



STN Workshops

Reaction Searching in CASREACT®

JUNE 2003



At the end of this workshop, you will be able to

- Use structures to locate chemical reactions of interest in CASREACT
- Use the reaction site and/or the reaction map feature to refine structure queries
- Use functional group search terms to locate broadly defined chemical reactions of interest in CASREACT
- Refine reaction results with yield, number of steps, other reaction participants, or additional reaction queries
- Display reaction results in a useful, cost-effective manner

Before you begin

This workshop is designed for searchers with a basic knowledge of organic chemistry who have experience building and searching structures with STN Express software.

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OVERVIEW

In this section, you will learn

- About the content of the CASREACT database
- About the information sources for the CASREACT database
- What an "answer" looks like in CASREACT
- About search terms commonly used in reaction searching

Content Overview

The CASREACT[®] database is an organic synthetic reaction database produced by CAS. It is a document-based file covering chemical reactions from 1907–present.

Reactions Covered

CASREACT contains synthetically useful reactions cited in the journal and patent literature. This includes

- Preparations
- New, more convenient, improved methods
- Procedures for improving yield
- Applications of new reagents

Substance preparations

CASREACT contains reactions used to prepare

- Aliphatic and alicyclic compounds
- Benzene and condensed benzene compounds
- Heterocyclic compounds
- Alkaloids, steroids, and carbohydrates
- Amino acids, small peptides, and small proteins
- Dyes and organic pigments
- Terpenes and terpenoids
- Organometallic compounds

Reaction types

In addition to straightforward single-step reactions, CASREACT contains

- Multistep reactions
- Stereospecific syntheses
- Biologically mediated reactions, such as enzymatic conversions
- "Pot" reactions (multistep reactions where the intermediates are not isolated)
- Failed reactions (if the intent was potentially useful)

note

CASREACT does not cover reactions used to prepare

- Inorganic compounds
- Polymers
- Surfactants and detergents

Reaction Sources

The reactions in CASREACT come from three sources.

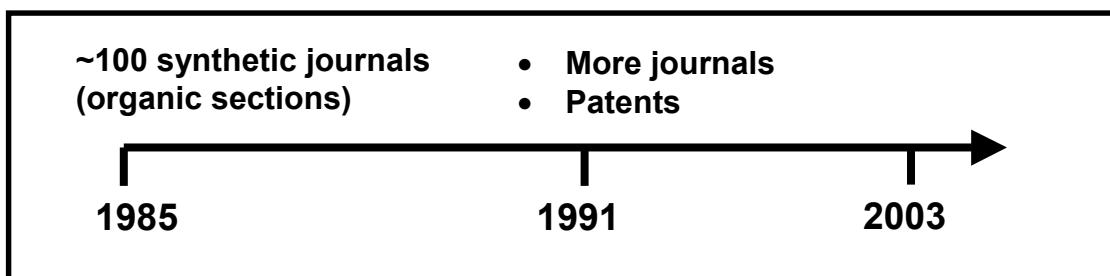
- CAS: journals, 1985–present; patents, 1991–present.
- InfoChem (InfoChem supplies the data from the VINITI/ZIC database): journals, 1974–1991; patents, 1982–1991.
- INPI (data from the French Core Reactions Database): 1907–1985.

All records are keyed to the appropriate CAplus record.

CAS Indexing

CAS indexes reactions based on synthetic utility and novelty. Coverage and indexing practices have changed over time.

Coverage changes:



Indexing practices:

Year range	Indexing practice:
1985–1990	All important reactions in a document
1991–present	<ul style="list-style-type: none">■ Reactions where author stresses synthetic utility or novelty■ Structurally representative reactions (for multiple reactions of same type)■ Patents in which a new process for preparing a compound is claimed■ Other sections: dyes and pigments, enzymes, fermentation and bioindustrial chemistry

Sample Record

CASREACT records contain

- One or more searchable/displayable reactions
- All of the information in the associated CPlus record

AN 137:87838 CASREACT [Full-text](#)
TI Antineoplastic Agents. 465. Structural Modification of Resveratrol:
Sodium Resverastatin Phosphate
AU Pettit, George R.; Grealish, Matthew P.; Jung, M. Katherine; Hamel,
Ernest; Pettit, Robin K.; Chapuis, J. Charles; Schmidt, Jean M.
CS Cancer Research Institute and Department of Chemistry and
Biochemistry, Arizona State University, Tempe, AZ, 85287-2404, USA
SO Journal of Medicinal Chemistry (2002), 45(12), 2534-2542
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 25
AB As an extension of structure/activity investigations of resveratrol,
phenstatin, and the cancer antiangiogenesis drug sodium
combretastatin A-4 phosphate, syntheses of certain related stilbenes
and benzophenones were undertaken. The tri-Me ether derivative of
(Z)-resveratrol exhibited the strongest activity (GI50 = 0.01-0.001
µg/mL) against a minipanel of human cancer cell lines. A
monodemethylated derivative was converted to prodrug (sodium
resverastatin phosphate) for further biol. evaluation. The
antitubulin and antimicrobial activities of selected compds. were
also evaluated.
ST antitumor resveratrol analog prepn structure activity
IT Structure-activity relationship
(antitumor; preparation and antitumor structure activity
relationships of resveratrol analogs)
IT Antimicrobial agents
Antitumor agents
Human
(preparation and antitumor structure activity relationships of
resveratrol analogs)
IT Tubulins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation and antitumor structure activity relationships of
resveratrol analogs)
IT 22255-22-7P 441351-32-2P 441351-38-8P 441351-40-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and antitumor structure activity relationships of
resveratrol analogs)

*Bibliographic information
and abstract are searchable.*

*All of the controlled
vocabulary is searchable,
except for the CAS RNs.*

(continued on next page)

IT 501-36-0P, Resveratrol 537-42-8P 33626-08-3P 58436-29-6P
61434-67-1P, cis-Resveratrol 94608-23-8P 94709-12-3P
129020-58-2P 192710-89-7P 412019-28-4P 441351-37-7P
441351-39-9P 441351-42-4P 441351-44-6P 441351-51-5P
441351-54-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation and antitumor structure activity relationships of
resveratrol analogs)

IT 117048-59-6, Combretastatin A-4 203448-32-2, Phenstatin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
(preparation and antitumor structure activity relationships of
resveratrol analogs)

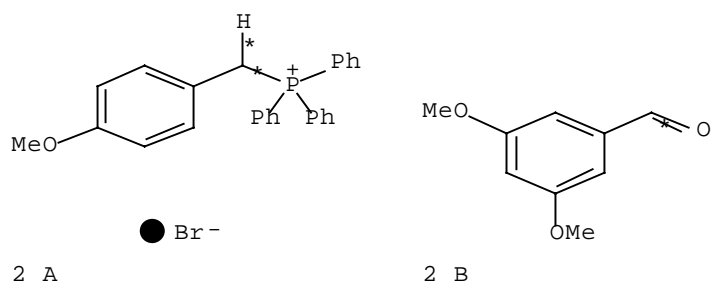
IT 104-92-7, 4-Bromoanisole 106-41-2, 4-Bromophenol 123-08-0,
4-Hydroxybenzaldehyde 603-35-0, Triphenyl phosphine, reactions
2746-25-0, 4-Methoxybenzyl bromide 7311-34-4, 3,5-
Dimethoxybenzaldehyde 7789-60-8, Phosphorus tribromide
17176-77-1, Dibenzyl phosphite 18162-48-6, Silyl chloride
26153-38-8, 3,5-Dihydroxybenzaldehyde 58479-61-1, tert-
Butyldiphenylsilyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antitumor structure activity relationships of
resveratrol analogs)

IT 1530-38-7P, 4-Methoxybenzyltriphenylphosphonium bromide
24131-30-4P, 3,5-Dimethoxybenzyltriphenylphosphonium bromide
67963-68-2P 116748-05-1P 116748-06-2P 120743-99-9P
187803-40-3P 192710-87-5P 192710-88-6P 441351-28-6P
441351-29-7P 441351-30-0P 441351-31-1P 441351-33-3P
441351-34-4P 441351-35-5P 441351-36-6P 441351-41-3P
441351-43-5P 441351-45-7P 441351-46-8P 441351-47-9P
441351-48-0P 441351-49-1P 441351-50-4P 441351-52-6P
441351-53-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT
(Reactant or reagent)
(preparation and antitumor structure activity relationships of
resveratrol analogs)

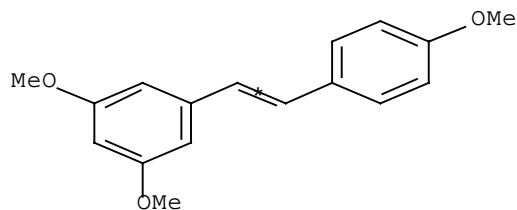
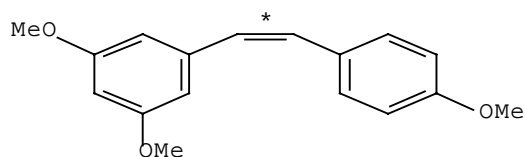
RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Adesanya, S; J Nat Prod 1999, V62, P1694 CAPLUS
(2) Arichi, H; Chem Pharm Bull 1982, V30, P1766 CAPLUS
(3) Chanvitayapongs, S; NeuroReport 1997, V8, P1499 CAPLUS
(4) Chaplin, D; Anticancer Res 1999, V19, P189 CAPLUS
(5) Chun, Y; Biochem Biophys Res 1999, V262, P20 CAPLUS
(6) Chun, Y; Biochem Biophys Res Commun 1999, V262, P20 CAPLUS
(7) Chung, M; Planta Med 1992, V58, P274 CAPLUS
(8) Cichewicz, R; J Nat Prod 1998, V61, P1313 CAPLUS
(9) Creasy, L; J Am Soc Hortic Sci 1988, V113, P230 CAPLUS
(10) Cushman, M; J Med Chem 1992, V35, P2293 CAPLUS
(11) de Ledinghen, V; Int J Oncol 2001, V19, P83 CAPLUS
(12) Eddarir, S; Tetrahedron Lett 2001, V42, P9127 CAPLUS
(13) Goldberg, D; Clin Chem 1995, V46, P159 CAPLUS
(14) Goldberg, D; Clin Chem 1996, V42, P113 CAPLUS
●
●
●

RX(1) OF 138 ...2 A + 2 B ==> C + D...

Records contain a **map** of the reaction - alphabetic identifiers for reaction participants.



Records contain a **diagram** of the reaction. Broken/formed bonds are marked with an asterisk.



