12 ...A + B ===> G + H...
```

When a reaction is the last step of a multistep reaction, dots precede the first participant in the map. RX(1) is an example of the final step in a multistep reaction.

```
RX(1) OF 12 ...A  +  B  ===> C + D
```

It is not possible to predict reaction numbers. The previous example is the final step but received reaction number one (i.e., RX(1)) in the document.

Documents with multistep reactions are retrieved when substances in separate steps are searched with the (L) operator. In the following example, the two substances are in separate steps (RX(1) and RX(2)) of the multistep reaction:

```
RX(29) OF 30 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(7),
                         RX(8)
RX(29)    A  +  B  +  H  +  R  +  AC  +  AG  ===>  AH
• • •
RX(1)     RCT  A 104-88-1, B 107-05-1

            STAGE(1)
               RGT  D 7439-95-4 Mg
               SOL  109-99-9 THF
               CON  SUBSTAGE(1) 1 hour, reflux
                    SUBSTAGE(2) 2 hours, reflux
• • •
RX(2)     RCT  C 14506-33-3, H 106-93-4
          RGT  J 7440-66-6 Zn, K 7758-89-6 CuCl
          PRO  I 123989-30-0
          SOL  71-43-2 Benzene
          CON  20 hours, reflux
• • •
```

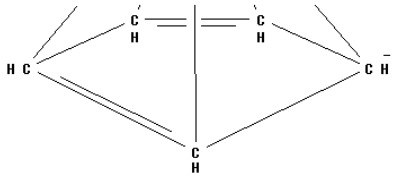
Documents with one substance in one reaction and the second substance in a different reaction not in the same multistep sequence are not retrieved when the (L) operator is used.

Structures Not Displayed

Some participants have structures that are not displayable. This is indicated by a message in the reaction diagram.

```
RX(2) OF 38      2 A  +  4 D  ===>  E
```

```
                                                              PAGE 2-A
```



```
2  A

                                  (2)
2  D      2  D
```

```
RX(2)      RCT  A 51812-05-6, D 630-08-0
           RGT  F 21324-39-0 NaPF6
           PRO  E 12154-95-9
           SOL  109-99-9 THF
```

The names of participants A, D, and E can be obtained by searching their CAS Registry Numbers in REGISTRY.

Chapter 7: Searching Functional Groups

Introduction

Functional group searching offers another approach to reaction searching. While broad types of reaction searches can be represented by the use of structures, often they do not sufficiently represent the desired reaction or substance class or the search will not complete within system limits.

Functional Groups

CASREACT has defined a set of functional groups, including several class terms that may be searched without having difficulties with system limits. These functional groups are derived from the structures of the reactants, reagents, and products in the database.

Functional Group Search Fields

The available search fields are:

Search Field	Description
/FG	Functional group in the reactant, reagent, or product
/FG.FORM	Functional group formed
/FG.NON	Nonreacting, but present, functional group
/FG.RCT	Functional group in the reactant
/FG.RGT	Functional group in the reagent
/FG.RXN	Reacting functional group
/FG.PRO	Functional group in the product
/FG.YD	Functional group yield
/FG.YDT	Functional group yield data

FG.RCT vs. FG.RXN

FG.RCT requires the functional group to be present in the reactant, but it may not be reacting in the hit reaction.

FG.RXN requires that the functional group be present in the reactant, and it also must be reacting in the hit reaction. It is a subset of FG.RCT.

FG.PRO vs. FG.FORM

FG.PRO requires that the functional group be present in the product, but it may not be formed in the hit reaction.

FG.FORM requires that the functional group be present in the product, and it also must be formed in the hit reaction. It is a subset of FG.PRO.

Functional Group HELP

You can see the list of functional groups online by entering HELP FGA at an arrow prompt in CASREACT.

List of Functional Groups

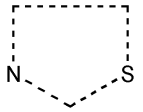
ACETAL
ACETYL
ACID HALIDE
ACYCLIC ALKENE
ACYCLIC KETONE
ACYLMETAL
ALCOHOLS
ALDEHYDE
ALKENES
ALKYL HALIDE
ALKYNE
ALKYNES
ALLENE
ALLYL ALCOHOL
ALLYL HALIDE
AMIDE
AMIDINE
AMINE OXIDE
AMINES
ANHYDRIDE
ARYL HALIDE
ARYLSULFONYL
AZIDE ENOL
AZINE
AZIRIDINE
AZO
AZOXY
CARBAMATE
CARBONATE
CARBONATE DERIVATIVES
CARBOXY DERIVATIVES
CARBOXYLATE
CARBOXYLIC
CEPHEM
CHLORAMINE
CYANAMIDE
CYANATE
CYANOHYDRIN
CYCLIC ALCOHOL
CYCLIC ALKENE
CYCLIC KETONE
CYCLOPROPYL
DIAZO
DIAZONIUM
DIENE
DIIMIDE
DISULFIDE
HALOHYDRIN
HEMIACETAL
HETEROCYCLES
HYDRAZIDE
HYDRAZINE
HYDRAZONE
HYDROPEROXIDE
HYDROXYLAMINE
IMIDE
IMINE
IMINO ETHER
ISOCYANATE
ISONITRILE
ISOTHIOCYANATE
KETAL
KETENE
KETENIMINE
KETONES
LACTAM
LACTONE
MESYL
METAL ARENE
METAL CARBENE
METAL CARBONYL
METAL CYCLOPENTADIENYL
METAL HALIDE
METAL HYDRIDE
METAL METAL BOND
METAL NITROGEN
METAL NITROSYL
METAL PHOSPHINE
METAL SULFUR
METALLOCARBOCYCLE
MU-CARBONYL
NITRILE
NITRILE OXIDE
NITRITE
NITRO
NITRONE
NITROSAMINE
NITROSO
NITROXIDE
NULL
O-QUINONE
ORGANOMETAL
ORGANOMETALLICS
ORTHO ESTER
PHOSPHITE
PHOSPHONATE
PHOSPHONIUM
PHOSPHORUS YLIDE
PI-ALKENE
PI-ALKYNE
PI-ALLYL
PRIMARY ALCOHOL
PRIMARY AMINE
PURINE
QUATERNARY AMMONIUM
S-O GROUP
SE GROUP
SECONDARY ALCOHOL
SECONDARY AMINE
SELENIDE
SELENOL
SILYL
SILYL ENOL ETHER
SULFENYL HALIDE
SULFIDE
SULFINATE
SULFINYL HALIDE
SULFONAMIDE
SULFONE
SULFONYL HALIDE
SULFONYLOXY
SULFOXIDE
SULFUR YLIDE
TE GROUP
TERTIARY ALCOHOL
TERTIARY AMINE
THIOACETAL
THIOAMIDE
THIOCARBONYL
THIOCARBOXY
THIOCYANATE
THIOKETAL
THIOL
THIONE
THIOPHENOL
THIOUREA
TRIAZENE
TRIHALIDE
UNSATD ACID
UNSATD ALDEHYDE
UNSATD AMIDE

(continued on next page)

ENAMINE	OXIME	UNSATD ESTER
ENOL	OXONIUM	UNSATD KETONE
ENOL ETHER	P-N GROUP	UNSATD NITRILE
ENYNE	P-O GROUP	UNSATURATED ACID
EPISULFIDE	P-QUINONE	UNSATURATED ALDEHYDE
EPOXIDE	P-S GROUP	UNSATURATED AMIDE
ETHER	PENAM	UNSATURATED ESTER
GEM-DIHALIDE	PEROXIDE	UNSATURATED KETONE
GLYCOL	PEROXY ACID	UNSATURATED NITRILE
GUANIDINE	PEROXY	UREA
HALIDES	PHENOL	VIC-DIHALIDE
HALOFORMATE	PHOSPHATE	VINYL HALIDE

Ring Terms

Ring terms describe 5- and 6-membered monocyclic rings with any type of bonding. For example, the term 1,3-C3NS represents:



The search term will retrieve any isolated or embedded ring system containing the 1,3-C3NS ring.

List of Ring Terms

1,2-C3N2	1,3-C3O2	1,4-C5N2
1,2-C3NO	1,3-C3OS	C2S
1,2-C3NS	1,3-C3S2	C3N
1,2-C3O2	1,3-C4N2	C3O
1,2-C3OS	1,3-C4NO	C3S
1,2-C3S2	1,3-C4NS	C4N
1,2-C4N2	1,3-C4O2	C4O
1,2-C4NO	1,3-C4OS	C4S
1,2-C4NS	1,3-C4S2	C5N
1,2-C4O2	1,4-C4N2	C5O
1,2-C4OS	1,4-C4NO	C5S
1,2-C4S2	1,4-C4NS	C6N
1,3-C3N2	1,4-C4O2	C6O
1,3-C3NO	1,4-C4OS	C6S
1,3-C3NS	1,4-C4S2	

Class Terms

Functional group class terms are a more general search term that allows searching a broader range of functionality. Searching a class term searches all of the specific functional groups in that class.

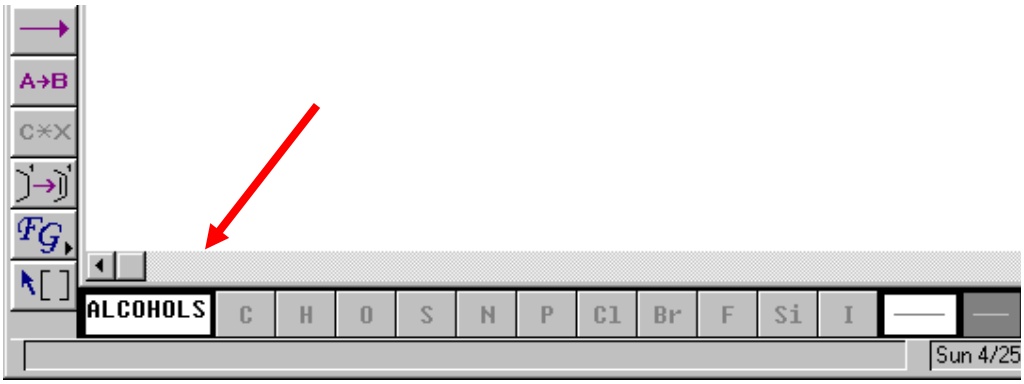
Class Term	Functional Groups Searched
ALCOHOLS	ALLYL ALCOHOL or CYANOHYDRIN or CYCLIC ALCOHOL or ENOL or GLYCOL or HALOHYDRIN or HEMIACETAL or HYDROXYLAMINE or PHENOL or PRIMARY ALCOHOL or SECONDARY ALCOHOL or TERTIARY ALCOHOL
ALKENES	ACYCLIC ALKENE or CYCLIC ALKENE
ALKYNES	ALKYNE or ENYNE or PI-ALKYNE
AMINES	AMINE OXIDE or AZIRIDINE or CHLORAMINE or CYANAMIDE or ENAMINE or HYDROXYLAMINE or IMINE or PRIMARY AMINE or SECONDARY AMINE or TERTIARY AMINE
CARBONATE DERIVATIVES	CARBAMATE or CARBONATE or GUANIDINE or HALOFORMATE or THIOUREA or UREA
CARBOXY DERIVATIVES	ACID HALIDE or AMIDE or AMIDINE or ANHYDRIDE or CARBOXYLATE or CARBOXYLIC or HALOFORMATE or IMIDE or LACTAM or LACTONE or PEROXY ACID or PEROXY ESTER or THIOAMIDE or THIOCARBOXY
HALIDES	ACID HALIDE or ALKYL HALIDE or ALLYL HALIDE or ARYL HALIDE or CHLORAMINE or GEM-DIHALIDE or HALOFORMATE or HALOHYDRIN or METAL HALIDE or SULFENYL HALIDE or SULFINYL HALIDE or SULFONYL HALIDE or TRIHALIDE or VIC-DIHALIDE or VINYL HALIDE
HETEROCYCLES	1,2-C3N2 or 1,2-C3NO or 1,2-C3NS or 1,2-C3O2 or 1,2-C3OS or 1,2-C3S2 or 1,2-C4N2 or 1,2-C4NO or 1,2-C4NS or 1,2-C4O2 or 1,2-C4OS or 1,2-C4S2 or 1,3-C3N2 or 1,3-C3NO or 1,3-C3NS or 1,3-C3O2 or 1,3-C3OS or 1,3-C3S2 or 1,3-C4N2 or 1,3-C4NO or 1,3-C4NS or 1,3-C4O2 or 1,3-C4OS or 1,3-C4S2 or 1,4-C4N2 or 1,4-C4NO or 1,4-C4NS or 1,4-C4O2 or 1,4-C4OS or 1,4-C4S2 or 1,4-C5N2 or C2S or C3N or C3O or C3S or C4N or C4O or C4S or C5N or C5O or C5S or C6N or C6O or C6S or AZIRIDINE or CEPHEM or EPISULFIDE or EPOXIDE or PENAM or PURINE
KETONES	ACYCLIC KETONE or CYCLIC KETONE or O-QUINONE or P-QUINONE
ORGANOMETALLICS	ACYLMETAL or METAL ARENE or METAL CARBENE or METAL CARBONYL or METAL CYCLOPENTADIENYL or METAL HALIDE or METAL HYDRIDE or METAL METAL BOND or METAL NITROGEN or METAL NITROSYL or METAL PHOSPHINE or METAL SULFUR or METALLOCARBOCYCLE or MU-CARBONYL or ORGANOMETAL or PI-ALKENE or PI-ALKYNE or PI-ALLYL

Viewing Functional Group Definitions

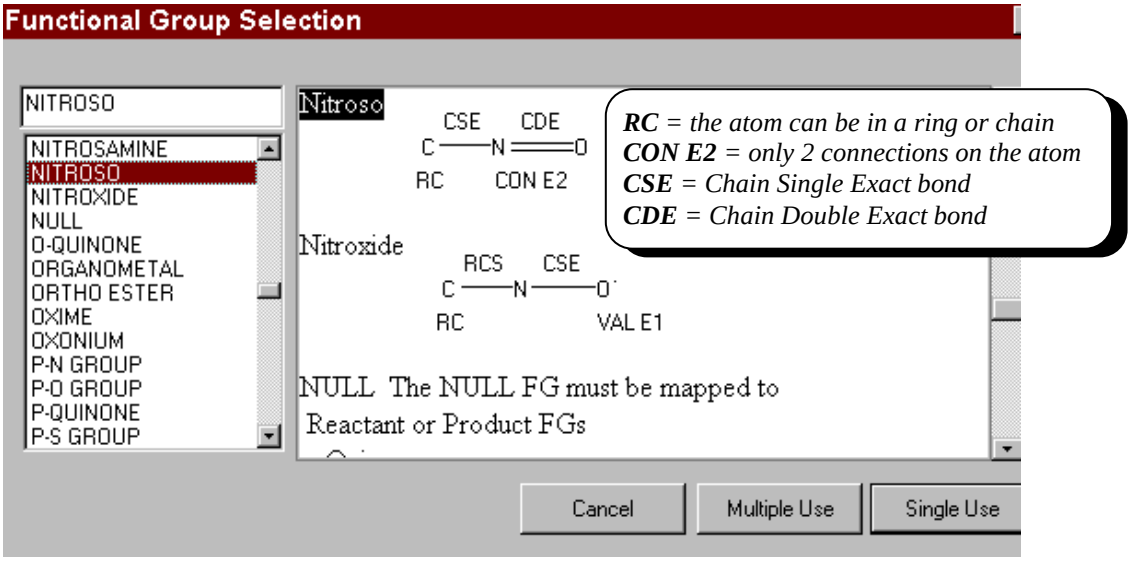
You can view the functional group definitions in the STN Express structure drawing window.

1. Click the **Functional Group** () button.

In "functional group mode", the current atom box changes to functional group terms and all structure drawing tools are inactive.



2. Click on the current atom box. An alphabetical listing of all functional group terms and their definitions appears.



Searching Functional Groups

The functional group search query may be entered directly online at an arrow prompt, or it may be drawn in STN Express and uploaded.

Online, it is a simple text search:

```
=> S PRIMARY AMINE/FG.RXN
L1   89319 PRIMARY AMINE/FG.RXN
```

Using Proximity Operators

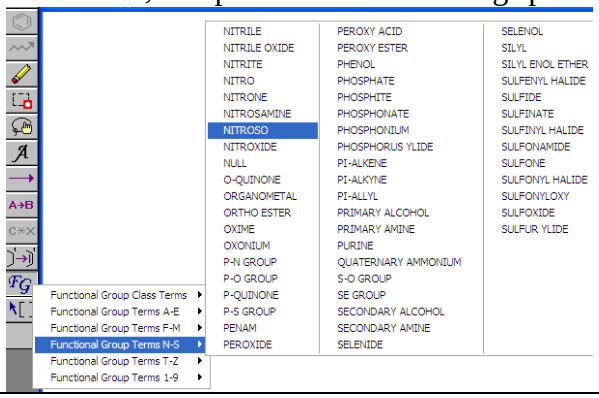
Most functional group searches use either the (L) proximity operator or the (S) proximity operator to connect participants in a reactant/product search.

The (S) operator is more precise because it includes atom mapping. At least one atom from the reacting functional group must also be present in the formed functional group. The following example illustrates the difference in results.

```
L1       12201 PRIMARY ALCOHOL/FG.RXN (L) KETONES/FG.FORM

L2        1967 PRIMARY ALCOHOL/FG.RXN (S) KETONES/FG.FORM
```

Using STN Express

Functional groups may be combined with structures or other functional groups. This example will search for nitroso compounds being converted to primary amines.

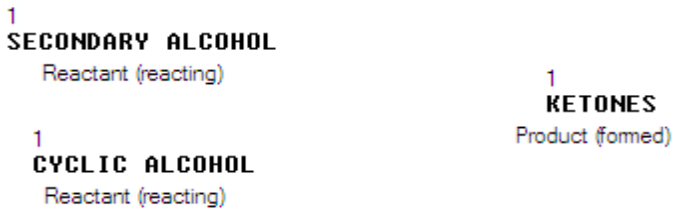
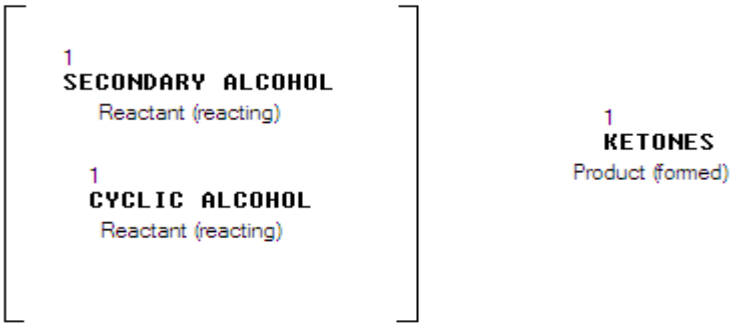
Step	Action
1	Open the structure drawing window, and click the **Functional Group** button () on the upper toolbar.
2	Click the **FG** button on the left, choose the N-S option, select NITROSO, and place it on the drawing space. 
3	Repeat the steps for PRIMARY AMINE.
4	Assign the reacting and formed roles.
5	Use the atom mapping tool.  
6	Save and upload the query.

7	Search the query.
	
	`=> que (NITROSO/fg.rxn (S) PRIMARY AMINE/fg.form)`
	
	`L1 QUE (NITROSO/FG.RXN (S) PRIMARY AMINE/FG.FORM)`
	
	`=> S L1`
	`1689 NITROSO/FG.RXN`
	`39018 PRIMARY AMINE/FG.FORM`
	`L2 221 (NITROSO/FG.RXN (S) PRIMARY AMINE/FG.FORM)`

OR Operator in STN Express

You can use the OR operator to create reaction queries using multiple alternative reactants or products.

For example, locate reactions of acyclic secondary alcohols or cyclic alcohols to form ketones.

Step	Action
1	Draw the three functional groups and include mapping. 
2	Use the **OR Operator** button (), and select the participants to be OR'ed. 

3	Save the query, and upload and search it.
	
	`=> que KETONES/fg.form (S) (SECONDARY ALCOHOL/fg.rxn OR CYCLIC ALCOHOL/fg.rxn)`
	
	`L1 QUE KETONES/FG.FORM (S) (SECONDARY ALCOHOL/FG.RXN OR CYCLIC ALCOHOL/FG.RXN)`
	
	`=> S L1`
	`79231 KETONES/FG.FORM`
	`71564 SECONDARY ALCOHOL/FG.RXN`
	`5526 CYCLIC ALCOHOL/FG.RXN`
	`L2 15291 KETONES/FG.FORM (S) (SECONDARY ALCOHOL/FG.RXN OR CYCLIC ALCOHOL/FG.RXN)`

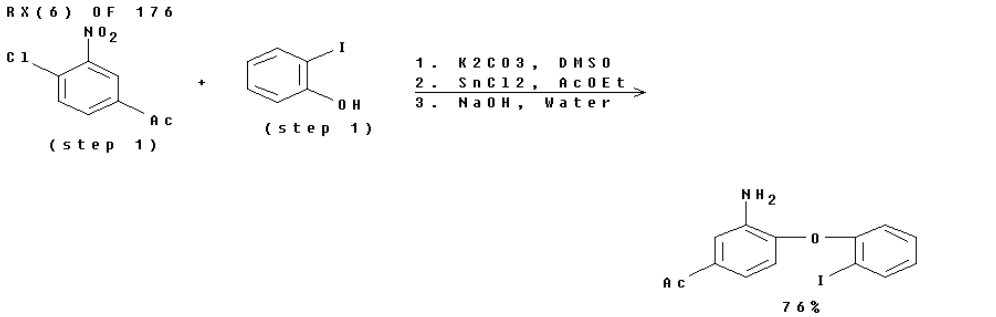
"In the Presence of…"

You may wish to do a search of the type "find reactions where nitro groups are converted to amines in the presence of ketones". This easy to formulate:

```
=> S NITRO/FG.RXN (S) AMINES/FG.FORM (L) KETONES/FG.NON
         20017 NITRO/FG.RXN
        127913 AMINES/FG.FORM
         89291 KETONES/FG.NON
L1        1032 NITRO/FG.RXN (S) AMINES/FG.FORM (L)
               KETONES/FG.NON
```

Note the use of the (S) operator between the reactant and the product and the (L) operator between the reacting participants and the nonreacting one.

```
=> D 3

L1   ANSWER 3 OF 1032  CASREACT  COPYRIGHT 2006 ACS on STN
```




```
REF:   Journal of the American Chemical Society, 127(42), 14776-14784;
       2005
NOTE:  starting nitrophenyl halide assumed
CON:   STAGE(1) 8 hours, 100 deg C
       STAGE(2) 18 hours, room temperature
       STAGE(3) room temperature
```

Yield Proximity

The yield search should be linked to the product using (A) proximity.

If you want to find:	Example
Products with a specified yield only	`=> S AMINES/FG.FORM (A) 90-100/FG.YD`
Products with a specified yield or with no yield stated	`=> S AMINES/FG.FORM (A) (90-100/FG.YD OR NONE/FG.YDT)`

Products of a specific reaction with a specified yield or with no yield stated	`L1. => S AMINES/FG.FORM (A) (90-100/FG.YD OR NONE/FG.YDT)`
	`L2. => S NITRO/FG.RXN (S) AMINES/FG.FORM`
	`L3. => S L2 (S) L1`

Chapter 8: Searching in Other Indexes

Basic Index Search Terms

If you do not append a search field to search terms in a query, the terms are searched in the Basic Index (/BI). The Basic Index contains single words from the notes (NTE), title (TI), abstract (AB), keywords (ST), and index entries (IT),[4] as well as reaction participant CAS Registry Numbers.

Reaction Participant CAS Registry Numbers

The Basic Index contains CAS Registry Numbers for all participants without their role assignment. You can enter CAS Registry Numbers directly or search the ones contained in a REGISTRY answer set by searching the REGISTRY L-number. A search of a CAS Registry Number in the Basic Index retrieves the documents that contain that substance in a reaction, regardless of the role it may play in that reaction.

Substance Example

The search for 106-93-4 (1,2-dibromoethane) in the Basic Index retrieves documents in which the substance is a reactant, product, reagent, solvent, and/or catalyst.

```
=> S 106-93-4
L1         2188 106-93-4
```

The search shows that there are 2188 document records with 1,2-dibromo-ethane in some role in a reaction.

As a reagent:

```
RX(3)      RCT  F 841244-87-9

             STAGE(1)
                RGT  G 109-72-8 BuLi
                SOL  109-99-9 THF
             STAGE(2)
                RGT  I 106-93-4 BrCH2CH2Br
           PRO  H 841244-78-8
           NTE  stereoselective
```

As a reactant:

```
RX(3)      RCT  J 106-93-4, F 479348-50-0
           RGT  L 1310-73-2 NaOH
           PRO  K 491832-72-5
           CAT  56-37-1 PhCH2NEt3 Cl
           SOL  7732-18-5 Water
           CON  4 hours, 45 deg C
```

(continued on next page)

[4]The CAS Registry Numbers in the IT are not searchable in the Basic Index or in the IT field. A search of any CAS Registry Number qualified with /IT yields 0 hits. A search of a CAS Registry Number in the Basic Index yields only hits for reaction participants regardless of whether they are indexed in the /IT or not.

As a product:

```
RX(18)    RCT  AE 107-21-1
          RGT  H 1643-19-2 Bu4N.Br, D 84-58-2 DDQ, E 603-35-0
                 PPh3
          PRO  AF 106-93-4
          SOL  75-09-2 CH2Cl2
          CON  room temperature
```

As a solvent:

```
RX(8)     RCT  Y 352-11-4

            STAGE(1)
               RGT  AB 7439-95-4 Mg
               SOL  109-99-9 THF, 106-93-4 BrCH2CH2Br
```

As a catalyst:

```
RX(35)    RCT  BJ 65426-00-8

            STAGE(1)
               RGT  BL 7439-95-4 Mg
               CAT  106-93-4 BrCH2CH2Br
               SOL  109-99-9 THF
```

REGISTRY L-Number Answer Set

An L-numbered answer set from REGISTRY may be searched in the Basic Index. In REGISTRY, all substances that are also indexed in CASREACT have CASREACT in the Locator (/LC) search field. Including this search term in the REGISTRY search assures that the CAS Registry Numbers in the answer set are in CASREACT. There is a limit of 10,000 CAS Registry Numbers allowed in a REGISTRY L-number searched in CASREACT.

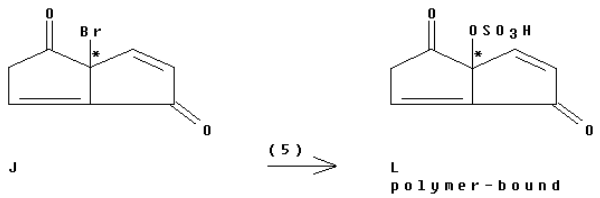
For example, if you are interested in reactions that contain 1,1- or 1,2-dibromoethane and do not know their CAS Registry Numbers, you could conduct the search in the following way.