RX(1) RCT A 1530-38-7

STAGE(1)

RGT E 109-72-8 BuLi

SOL 109-99-9 THF

STAGE(2)

RCT B 7311-34-4

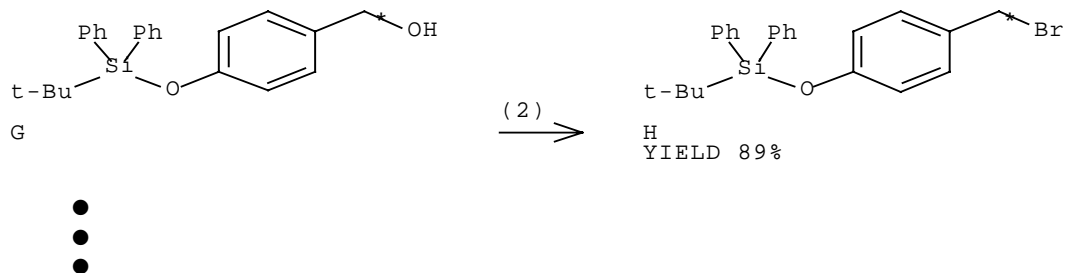
SOL 109-99-9 THF

PRO C 94608-23-8, D 22255-22-7

NTE stereoselective, 91 % overall yield

Records contain a **summary** of the reaction. CAS RNs and roles for each reaction participant are identified.

RX(2) OF 138 ...G ==> H...



Reaction Search Terms

A variety of search terms can be used to

- Define a reaction
- Refine a set of reactions
- Refine reaction search results

Defining a Reaction

Reactions may be defined initially via

- Structure diagram
- Functional group

Refining a Set of Reactions

The following information may be used to more precisely define reactions of interest:

- Yield
- Number of steps
- CAS RNs for other reaction participants (e.g., catalyst)

Refining Reaction Search Results

Typical text refinement strategies can be used to refine reaction answer sets:

- Document type
- Publication year
- Author
- Company name

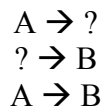
STRUCTURE SEARCHING

In this section, you will learn to

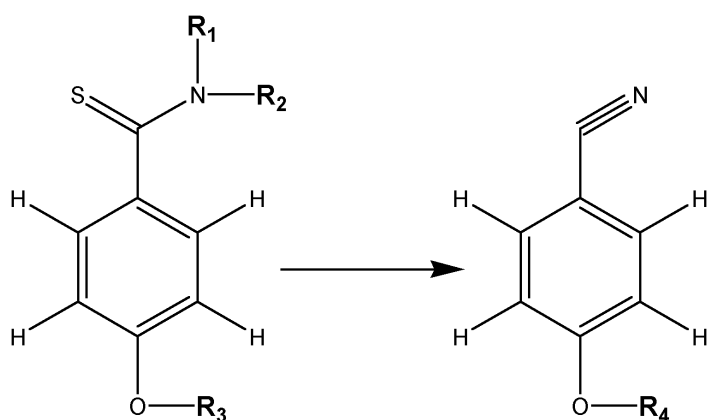
- Build structure queries for reaction searching
- Upload a reaction query and run a reaction search
- Display the reaction information for the answers retrieved in a reaction search
- Improve the precision of a reaction search by specifying reaction sites and/or mapping atoms from reactants to products
- Build queries involving two reactants and a product

Reactant → Product Structure Searching

Structure-based reaction searching is used to locate reactions of the type:



Search Question: *Locate methods for converting the following thioamides to the corresponding nitriles:*



$R_1, R_2, R_3, R_4 = \text{Anything, including hydrogen}$

Search Strategy

- Step 1** Build and save the reaction query.
- Step 2** Logon to STN and enter CASREACT.
- Step 3** Upload the reaction query.
- Step 4** Run the reaction search.
- Step 5** Display the reactions.

Step 1: Build and Save the Reaction Query

To build a reactant → product reaction query, do the following:

- Draw the structure diagrams.
- Specify the reaction features.
- Save the reaction query.

A. Draw the structure diagrams








- Click the *Prepare Query* icon to open the structure drawing screen.
- Draw the structures for the reactant and the product in the same window.

B. Specify the reaction features

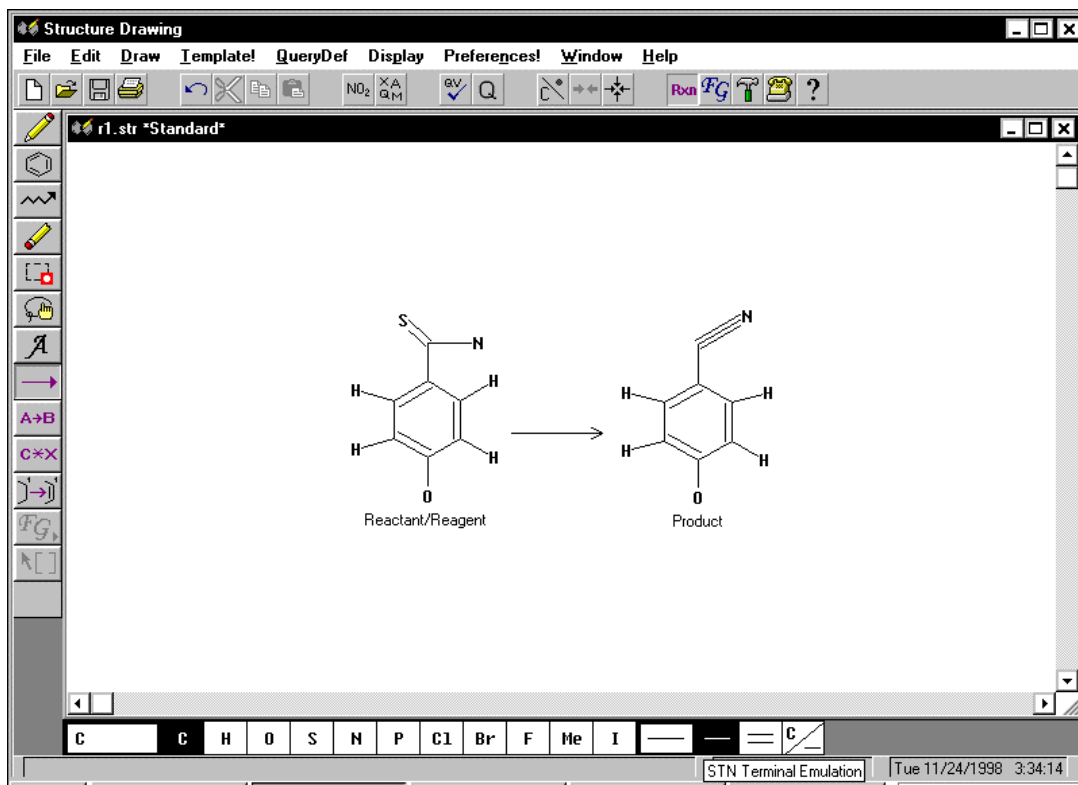


- Click on the *Reaction* icon to activate the reaction tools.

To assign a	Use the
Reaction direction	Reaction Arrow tool 
Fragment role	Reaction Role tool 
Bond that is changed/unchanged in the reaction	Reaction Site tool 
Mapping between an atom in the reactant and product	Atom Mapping tool 

2. To specify reactant and product, right click the **Reaction Arrow tool**  and draw an arrow from the reactant to the product.

The role reactant/reagent is assigned to the structure to the left of the arrow, and the role product is assigned to the structure to the right of the arrow.



note

The role reactant/reagent is assigned instead of reactant because a compound may be considered to be a reactant in one paper and a reagent in others. To maximize the number of reactions retrieved, the broader role of reactant/reagent is assigned to the starting material.

C. Save the reaction query



1. Click the **Save** icon. The **Save Query As** dialog box appears.
2. In the **File Name:** entry box type a name for the query.
Click **OK**.
3. On the **Saving** screen, click **Save**.

Step 2: Logon to STN and Enter CASREACT



1. Logon to STN by clicking the *Logon* icon

You are placed in the HOME file on STN.

2. Use the **FILE** command to enter a reaction database.

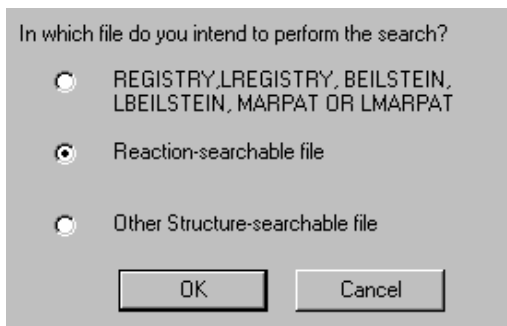
```
* * * * * STN Columbus * * * * *  
  
FILE 'HOME' ENTERED AT ...  
  
=> FILE CASREACT
```

Step 3: Upload the Reaction Query



1. Click the *Upload Structure Query* icon
2. Choose the name of the structure to upload. Click *Open*.

Select the type of database in which you will do the search. Click **OK**.



note

The query will be uploaded as a reaction only in the reaction-searchable databases. In the other databases, the reactant and product will be uploaded as separate structure queries.

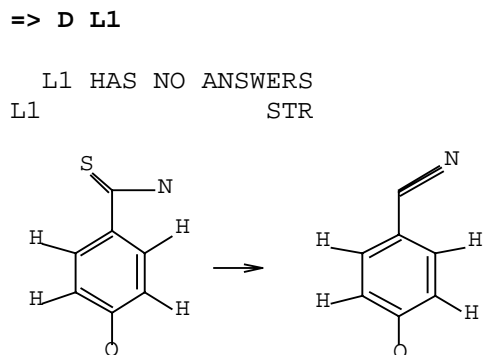
When the structure upload is completed, an L-number is assigned to the structure reaction query.

```
=>
Uploading r1.str

L1      STRUCTURE UPLOADED
```

Option: Verify the reaction query online

Display the uploaded reaction and verify that it corresponds to the reaction you wish to search.



Step 4: Run the Reaction Search

The **SEARCH** command is used to run a reaction search.

Running a reaction search involves three steps:

1. Run a **SAMPLE** search.
2. Evaluate answers.
3. Run a **FULL** search.

Run the SAMPLE search

```
=> S L1 SSS SAM

SAMPLE SEARCH INITIATED 14:37:13 FILE 'CASREACT'
SCREENING COMPLETE -      3 REACTIONS TO VERIFY FROM      3 DOCUMENTS
100.0% DONE      3 VERIFIED      2 HIT RXNS      2 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                       BATCH   **COMPLETE**
PROJECTED VERIFICATIONS: 3 TO    163
PROJECTED ANSWERS:      2 TO    124

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

The search is projected to complete in the full database.

↑
Each answer is a document record.

↑
Each answer contains one or more reactions that match the query.

Evaluate answers with D SCAN

In CASREACT, the no-cost D SCAN feature shows the

- Title of the publication
- First hit reaction in a condensed form

```
=> D SCAN

L2  2 ANSWERS  CASREACT  COPYRIGHT 2003 ACS

TI  Nitrile-formamide chloride adducts. X. Formation of nitriles by
    base-induced fragmentation of N-acylamides and their heteroanalogous
    derivatives