```
=> FIL REGISTRY
=> S (1,1-DIBROMOETHANE/CN OR 1,2-DIBROMOETHANE/CN)AND
      CASREACT/LC
             1 1,1-DIBROMOETHANE/CN
             1 1,2-DIBROMOETHANE/CN
       3855587 CASREACT/LC
L1           2 (1,1-DIBROMOETHANE/CN OR 1,2-
               DIBROMOETHANE/CN)AND CASREACT/LC

=> FILE CASREACT;S L1
L2        2220 L1
```

Nonspecific Derivatives of Substances

Some of the reaction participants are nonspecific derivatives of substances. These are indexed as the CAS Registry Number of the specific substance with a D appended. When you search a REGISTRY answer set L-number, the CAS Registry Numbers and the CAS Registry Numbers with the D appended are automatically searched by the system in CASREACT. If you are directly entering the CAS Registry Numbers, you must append the D, if these derivatives are of interest.

```
=> S 108347-23-5D
L4            1 108347-23-5D

=> D FHIT CBIB

L4   ANSWER 1 OF 1  CASREACT  COPYRIGHT 2005 ACS on STN

RX(5) OF 61     ...J  ===>  L...
```



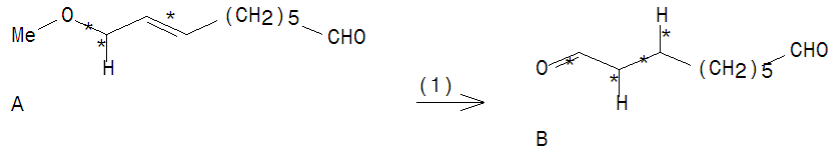

```
RX(5)     RCT  J 108347-28-0
          PRO  L 108347-23-5D
          SOL  123-91-1 Dioxane
          NTE  polymeric silver sulfonate reactant
107:96364  Existence and reactivity of bicyclic annulenones.
     2. Bicyclo[3.3.0]octa-1(5),3,7-triene-2,6-dione.  Gavina,
     Francisco; Costero, Ana M.; Gonzalez, Ana M.; Luis,
     Santiago V.  (Col. Univ. Castellon, Univ. Valencia,
     Castellon de la Plana, Spain).  Journal of Organic
     Chemistry, 52(14), 2997-9 (English) 1987.  CODEN: JOCEAH.
     ISSN: 0022-3263.
```

When the nonspecific substance is a reactant or product, the derivative information displays under the specific substance in the reaction diagram. However, if the substance is a reagent, solvent, or catalyst, no derivative information is displayed, only the appended D indicates that a nonspecific derivative was used.

```
=> S 7440-48-4D
L1          50 7440-48-4D
```

(continued on next page)

```
=> D FHIT CBIB

L1   ANSWER 1 OF 50  CASREACT  COPYRIGHT 2006 ACS on STN

RX(1) OF 2     A  ===>  B
```



A B

```
RX(1)     RCT  A 107605-39-0

            STAGE(1)
               RGT  C 1333-74-0 H2
               CAT  7440-48-4D Co
               CON  2 hours, 140 deg C

            STAGE(2)
               RGT  D 7664-93-9 H2SO4
               SOL  7732-18-5 Water
               CON  1 hour, room temperature

          PRO  B 51651-40-2
143:193720  Preparation of nonanedial or methyloctanedial.
     Hori, Hiroshi; Tokuyasu, Hitoshi; Iwasaki, Shuji (Kuraray
     Co., Ltd., Japan).  Jpn. Kokai Tokkyo Koho JP 2005225765
     A2 20050825, 6 pp.  (Japanese).  CODEN: JKXXAF.
     APPLICATION: JP 2004-33014 20040210.
```

Additional Information in the Indexing

Try displaying the indexing information to find additional information about the type of derivative being used.

```
=> D IT

L1   ANSWER 1 OF 50  CASREACT  COPYRIGHT 2006 ACS on STN
IT   Isomerization catalysts
        (prepn. of nonanedial or methyloctanedial from
        alkoxynonenals or alkoxymethyloctenals via
        isomerization and hydrolysis)
IT   7440-48-4DP, Cobalt, hydride complexes
     RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
        (Preparation);
     USES (Uses)
        (prepn. of nonanedial or methyloctanedial from
        alkoxynonenals or alkoxymethyloctenals via
        isomerization and hydrolysis)
        • • •
```

Text Terms

In addition to CAS Registry Numbers, the Basic Index contains single words from the notes (NTE), title (TI), abstract (AB), supplementary terms (ST), and index entries (IT).

In CASREACT, you may search the words appearing next to the CAS Registry Numbers in the ITs. Stopwords, non-indexed terms found in the fields of the Basic Index or the NTE, are not searchable. They are searchable in the specific fields (e.g., TI, AB, ST, IT). The stopwords are:

AN	AT	FROM	OF	THE
AND	BY	IN	ON	TO
AS	FOR	NOT	OR	WITH

Using EXPAND in CASREACT

Before searching a CAS Registry Number or word in the Basic Index, it is a good practice to EXPAND first to be sure that the term is present in the database.

```
=> E REGIOSELECTIVE
E1            1     REGIOSELECTIONS/BI
E2            1     REGIOSELECTIV/BI
E3       172349 --> REGIOSELECTIVE/BI
E4            1     REGIOSELECTIVED/BI
E5            1     REGIOSELECTIVEDEUTERATION/BI
E6         4302     REGIOSELECTIVELY/BI
E7            1     REGIOSELECTIVEN/BI
E8            1     REGIOSELECTIVEPOLYMETHYLATION/BI
E9            1     REGIOSELECTIVES/BI
E10           1     REGIOSELECTIVETY/BI
E11           2     REGIOSELECTIVIE/BI
E12           1     REGIOSELECTIVIT/BI
```

The E-numbers may be searched directly or used to determine what truncation stem to use.

Truncation

Both left and right truncation are available when searching in the Basic Index. EXPAND gives you an indication of the proper place to truncate. The standard STN truncation symbols are valid for searches in CASREACT. For further details, enter HELP TRUNCATION at an arrow prompt.

Symbol	Meaning	Example	Retrieves
!	One character (may be used internally or externally)	S AMI**!**E S AMIN**!**	AMINE, AMIDE AMINE, AMINO
#	Zero or one character	S AMINE#	AMINE, AMINES
?	Any number of characters including zero	S AMINO? S ?AMINO?	AMINO, AMINOALKYL, AMINOLYSIS, etc. AMINO, AMINOALKYL, ALKYLAMINES

With left truncation, the search term must consist of at least four characters.

Proximity Operators

The proximity operators (W), (nW), (xW), (NOTW), (A), (nA), (xA), (NOTA), (L), and (NOTL) may be used to combine text terms when searching in the Basic Index. Only the (L) operator is useful to combine text terms with the CAS Registry Number in the Basic Index. For more information, enter HELP (operator), where (operator) is (W), (A), or (L), at an arrow prompt in CASREACT.

If two or more terms are combined without an operator, the (W) operator is implied and the system automatically adds it to the search profile. The example also has the plurals feature set to ON.

```
=> S AMINO ACID
          64584 AMINO
              2 AMINOS
          64586 AMINO
                  (AMINO OR AMINOS)
         182878 ACID
          58403 ACIDS
         193982 ACID
                  (ACID OR ACIDS)
L1        15549 AMINO ACID
                  (AMINO(W)ACID)
=> D HIT 6

L1   ANSWER 6 OF 15549  CASREACT  COPYRIGHT 2006 ACS on STN
IT   Amino acids, preparation
     RL: PAC (Pharmacological activity); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation)
        (syntheses and hypoglycemia activities of N-(trans-4-
        isopropylcyclohexylcarbonyl)-.beta.-ring substituted
        phenylalanines)
```

(L) Operator

The (L) operator requires that the combined terms be in the same information unit, e.g., in the title, in one set of keywords, in one index entry. Within the reaction information, (L) is a powerful tool that restricts the terms to the same single-step or multistep reaction. For example, if you are interested in reactions that use 1,2-dibromoethane (106-93-4) and THF (109-99-9), conduct the search in the following way.

```
=> S 106-93-4 (L) 109-99-9
           2281 106-93-4
         124562 109-99-9
L2         1015 106-93-4 (L) 109-99-9
```

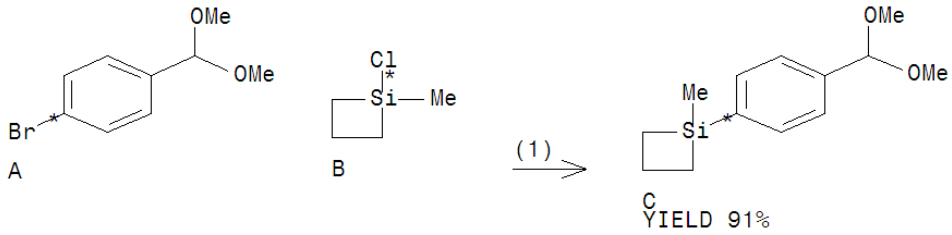
All documents containing the two substances in a single-step reaction are retrieved, such as the one shown here.

(continued on next page)

=> **D FHIT**

L2 ANSWER 1 OF 1015 CASREACT COPYRIGHT 2006 ACS on STN

RX(1) OF 56 A + B ===> C...



RX(1)

STAGE(1)
RGT D 7553-56-2 I2, E 7439-95-4 Mg, F **106-93-4** BrCH2CH2Br
SOL **109-99-9** THF
CON 10 minutes, 0 deg C

STAGE(2)
RCT A 24856-58-4

STAGE(3)
RCT B 2351-34-0
SOL **109-99-9** THF
CON SUBSTAGE(1) 45 minutes, 0 deg C
SUBSTAGE(2) 1 hour, 0 deg C
SUBSTAGE(3) overnight, 0 deg C -> room temperature

STAGE(4)
RGT G 7732-18-5 Water

PRO C 873292-73-0

(L) Operator and Text Terms

Terms in the NTE field are the only text terms in the same information unit as the reaction participant CAS Registry Number.

Combining an IT CAS Registry Number with its associated text using (L) proximity will result in zero hits.

(NOTL) Operator

(NOTL) provides a way to eliminate undesirable substances from a reaction information search. For example, if you want to perform a search for dibromoethane and THF, but you need to eliminate any reaction that also uses benzene, do the following search. You may combine an answer set with additional terms using proximity operators.

```
=> S (106-93-4 (L) 109-99-9) (NOTL) 71-43-2
          2281 106-93-4
        124562 109-99-9
         55293 71-43-2
L2         989 (106-93-4 (L) 109-99-9) (NOTL) 71-43-2
```

Boolean Operators

The Boolean operators AND, NOT, and OR may be used to combine two or more words or CAS Registry Numbers. These operate at the document level, not the reaction level. Therefore, when you search for reaction information, (L) and (NOTL) give you more precise answers than AND and NOT. However, when combining words in fields other than the NTE with CAS Registry Numbers, you must use the Boolean operators.

Chapter 9: Combining Structure Search Results with Other Index Searches

Introduction

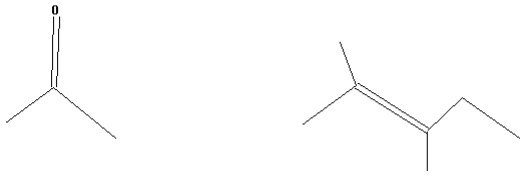
It is not possible to combine structure queries and text queries into a single search query. However, it is possible to combine a structure search answer set with terms in the Basic Index by using either Boolean or proximity operators.

Structure Result and Other Reaction Terms

Only reactants, reagents, and products may be searched with a structure query. Therefore, if you require other reaction participants, e.g., a solvent or a catalyst, search for the reactants/reagents and products with a structure search and separately search the CAS Registry Numbers of the other required substances. Combine the L-number answer sets using the (L) operator to require all participants be in the same reaction.

For example, to find reactions with this type of double bond formation in the presence of THF:

```
=>
Uploading C:\CASNC\STN Express\Queries\rxn6.str
L1      STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1              STR
```



```
Structure attributes must be viewed using STN Express query
preparation.