RX(2) OF 5
```

COc1ccc(cc1)C(=O)N=CHN.CN>>COc1ccc(cc1)C#N

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN?: 0

Run the FULL search

=> S L1 SSS FULL

FULL SEARCH INITIATED 14:37:49 FILE 'CASREACT'
SCREENING COMPLETE - 33 REACTIONS TO VERIFY FROM 20 DOCUMENTS
100.0% DONE 33 VERIFIED 11 HIT RXNS 9 DOCS
SEARCH TIME: 00.00.01

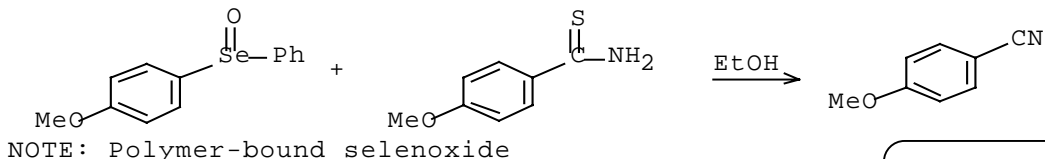
L3 9 SEA SSS FUL L1 (11 REACTIONS)

=> D SCAN

L3 9 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Mild and selective oxidations with polystyrene-bound
diaryl selenoxide

RX(20) OF 27

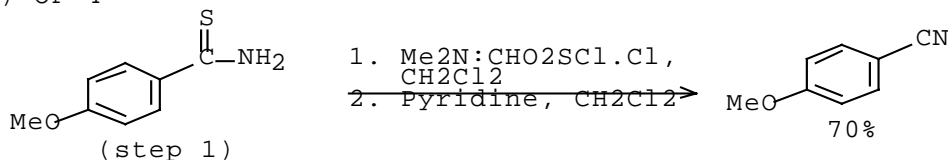


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 9 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI A new, efficient one-pot preparation of nitriles from
thiocarboxamides

RX(1) OF 4



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

The FULL search retrieved 9 documents containing a total of 11 reactions that match the query.

D SCAN randomly selects answers from the answer set for display.

Type "0" or "END" to exit from D SCAN.

Step 5: Display Reactions

Many display formats are available in CASREACT to view additional information from an answer.

Use this format	To display
OCC	The number of hit reactions in each answer
CRD	All hit reactions for each answer in the compact format
FCRDREF (default)	First hit reaction for each answer in the compact format, plus the reference
CRDREF	All hit reactions for each answer in the compact format, plus the reference
FHIT	First hit reaction for each answer in the full format (Map, Diagram, and Summary - includes CAS RNs for each participant)
HIT	All hit reactions for each answer in the full format (Map, Diagram, and Summary - includes CAS RNs for each participant)
BIB	Full bibliographic information
ABS	Abstract from printed <i>Chemical Abstracts</i>

Occurrence display (OCC):

OCC displays information about the "hits" in the answer. The first line shows the number of reactions that matched the search query.

```
=> D L3 1-4 OCC
```

```
L3 ANSWER 1 OF 9 CASREACT COPYRIGHT 2003 ACS
NUMBER OF HIT REACTIONS          2
NUMBER OF REACTIONS IN PATH      2
NUMBER OF REACTIONS IN SPATH     2
FIELD                             COUNT
RX(4)                             2
RX(5)                             2
```

```
L3 ANSWER 2 OF 9 CASREACT COPYRIGHT 2003 ACS
NUMBER OF HIT REACTIONS          1
NUMBER OF REACTIONS IN PATH      1
NUMBER OF REACTIONS IN SPATH     1
FIELD                             COUNT
RX(1)                             2
```

```
L3 ANSWER 3 OF 9 CASREACT COPYRIGHT 2003 ACS
NUMBER OF HIT REACTIONS          1
NUMBER OF REACTIONS IN PATH      1
NUMBER OF REACTIONS IN SPATH     1
FIELD                             COUNT
RX(2)                             2
```

```
L3 ANSWER 4 OF 9 CASREACT COPYRIGHT 2003 ACS
NUMBER OF HIT REACTIONS          2
NUMBER OF REACTIONS IN PATH      2
NUMBER OF REACTIONS IN SPATH     2
FIELD                             COUNT
RX(45)                           2
RX(59)                           2
```

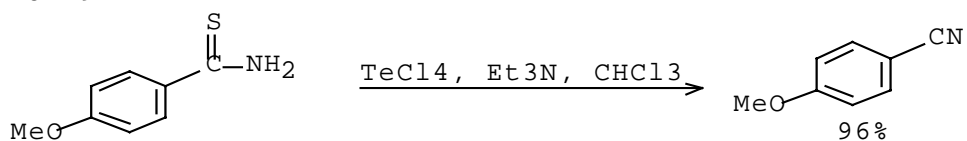
Compact reaction display (CRD):

CRD shows all hit reactions for an answer.

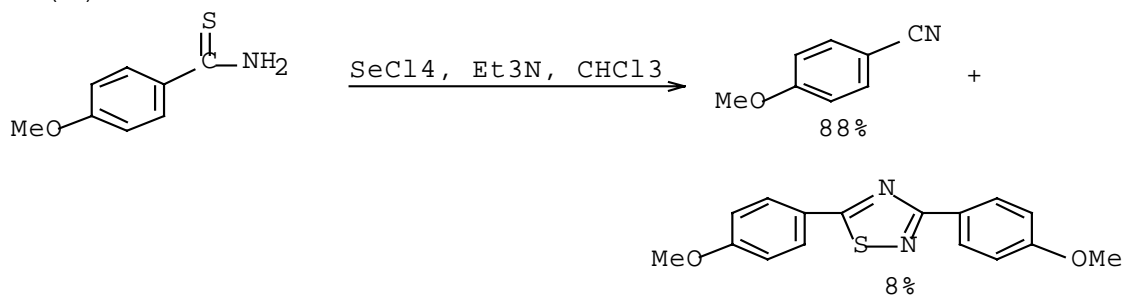
=> D L3 1 CRD

L3 ANSWER 1 OF 9 CASREACT COPYRIGHT 2003 ACS

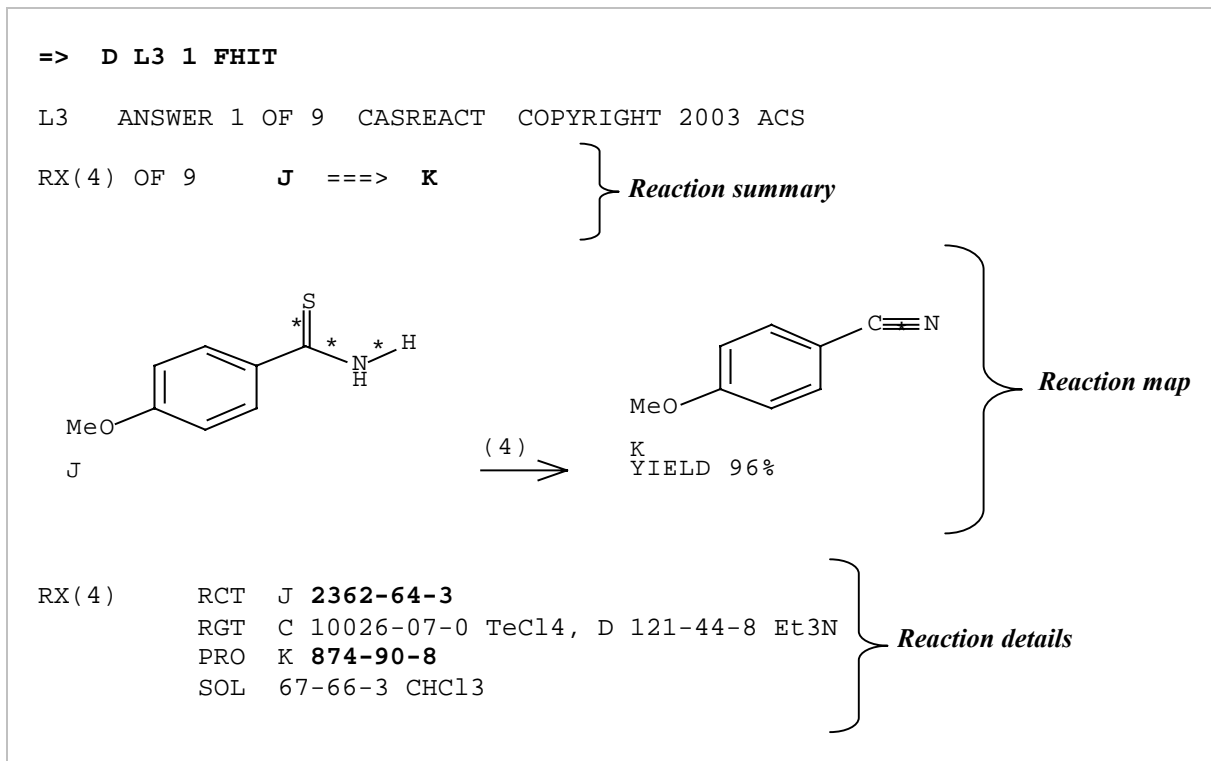
RX(4) OF 9



RX(5) OF 9



First hit reaction display (FHIT):



Helpful HINT

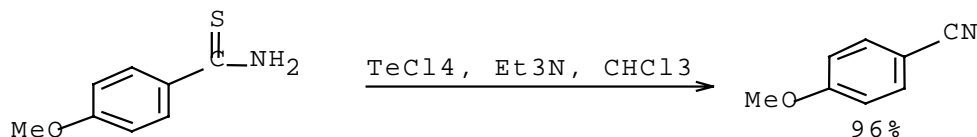
The FHIT and HIT formats are useful when you need to see the CAS RNs for one or more of the reaction participants.

Default display (FCRDREF):

=> D L3 1

L3 ANSWER 1 OF 9 CASREACT COPYRIGHT 2003 ACS

RX(4) OF 9



REF: Journal of Chemical research, Synopses, (4), 152-3; 1995

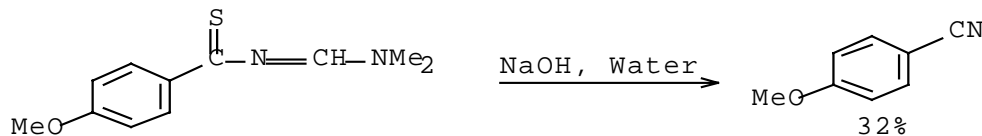
If a display format is not specified on the command line, STN uses the default format for the database to display the results.

Including the abstract in the display with ABS:

=> D L3 3 CRDREF ABS

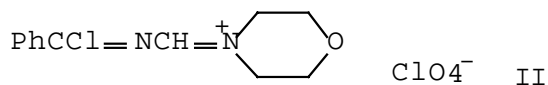
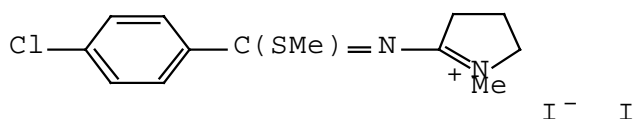
L3 ANSWER 3 OF 9 CASREACT COPYRIGHT 2003 ACS

RX(2) OF 5



REF: Journal fuer Praktische Chemie (Leipzig), 330(5), 847-50; 1988

GI



AB 4-MeOC6H4CN was obtained by treatment of 4-MeOC6H4CCl:NCH:N+Me2 ClO4- or 4-MeOC6H4CSN:CHNMe2 with base. 4-ClC6H4CN was similarly obtained from the pyrrolinium salt I and 3-morpholino-2-phenylacrylonitrile from the iminium salt II. 3-Phthalimidopropionitrile was prepd. from N-(3-phthalimidopropionyl) formamide and MeNHNH2.

Helpful HINT

To permanently change the default display format:

1. Define the new format using SET FORMAT.

```
=> SET FORMAT
```

```
ENTER FORMAT NAME OR (?): .MYRXN
```

```
ENTER FORMAT DEFINITION OR (?): TI CRDEF
```

```
SET COMMAND COMPLETED
```

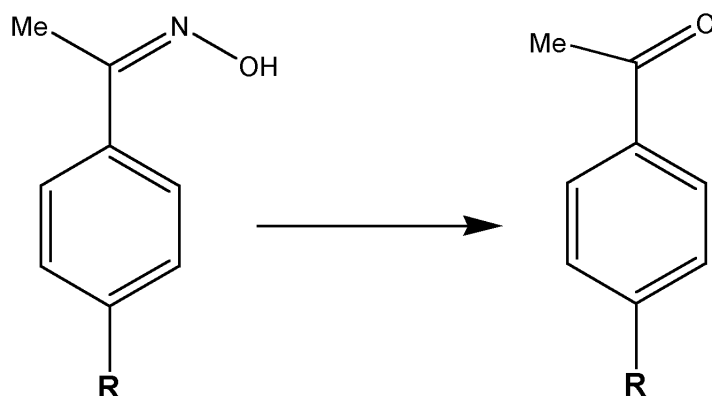
2. Permanently change the default to the new format.

```
=> SET DFORMAT PERM .MYRXN
```

```
SET COMMAND COMPLETED
```

Skills Practice

1. Locate the requested information about the conversion of the following ketoximes to the corresponding ketones:

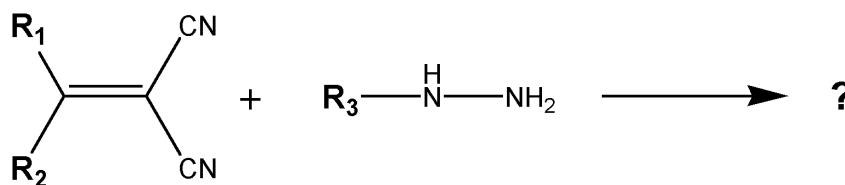


R = any non-hydrogen ring or chain substituent
Rings may have other rings fused to them
Any substitution at all open sites

- A. Build the query.
- B. Test it with a SAMPLE search.
Will the search run within system limits in the FULL database?
- C. Run the search in the FULL database.
How many documents were retrieved?
How many total hit reactions were in the documents?
- D. Display the Title (TI) and CRDREF information for all of the answers.
How many different methods were reported for carrying out the conversion?

Skills Practice

2. What types of products have been formed from the reaction of the following two starting materials?



R₁ and R₂ may be any atom *including* hydrogen.
R₃ may be any atom *except* hydrogen.

Precision Tools for Reaction Searching

When many reactions of the same type are reported in a paper, generally only synthetically useful or structurally representative reactions are included in CASREACT. To maximize the retrieval of papers that may contain transformations of interest, do the following:

1. Draw the initial reaction query as broadly as possible.
2. Apply precision tools to refine results.

Search Question: *Locate methods for converting the primary amine to a nitro group in the following types of compounds:*



R = *any type of carbocyclic ring system, e.g., benzene, cyclopentane, etc.*

Any other substitution in addition to that shown in the structure is allowed

Test the Broad Query

=> FILE CASREACT

=>

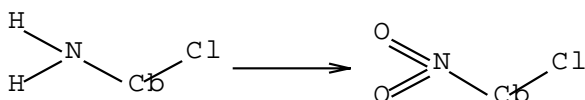
Uploading rx2.str

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



=> S L1 SSS SAM

SAMPLE SEARCH INITIATED 15:20:23 FILE 'CASREACT'
SCREENING COMPLETE - 1413 REACTIONS TO VERIFY FROM 330 DOCUMENTS
100.0% DONE 1413 VERIFIED 45 HIT RXNS 16 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 26010 TO 30510
PROJECTED ANSWERS: 81 TO 559

L2 16 SEA SSS SAM L1 (45 REACTIONS)

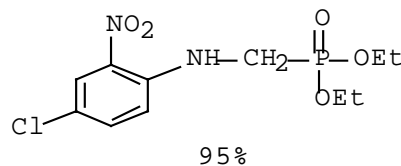
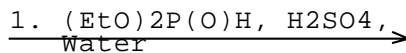
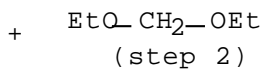
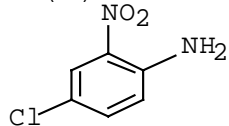
Evaluate answers with D SCAN:

=> D SCAN

L2 16 ANSWERS CASREACT COPYRIGHT 2000 ACS

TI Preparation of benzimidazole phosphono-amino acids useful as NMDA Antagonists

RX(2) OF 3

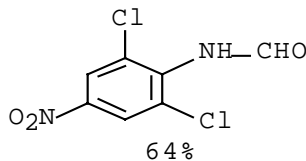
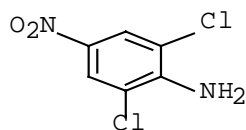


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 16 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Radioiodinated p-iodoclonidine. A high-affinity probe for the .alpha.2-adrenergic receptor

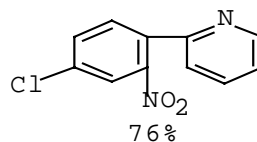
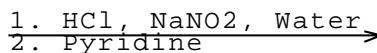
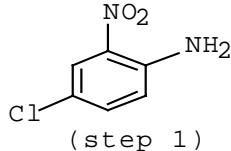
RX(12) OF 50



L2 16 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Synthesis of the new pyrido[1,2-c]benzo-v-triazinium system via valence bond isomerization

RX(9) OF 22



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN?:0



=>

Worksheet

Directions: Look at the reactions retrieved in the SAMPLE search. How many of those reactions are the transformation of interest?

Add Precision to Reaction Results

Two tools are available for improving the precision of reaction structure queries.

Use this tool	When you need to specify that
Atom mapping 	An atom in the reactant is the same atom in the product
Reaction site 	A bond is completely changed, partially changed, or unchanged in the reaction

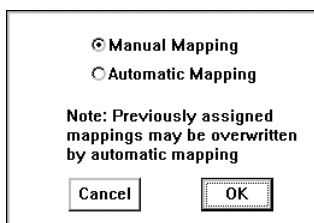
Atom Mapping

To map atoms in a reaction query:

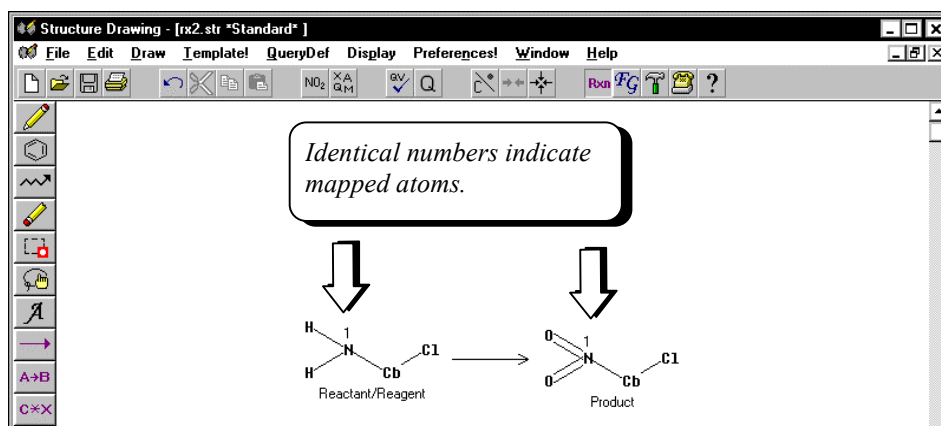
1. Click on the *Atom mapping tool*



2. A list of options appears. Select **Manual Mapping**. Click **OK**.



3. Click on an atom in the reactant and the corresponding atom in the product.




note

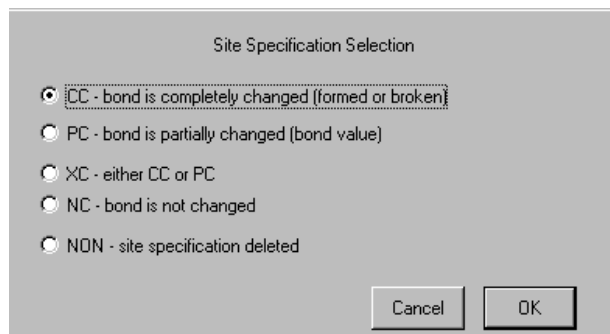
Mapping may NOT be used with

- Shortcut symbols
- Variable groups
- G-groups
- Different elements, e.g. you cannot map C to N

Reaction Sites

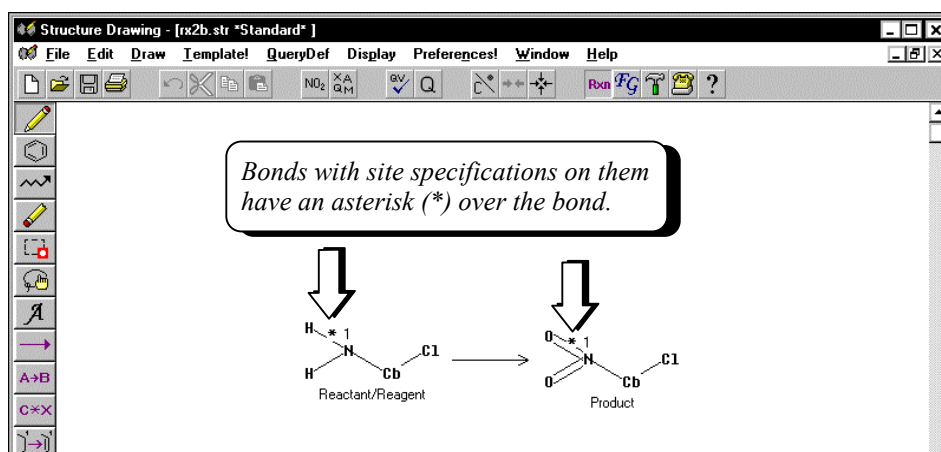
To specify a reaction site in a reaction query:

1. Click on the *Reaction site tool* .
2. Click on a bond in the query that you want to specify as a reaction site.
3. A list of options appears. Select the desired option. Click **OK**.



4. Repeat Steps 2 and 3 for other bonds in the structure.
5. Save the modified query.

For the search query in this example, **one** H–N and **one** O=N bond is specified as XC.



Helpful HINT

Over-specification of bond sites and atom mapping may cause the loss of relevant atoms. Specify only the minimum requirements needed to eliminate non-relevant answers.

Test the Modified Query

Determine the impact of the change you made with another SAMPLE search.