=> S L1
SAMPLE SEARCH INITIATED 13:29:59
SCREENING COMPLETE -2828 REACTIONS TO VERIFY FROM 192 DOCUMENTS
100.0% DONE    2828 VERIFIED      55 HIT RXNS    18 DOCS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:     53378 TO    59742
PROJECTED ANSWERS:             106 TO      614

L2           18 SEA SSS SAM L1 (    55 REACTIONS)
```

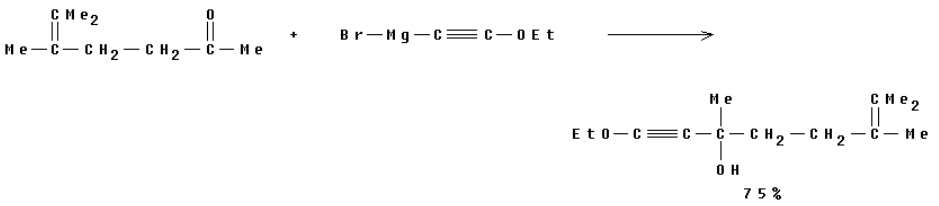
(continued on next page)

=> **D SCAN**

L2 18 ANSWERS CASREACT COPYRIGHT 2006 ACS on STN

TI Studies on volatile plant substances. CXV. Synthesis of 3-methylcitral stereoisomers by the Arens and van Dorp reaction

RX(5) OF 9



NOTE: Classification: C-Alkylation; Addition; # Conditions: 10mn -5 deg; 15mn

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):**0**

=> **S L1 FUL**

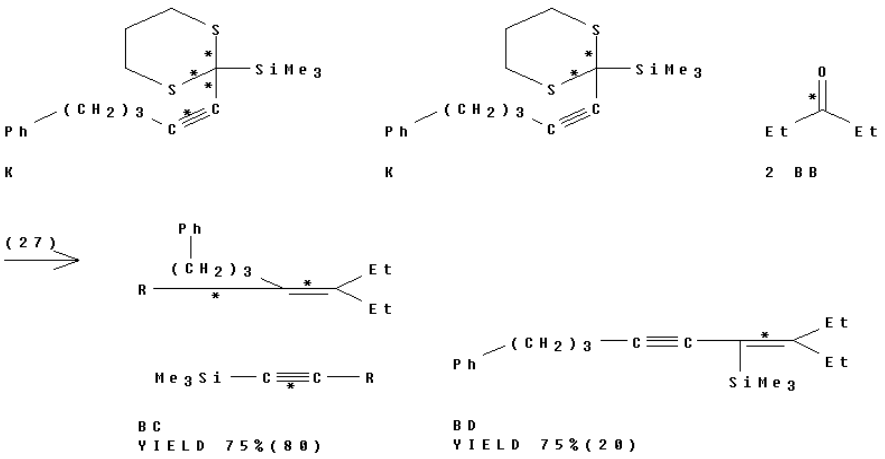
FULL SEARCH INITIATED 13:32:09
SCREENING COMPLETE -64599 REACTIONS TO VERIFY FROM 3998 DOCUMENTS
100.0% DONE 64599 VERIFIED 1809 HIT RXNS 323 DOCS
SEARCH TIME: 00.00.03
L3 323 SEA SSS FUL L1 (1809 REACTIONS)

=> **S L3 (L) 109-99-9**
124562 109-99-9
L4 95 L3 (L) 109-99-9

=> **D FHIT**

L4 ANSWER 1 OF 95 CASREACT COPYRIGHT 2006 ACS on STN

RX(27) OF 169 ...2 K + 2 **BB** ===> **BC** + BD



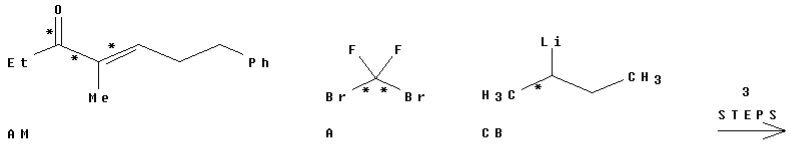
(continued on next page)

```
RX(27)    RCT  K 765943-35-9

            STAGE(1)
               RGT  AE 185991-38-2 Titanium, bis(.eta.5-2,4-
                    cyclopentadien-1-yl)bis(triethylphosphite-
                    .kappa.P)-
               SOL  109-99-9 THF
               CON  10 minutes, 25 deg C

            STAGE(2)
               RCT  BB 96-22-0
               SOL  109-99-9 THF
               CON  1 hour, 25 deg C

          PRO  BC 765943-38-2, BD 765943-40-6
          NTE  titanocene phosphite complex was prepd. in situ
               at 1st step
```

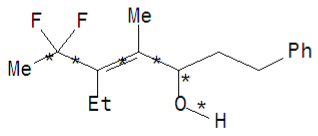
Structure Result and Nonreaction Terms

If the search terms occur in the *nonreaction* information, i.e., the bibliographic, abstract, or text indexing information, combine them with the structure search results by using the Boolean operators. For example, you could combine the previous structure search results with WITTIG to see if the Wittig reaction is mentioned in any of the documents.