```
=>
Uploading rx2b.str

L3      STRUCTURE UPLOADED

=> S L3 SSS SAM

SAMPLE SEARCH INITIATED 15:22:14 FILE 'CASREACT'
SCREENING COMPLETE - 1413 REACTIONS TO VERIFY FROM 330 DOCUMENTS
100.0% DONE 1413 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 26010 TO 30510
PROJECTED ANSWERS:      1 TO 79
```

A SAMPLE search searches the same portion of the database each time, so you can easily see the impact of the changes you made.

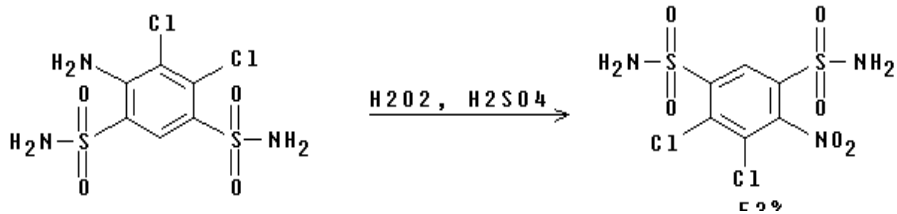
```
L4      1 SEA SSS SAM L3(1 REACTIONS)
```

```
=> D SCAN
```

```
L4      1 ANSWERS CASREACT COPYRIGHT 2003 ACS
```

```
TI      The synthesis of some substituted m-benzenedisulfonamides
```

```
RX(1) OF 2
```



```
ALL ANSWERS HAVE BEEN SCANNED
```

Run the FULL Search

=> S L3 SSS FULL

FULL SEARCH INITIATED 15:41:00 FILE 'CASREACT'
SCREENING COMPLETE - 28981 REACTIONS TO VERIFY FROM 6743 DOCUMENTS

100.0% DONE 28981 VERIFIED 41 HIT RXNS 23 DOCS
SEARCH TIME: 00.00.03

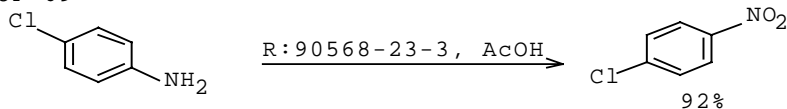
L5 23 SEA SSS FUL L3 (41 REACTIONS)

=> D SCAN

L5 23 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Functional group oxidation using sodium perborate

RX(7) OF 69

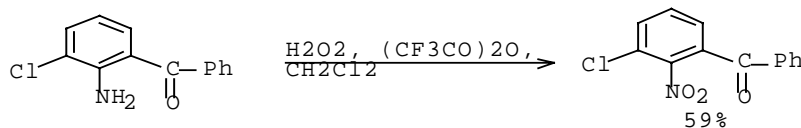


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L5 23 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Antiinflammatory agents. 4. Syntheses and biological evaluation of potential pro-drugs of 2-amino-3-benzoylbenzeneacetic acid and 2-amino-3-(4-chlorobenzoyl)benzeneacetic acid

RX(22) OF 83



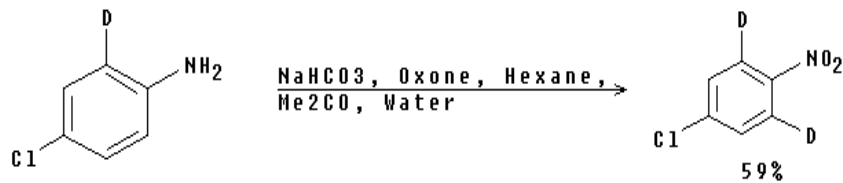
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Default display:

=> D L5 1-3

L5 ANSWER 1 OF 23 CASREACT COPYRIGHT 2003 ACS

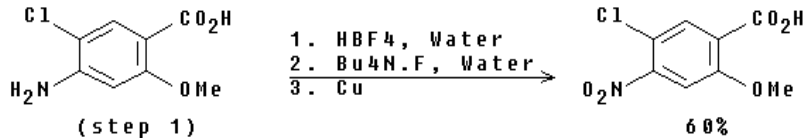
RX(4) OF 48



REF: Tetrahedron, 57(22), 4753-4757; 2001

L5 ANSWER 2 OF 23 CASREACT COPYRIGHT 2003 ACS

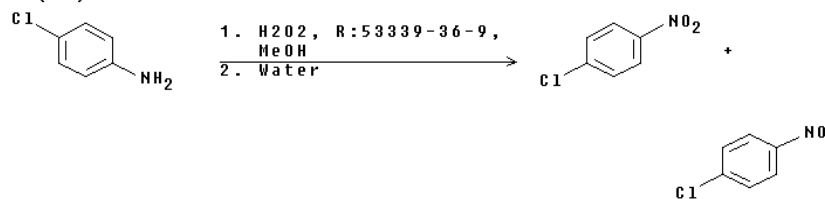
RX(1) OF 66



REF: Span., 2138902, 16 Jan 2000

L5 ANSWER 3 OF 23 CASREACT COPYRIGHT 2003 ACS

RX(10) OF 16



REF: Angewandte Chemie, International Edition, 40(2), 405-408; 2001
NOTE: 100% conversion

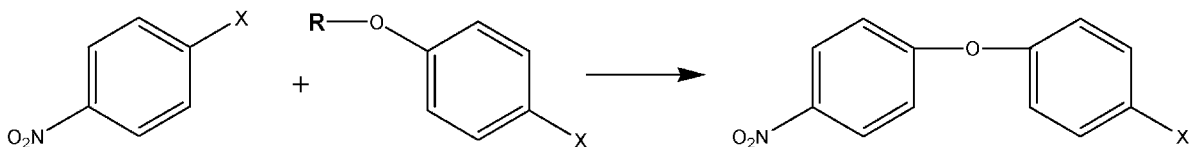
The default format displays the first hit reactions and its associated reference.

Reaction Queries with Multiple Reactants

Many types of reaction structure queries may be searched in CASREACT:

$A + B \Rightarrow C$	(two reactants leading to a product)
$A + B \Rightarrow ?$	(two reactants going to any product)
$A \Rightarrow ?$	(reactant going to any product)
$? \Rightarrow B$	(any reactant going to a specific product)

Search Question: *Locate methods for converting the two starting materials shown below to the specified ether.*



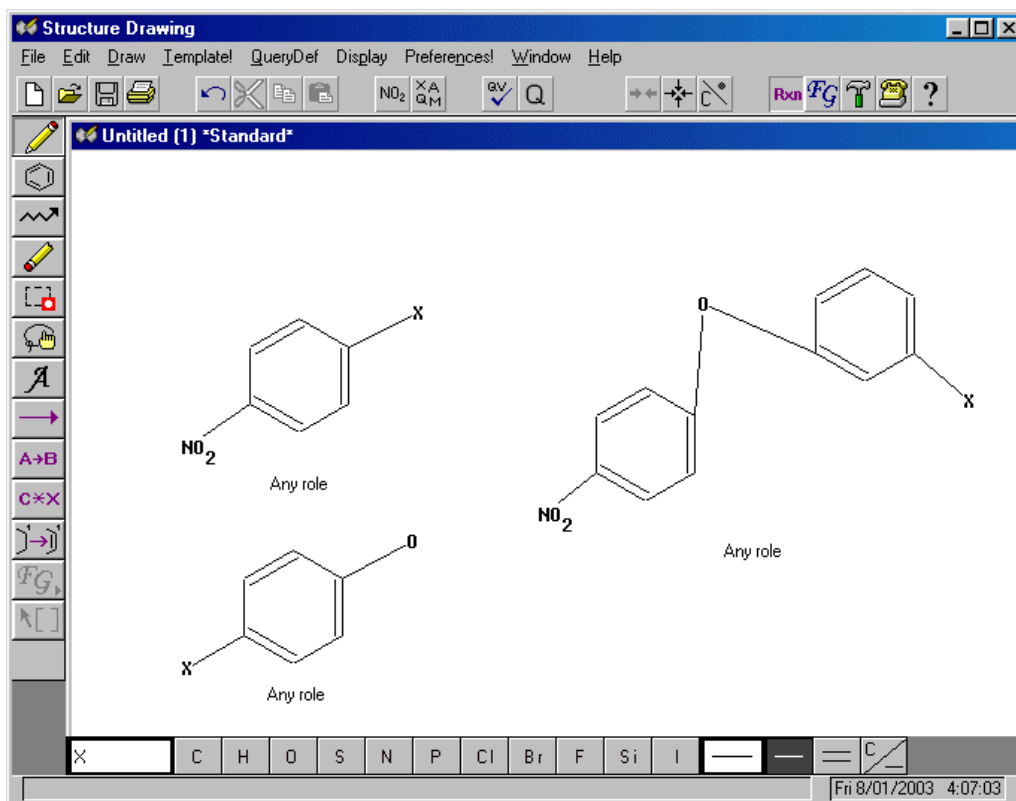
R = anything, including hydrogen
Benzene rings may have other rings fused onto them
Any substitution at all open sites

Search Strategy

For reactions with multiple reactants


- Step 1** Draw all reaction participants on the same structure drawing screen.
- Step 2** Specify reaction roles.
- Step 3** Specify precision.
- Step 4** Run the search.

Draw Reaction Participants



Specify Reaction Roles

To specify the reaction role for the structure fragment(s):

1. Click on the **Reaction role tool** .
2. Click an atom in the structure for which you want to specify a role.

A menu of roles displays. Select the desired role. Click **OK**.

The dialog box is titled 'Role Specification Selection'. It contains five radio button options: 'Reactant', 'Reagent', 'Product', 'Reactant/Reagent', and 'Any role (no role assigned)'. The 'Reactant/Reagent' option is selected. At the bottom of the dialog are 'Cancel' and 'OK' buttons.

Specify Precision

Specify the following bonds as completely changed:

- from the benzene ring to X in one reactant
- from nitrobenzene ring to O in the product

Run the Search

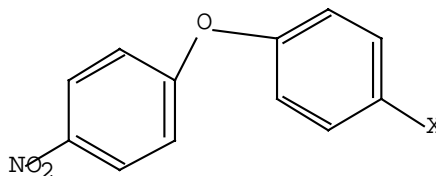
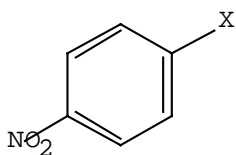
```
=>
Uploading rx3.str
```

```
L1      STRUCTURE UPLOADED
```

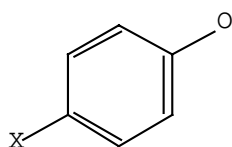
```
=> D L1
```

```
L1 HAS NO ANSWERS
```

```
L1      STR
```



Reaction roles do not display with the structures on STN.



```
=> S L1 SSS SAM
```

```
SAMPLE SEARCH INITIATED 16:20:47 FILE 'CASREACT'
SCREENING COMPLETE -      97 REACTIONS TO VERIFY FROM      15 DOCUMENTS
100.0% DONE      97 VERIFIED      4 HIT RXNS      2 DOCS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
```

```
                        BATCH   **COMPLETE**
```

```
PROJECTED VERIFICATIONS:      1350 TO      2530
```

```
PROJECTED ANSWERS:           2 TO      124
```

```
L2      2 SEA SSS SAM L1 (4 REACTIONS)
```

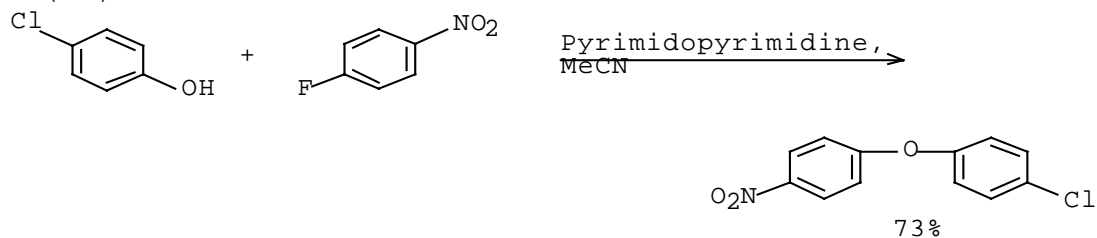
Evaluate answers with D SCAN:

=> D SCAN

L2 2 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Polymer-supported bases in combinatorial chemistry: synthesis of aryl ethers from phenols and alkyl halides and aryl halides

RX(14) OF 15



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN?: 0

Run the FULL Search:

=> S L1 SSS FULL

FULL SEARCH INITIATED 15:45:42 FILE 'CASREACT'
SCREENING COMPLETE - 1277 REACTIONS TO VERIFY FROM 333 DOCUMENTS

100.0% DONE 1277 VERIFIED 63 HIT RXNS 39 DOCS
SEARCH TIME: 00.00.01

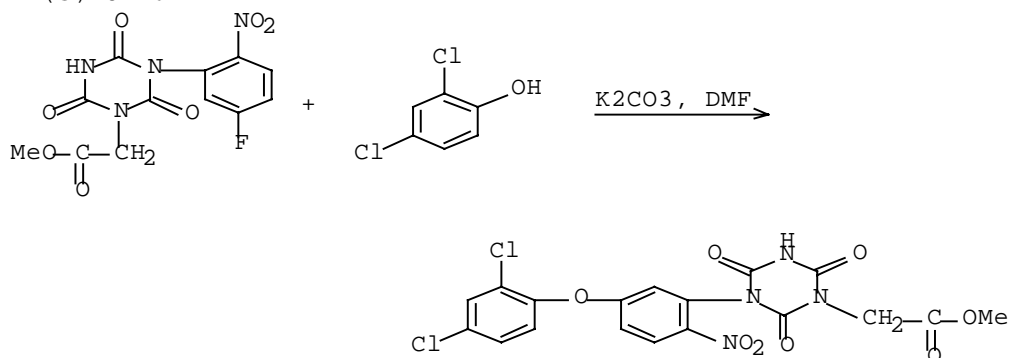
L3 39 SEA SSS FUL L1 (63 REACTIONS)

=> D SCAN

L3 39 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI 3-(3-Aryloxyphenyl)-1-(substituted methyl)-s-triazine-2,4,6-trione
or -thiotrione herbicidal agents

RX(3) OF 6

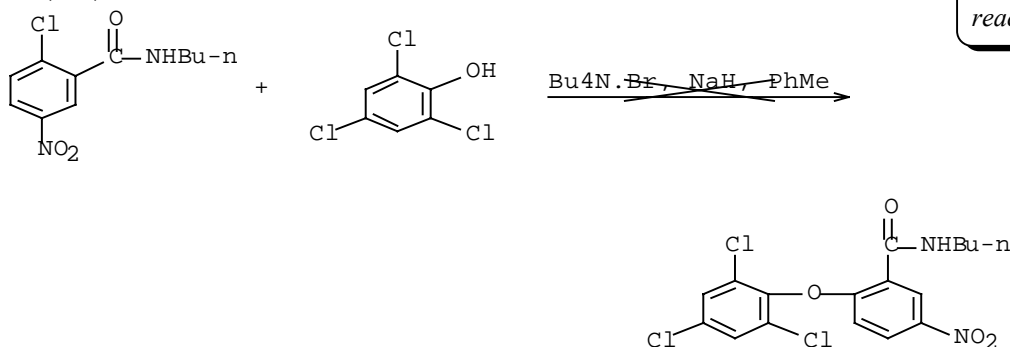


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 39 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Synthesis of 2-alkoxy-5-nitrobenzamides by phase-transfer catalyzed
nucleophilic substitution of 2-chloro-5-nitrobenzamides

RX(19) OF 19



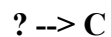
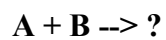
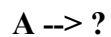
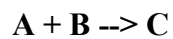
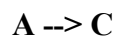
Note how "failed
reactions" display.

NOTE: FAILED REACTION





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

Summary

Reaction queries may be of the following types:

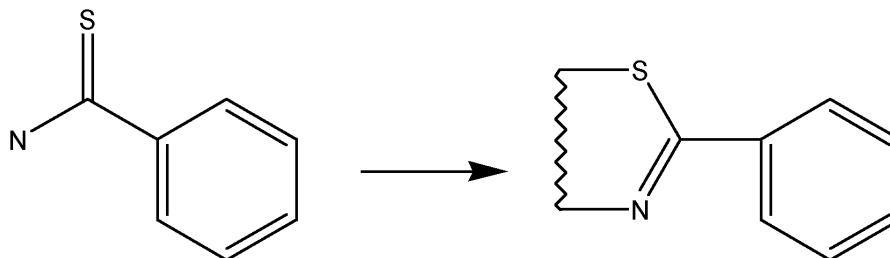


Precision tools are available to focus on the desired types of reactions.

To assign a	Use the
Reaction direction	Reaction Arrow Tool 
Fragment role	Reaction Role Tool 
Bond that is changed/unchanged in the reaction	Reaction Site Tool 
Mapping between an atom in the reactant and product	Atom Mapping Tool 

Skills Practice

Locate methods for carrying out the following ring-forming reaction:



Additional substitution is allowed at all open sites
Additional ring fusion is allowed
The $\text{C}\sim\text{C}$ bond can be single, double, or triple

FUNCTIONAL GROUP SEARCHING

In this section, you will learn to

- Search for broadly defined transformations using functional groups
- Specify non-reacting functional groups

Why Use Functional Group Queries?

While structure queries could be created to search for broadly defined reactions, this approach may

- Not run to completion within system limits
- Take a long time to complete

Consider using functional group queries when you

- Want an overview of current methods being used to carry out a broadly defined transformation
- Are not retrieving answers with a precisely defined structure query
- Are looking for a broadly defined transformation in the presence of a non-reacting functional group

Functional group terms are assigned to approximately 200 different structural groups in CASREACT. Groups are identified as

- Reacting functionalities
- Formed functionalities