```
=> S L3 AND WITTIG
         10267 WITTIG
L5          18 L3 AND WITTIG

=> D HIT

L5   ANSWER 1 OF 18  CASREACT  COPYRIGHT 2006 ACS on STN

RX(158) OF 208 COMPOSED OF RX(23), RX(2), RX(43)
RX(158)   AM  +  A  +  CB  ===>  CJ
```



AM A CB



CJ
YIELD 52%

Note: *D FHIT will not display the highlighted hit information for the nonreaction search terms. Use HIT instead.*

(continued on next page)

RX(23) RCT AM **791809-35-3**
RGT BA 1310-73-2 NaOH, BB 7722-84-1 H2O2
PRO I 791809-45-5
SOL 7732-18-5 Water, 67-56-1 MeOH
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> room temperature
SUBSTAGE(3) 5 hours, room temperature
NTE stereoselective

• • •

RX(43) RCT J 791809-63-7, CB 598-30-1

STAGE(1)
SOL 109-99-9 THF
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 2 hours, 0 deg C

STAGE(2)
RGT BZ 12125-02-9 NH4Cl
SOL 7732-18-5 Water

PRO CJ **791809-76-2**
NTE stereoselective, E/Z 63:37

• • •

IT 104-87-0, 4-Methylbenzaldehyde 555-16-8, 4-Nitrobenzaldehyde, reactions 1439-36-7, (2-Oxopropylidene)-triphenylphosphorane
RL: RCT (Reactant); RACT (Reactant or reagent)
(**Wittig**; prepn. and regio- and stereoselective SN2' ring opening of gem-difluorinated vinyloxiranes with RLi leading to difluorinated allylic alcs. and theor. PES study of the reaction mechanism)

IT 680-31-9P, HMPA, reactions
RL: BYP (Byproduct); RGT (Reagent); PREP (Preparation); RACT (Reactant or reagent)
(formation as byproduct from hexamethylphosphorus triamide **Wittig** reagent and use as chelating agent)

Summary of Text Search Strategy

If you want:	Then:
Substances in any reaction role	Search the CAS RN in the Basic Index
Substances in a specific role	Search the CAS RN qualified with that role
Multiple substances in the same reaction	Search their CAS RNs combined with (L)
A few specific substances participating in the reaction	Search their CASRN qualified with the appropriate roles and combined with (L)
Reaction conditions or health or safety information	Search text in the reaction notes combined with other specifications using (L)
To combine reaction information with terms from the bibliographic, abstract, and/or indexing information	Combine the reaction search terms with the other word search terms using Boolean operators.
Create a L-number for a subset reaction search	Use word search strategy to create the subset L-number, then do the subset reaction search

Bibliographic Data

The bibliographic search fields in CASREACT are the same as those in CAplus. See the CASREACT Database Summary Sheet at www.cas.org for the complete list of search and display fields.

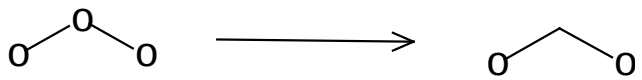
Bibliographic search terms are usually used to refine a search to a smaller number of documents or to create a subset of the database to be used in a structure search.

Boolean Operators

You may combine bibliographic search terms with reaction search terms using the Boolean operators. You may do the combination directly in a single query or combine the terms with the L-number answer set.

Refining a Reaction Search

For example, to determine if any of the work done with this reaction was conducted at The Ohio State University, do the following:



Reactant/Reagent Product

```
=> S L1 FUL
FULL SEARCH INITIATED 14:48:59
SCREENING COMPLETE - 116622 REACTIONS TO VERIFY FROM 5436 DOCUMENTS

100.0% DONE  116622 VERIFIED 34188 HIT RXNS 2076 DOCS
SEARCH TIME: 00.00.04

L3         2076 SEA SSS FUL L1 ( 34188 REACTIONS)

=> S L3 AND (OHIO STATE)/CS
          1832 OHIO/CS
         19241 STATE/CS
          1747 (OHIO STATE)/CS
                 ((OHIO(S)STATE)/CS)
L4          28 L3 AND (OHIO STATE)/CS
```

Chapter 10: Searching Subsets in CASREACT

Introduction

If a structure query will not complete its search within system limits and none of the query refinement options will resolve the issue, then a subset search may be the solution.

Creating a Subset

A CASREACT subset may be created in a number of ways:

- A text term search in the Basic Index or other text search indexes
- A functional group search
- Another structure search that will complete

Solvent Subsets

Search terms in the /SOL field may be used to create a subset definition for a structure search. The results are the same as when you link (L) the /SOL field with the structure search results. However, the /SOL search term that defines the subset is not highlighted in the subset search answer set. Only the substances that match the structure query are highlighted.

Catalyst Subsets

Search terms in the /CAT field may be used to create a subset definition for a structure search. The results are the same as when you link (L) the /CAT field with the structure search results. However, the /CAT search term that defines the subset is not highlighted in the subset search answer set. Only the substances that match the structure query are highlighted.

Using Basic Index Results as Subsets

By searching words in the Basic Index, you can easily create a subset of the database that contains terms relevant to your search. This subset can then be used to run a structure search containing small substructures that would exceed system limits if run in the full database.

Step	Action
1	Search the text terms.
2	Use the L-number of the answer set as the subset definition for the structure search.

Subset Search Example

For more information on subset searching, type HELP SUBSET at an arrow prompt while online.

Find reactions where alkyl amines are oxidized to alkyl nitrates.

```
=>
Uploading C:\CASNC\STN Express\Queries\rxn7.str
L1      STRUCTURE UPLOADED
=> D L1
L1 HAS NO ANSWERS
L1              STR
```

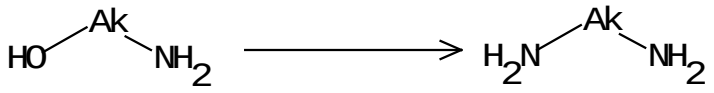
```
Structure attributes must be viewed using STN Express query
preparation.
=> S L1
SAMPLE SEARCH INITIATED 10:00:18
SCREENING COMPLETE -  53736 REACTIONS TO VERIFY FROM   3949 DOCUMENTS
  9.3% DONE    5000 VERIFIED      43 HIT RXNS            2 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:   1061538 TO  1087902
PROJECTED ANSWERS:              208 TO      814

L2            2 SEA SSS SAM L1 (    43 REACTIONS)
```

To reduce the number of documents and reactions that must be processed, create a subset of the database. Find documents that mention OXIDATION or the abbreviation OXIDN in the title, keywords, or index terms. Then use that set of documents as the basis for the structure search. Any answer set created in CASREACT may be used as the basis of a subset search in the database.

```
=> S OXIDATION OR OXIDN
    • • •
L3       71526 OXIDATION OR OXIDN

=> S L1 SUB=L3 FUL
FULL SUBSET SEARCH INITIATED 10:06:47
SCREENING COMPLETE -171782 REACTIONS TO VERIFY FROM   10523 DOCUMENTS
100.0% DONE  171782 VERIFIED  289 HIT RXNS (   1 INCOMP)      82 DOCS
SEARCH TIME: 00.00.04

L4           82 SEA SUB=L3 SSS FUL L1 (   289 REACTIONS)
```

Creating a Subset for a Reaction Search

The results of a bibliographic search may also be used as the subset definition for a structure search. Doing the bibliographic search first creates a subset of the database that allows the structure search to run within system limits. For example, you can retrieve patents that illustrate the desired reaction with the following search.



Reactant/Reagent Product

```
=> S L1 CSS
SAMPLE SEARCH INITIATED 15:00:27
SCREENING COMPLETE - 187119 REACTIONS TO VERIFY FROM 10512 DOCUMENTS

  2.7% DONE    5000 VERIFIED       0 HIT RXNS   0 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED VERIFICATIONS:   3721501 TO  3763259
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA CSS SAM L1 (     0 REACTIONS)

=> S P/DT
L3       76501 P/DT

=> S L1 CSS SUB=L3 FULL
FULL SUBSET SEARCH INITIATED 15:01:36
SCREENING COMPLETE - 285474 REACTIONS TO VERIFY FROM  29233 DOCUMENTS

100.0% DONE  285474 VERIFIED      23 HIT RXNS     21 DOCS
SEARCH TIME: 00.00.07

L4           21 SEA SUB=L3 CSS FUL L1 (    23 REACTIONS)
```

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