- Non-reacting functionalities

Functional groups are divided into terms for

- Rings
- Functionalities

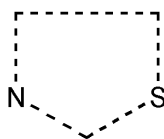
Ring Terms

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	

Ring terms describe 5- and 6-membered rings with any type of bonding.

For example:

The term **1,3-C3NS** describes this type of ring



where the N and S are in the 1 and 3 positions and other rings may be fused to the structure.

Functionality Terms

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

Reaction Searching Using Functional Group Terms

Search Question: *Locate methods for converting a nitroso group to a primary amine.*

Search Strategy

- Step 1** Build and save the functional group reaction query.
- Step 2** Logon to STN and enter CASREACT.
- Step 3** Upload the reaction query.
- Step 4** Run the reaction search.
- Step 5** Display the results.

Build the Functional Group Query

Functional group queries are created in the structure drawing window.

Building a functional group query is accomplished in three steps:

- A. Select the functional groups for the query
- B. Assign reaction roles to functional groups
- C. Save the query

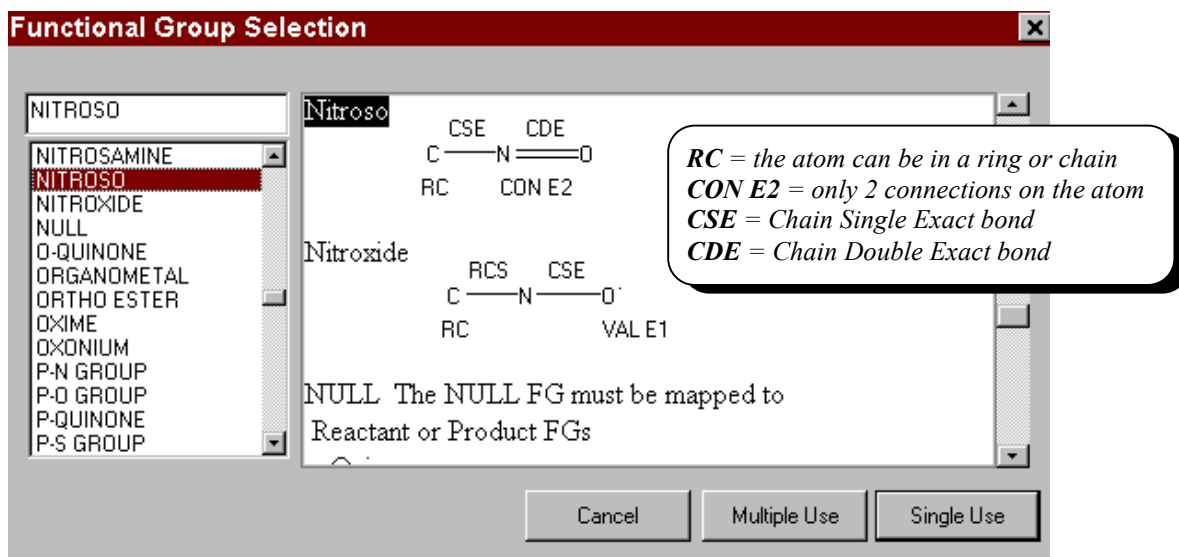
A. Select the functional groups for the query

1. Click on the *Functional Group* icon .

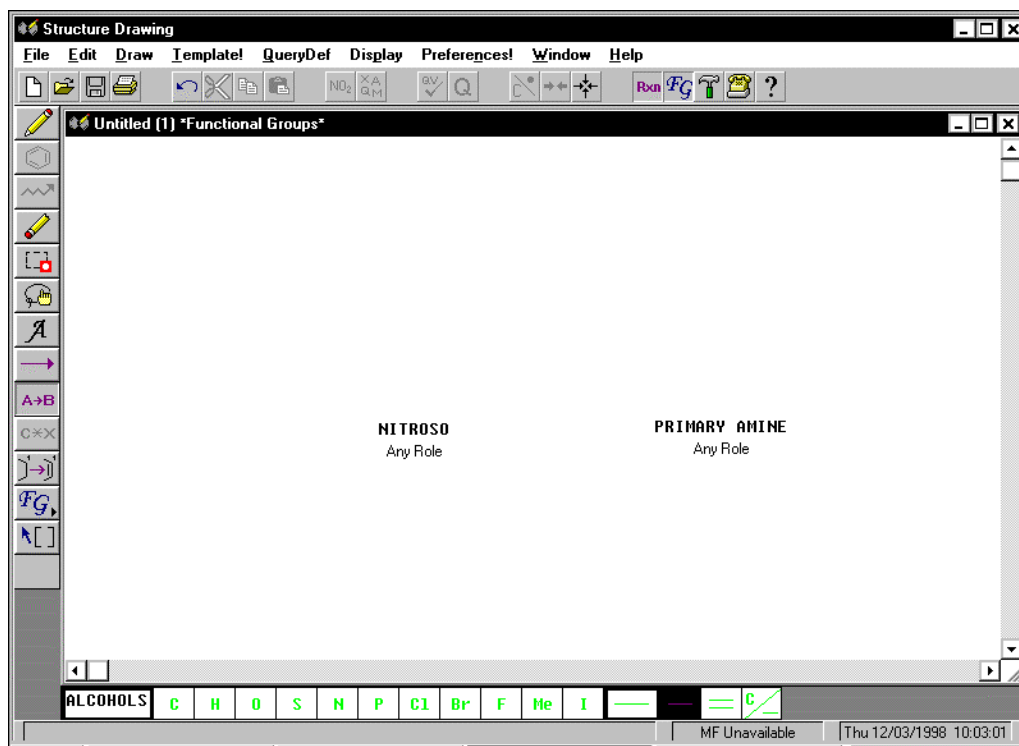
In "functional group mode" the current atom box changes to functional group terms and all structure drawing tools are inactive.




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

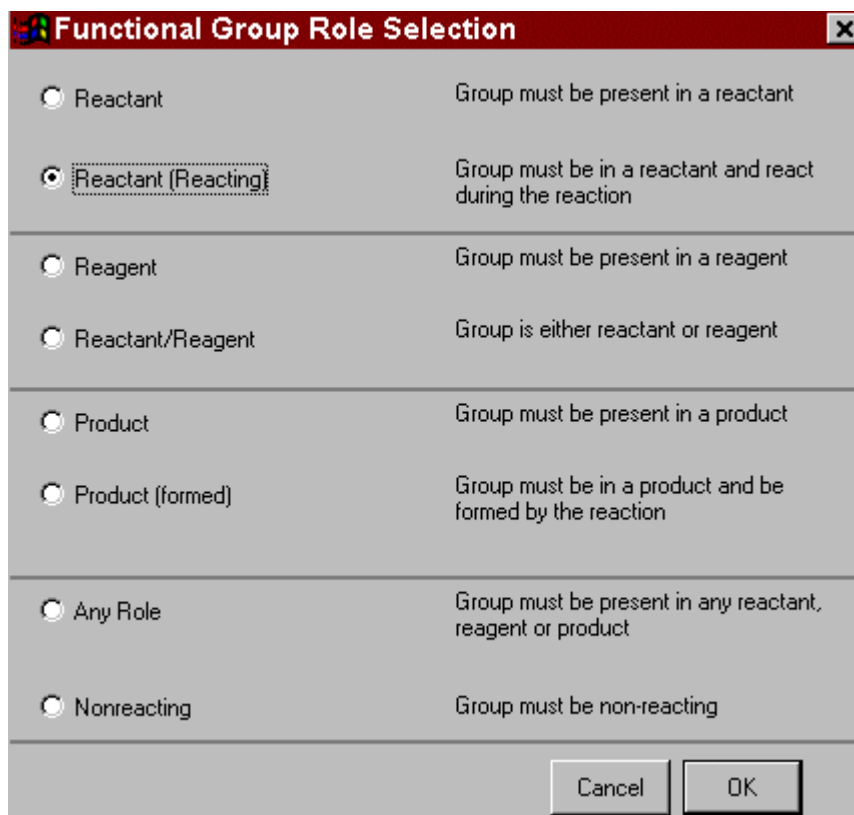


- Click on the name of the desired functional group and select **Single Use** or **Multiple Use**. Click at the position on the structure drawing screen where you want to position the functional group.
- Repeat Step 3 for each functional group in the query.



B. Assign reaction roles to functional groups

1. Click on the *Reaction Role tool* .
2. Click on the functional group to which you want to assign a role. A box with all of the functional group roles appears.



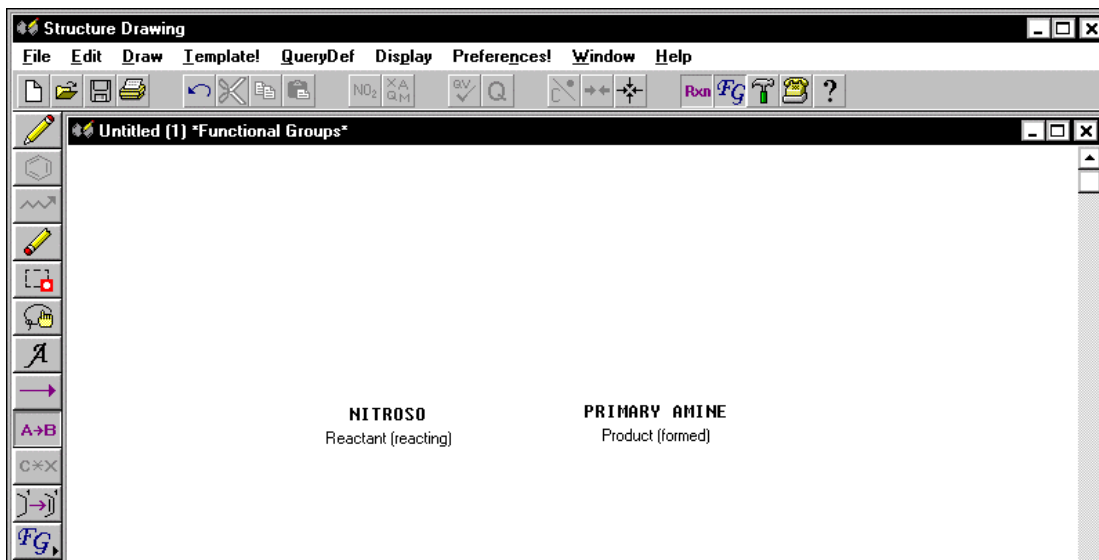
Role	Description
<input type="radio"/> Reactant	Group must be present in a reactant
<input checked="" type="radio"/> Reactant (Reacting)	Group must be in a reactant and react during the reaction
<input type="radio"/> Reagent	Group must be present in a reagent
<input type="radio"/> Reactant/Reagent	Group is either reactant or reagent
<input type="radio"/> Product	Group must be present in a product
<input type="radio"/> Product (formed)	Group must be in a product and be formed by the reaction
<input type="radio"/> Any Role	Group must be present in any reactant, reagent or product
<input type="radio"/> Nonreacting	Group must be non-reacting


Cancel OK

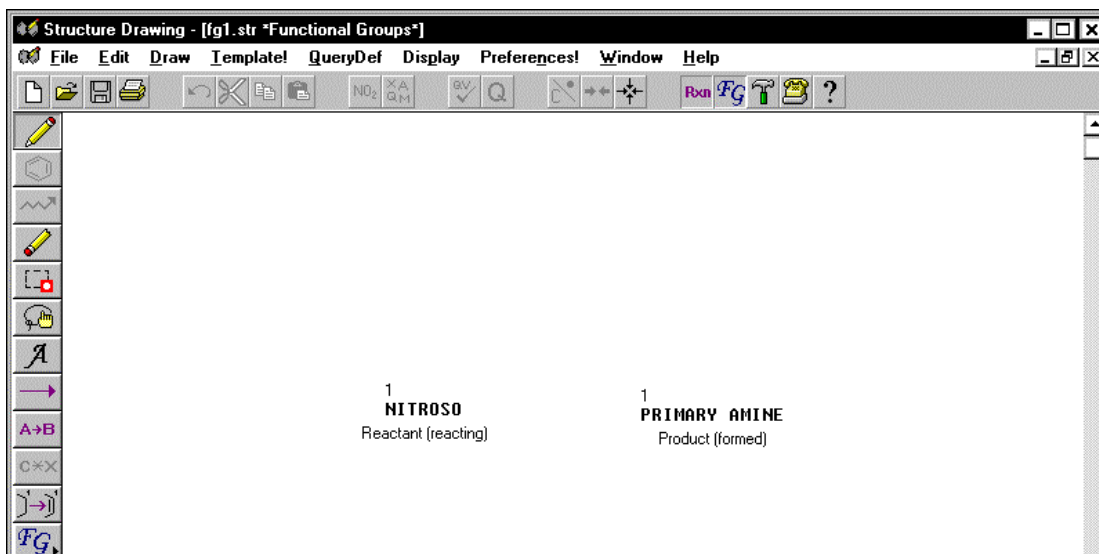
Select the role that applies to the functional group. Click **OK**.

3. Click on the next functional group and repeat Step 2 for it.

Role assignments appear on the screen.



4. Use the *Atom mapping* tool  to guarantee that at least one atom from the reacting group appears in the formed group.



Helpful HINT

If atom mapping is not used, the search will retrieve more answers, but the conversion of the reacting functional group into the formed functional group is not guaranteed.

C. Save the query

Save the functional group query using the same procedure used to save a structure query.

Run the Functional Group Search

Upload the query:

```
=> FILE CASREACT  
  
=> QUE (NITROSO/FG.RXN (S) PRIMARY AMINE/FG.FORM)  
  
L1   QUE (NITROSO/FG.RXN (S) PRIMARY AMINE/FG.FORM)
```

The uploaded "text" query is assigned an L-number.

The functional group query is converted to a 'text' query when you save it. The 'text' query includes

- Search fields to indicate
 - ◆ Reacting functional groups (/FG.RXN)
 - ◆ Formed functional groups (/FG.FORM)
- The (S) operator which maps one atom from the reacting group to an atom in the product group

Helpful HINT

For a functional group query, as with any other text query, you *cannot* specify a search type (SSS/CSS) or a search scope (SAM/FULL).

Run the search:

```
=> S L1  
  
      1396 NITROSO/FG.RXN  
      28186 PRIMARY AMINE/FG.FORM  
L2     188 (NITROSO/FG.RXN (S) PRIMARY AMINE/FG.FORM)
```

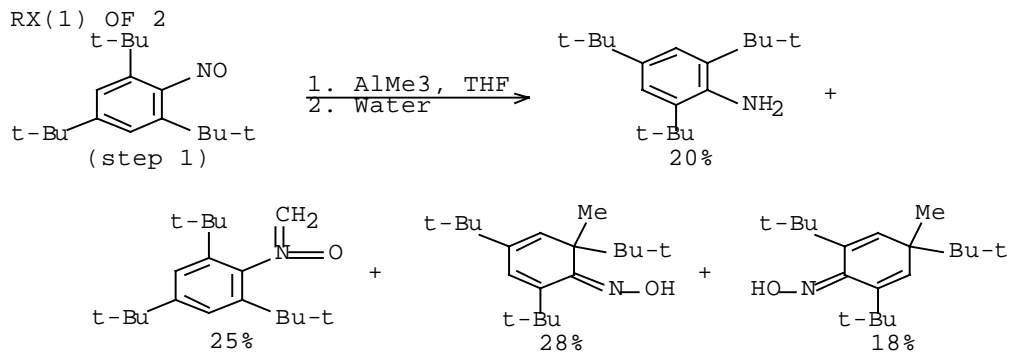
Each answer to a functional group search is a document record containing one or more reactions that match the specified transformation.

Display the results:

=> D SCAN

L2 188 ANSWERS CASREACT COPYRIGHT 2003 ACS

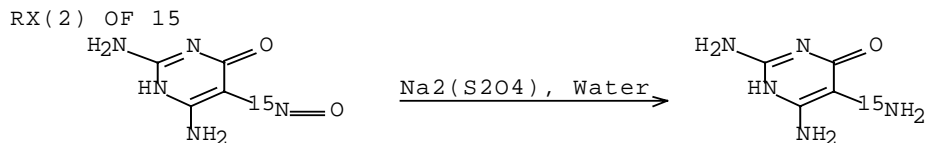
TI Reactions of trimethyl- and triethylaluminum with 2,4,6-tri-tert-butyl-
nitrosobenzene



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

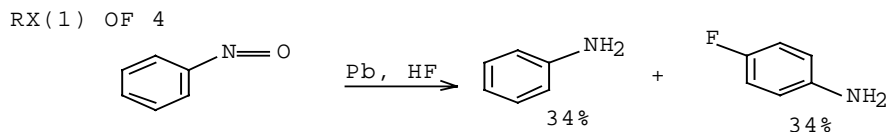
L2 188 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI [7-15N]guanosine-labeled oligonucleotides as a nuclear magnetic
resonance probe for protein-nucleic acid interaction in the major
groove



L2 188 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Process for the reductive halogenation of aromatic nitro or nitroso
compounds to haloaromatic amines

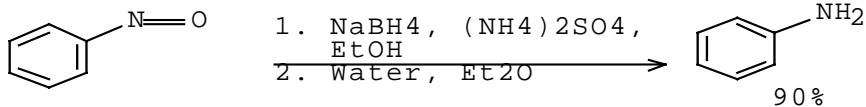


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Search Question: Find out more about this D SCAN hit:

TI A new and efficient method for the selective reduction of nitroarenes: use of ammonium sulfate-sodium borohydride

RX(11) OF 13



Search Strategy

To display a D SCAN answer in more detail

- Step 1** Select a unique word from the title.
- Step 2** Search the answer L-number AND *word*/TI.
- Step 3** Display the resulting answer in more detail.

Example:

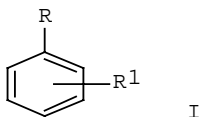
=> S L2 AND NITROARENES/TI

Search the answer L-number and a unique word from the title.

123 NITROARENES/TI
L3 1 L1 AND NITROARENES/TI

=> D L3 1 BIB ABS

L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2003 ACS
AN 123:338641 CASREACT
TI A new and efficient method for the selective reduction of
nitroarenes: use of ammonium sulfate-sodium borohydride
AU Gohain, Sujata; Prajapati, Dipak; Sandhu, Jagir S.
CS Reg. Res. Lab., Assam, 785 006, India
SO Chem. Lett. (1995), (8), 725-6
CODEN: CMLTAG; ISSN: 0366-7022
DT Journal
LA English
GI

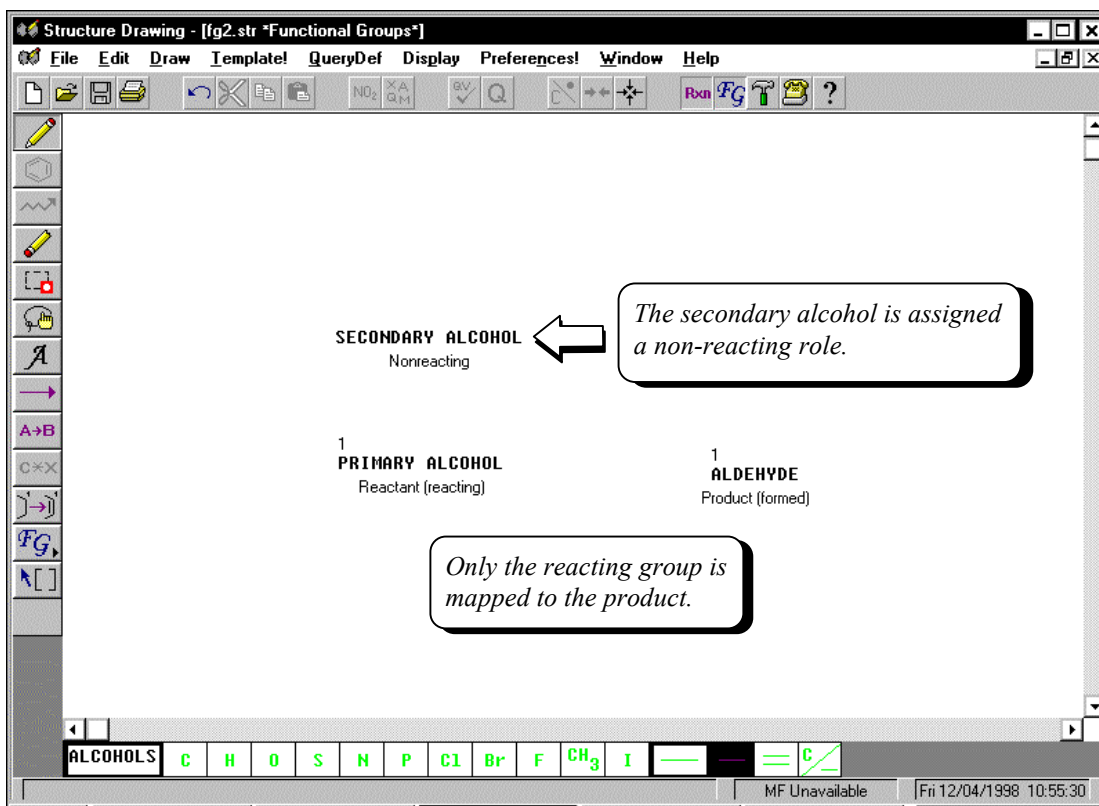


AB Nitroarenes I (R = NO₂; R₁ = e.g., 4-Cl, 2-, 4-CO₂H, 4-Ac, 4-cyano, 3-vinyl) were selectively and rapidly reduced to 75-90% corresponding amino compds. I (R = NH₂) using (NH₄)₂SO₄-NaBH₄. This method is typically complete in 30 min and shows no byproducts usually seen using other methods.

Specifying a Non-reacting Functional Group

Search Question: Locate methods for converting a primary alcohol to an aldehyde in the presence of a non-reacting secondary alcohol.

Build the Functional Group Query:



Upload and search the query in CASREACT:

```
=> FILE CASREACT
```

```
=> QUE SECONDARY ALCOHOL/FG.NON (L) (PRIMARY ALCOHOL/FG.RXN (S)  
ALDEHYDE/FG.FORM)
```

```
L1  QUE SECONDARY ALCOHOL/FG.NON (L) (PRIMARY ALCOHOL/FG.RXN (S)  
ALDEHYDE/FG.FORM)
```

```
=> S L1
```

```
32742 SECONDARY ALCOHOL/FG.NON
```

```
69845 PRIMARY ALCOHOL/FG.RXN
```

```
27167 ALDEHYDE/FG.FORM
```

```
L2  331 SECONDARY ALCOHOL/FG.NON (L) (PRIMARY ALCOHOL/FG.RXN (S)  
ALDEHYDE/FG.FORM)
```

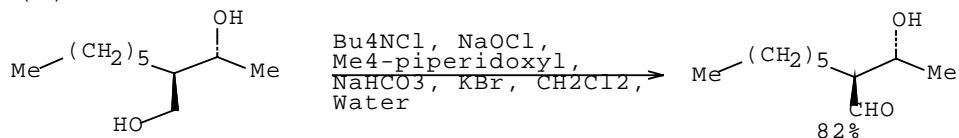
Display the results:

=> D SCAN

L2 331 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Selective oxidation of primary hydroxy groups in primary-secondary diols

RX(1) OF 1

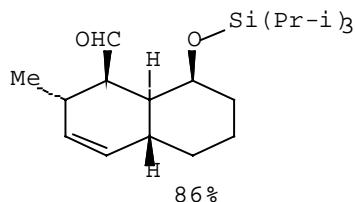
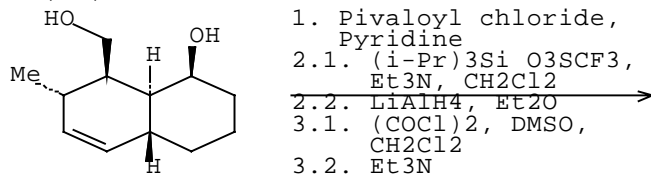


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 331 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Total synthesis of (+)-compactin by a double Michael protocol

RX(78) OF 409 - 3 STEPS



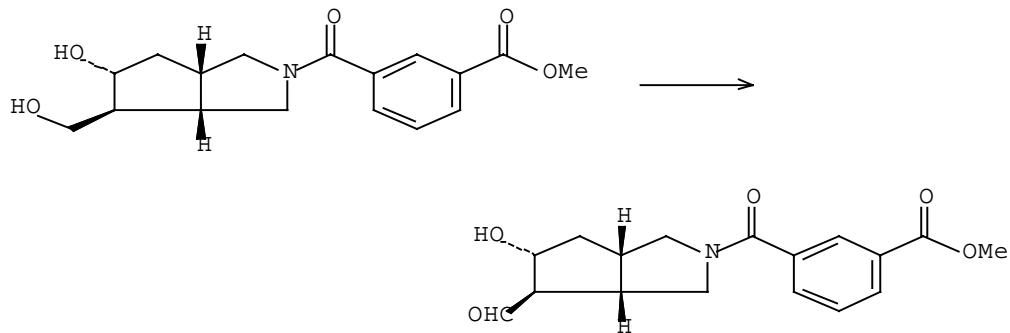
NOTE: 2) (99%/99%)

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

L2 331 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Prostanoid and related compounds. Part II. Synthesis of biologically active 6-azaprostacyclin derivatives

RX(6) OF 69



NOTE: Pfitzner-Moffatt reagent

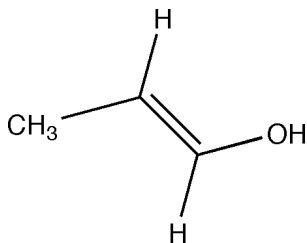
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Functional Group Classes

When a reaction is entered into the CASREACT database, the most *precise* functional group term that applies to a structure group is assigned. *Broader* functional group terms are *not* also assigned.

Example:

For this structure:



The functional group term ENOL is assigned, but the terms PRIMARY ALCOHOL and ACYCLIC ALKENE are not.

Use **class terms**, which encompass specific functional group terms for that class, to search for *all* specific functionalities in a broader functional group.

Class Terms	
Alcohols	Carboxy derivatives
Alkenes	Halides
Alkynes	Heterocycles
Amines	Ketones
Carbonate derivatives	Organometallics

Specific Functionalities in Class Term Categories

ALCOHOLS	ALLYL ALCOHOL CYANOHYDRIN CYCLIC ALCOHOL ENOL GLYCOL HALOHYDRIN	HEMIACETAL HYDROXYLAMINE PHENOL PRIMARY ALCOHOL SECONDARY ALCOHOL TERTIARY ALCOHOL
ALKENES	ACYCLIC ALKENE CYCLIC ALKENE	
ALKYNES	ALKYNE ENYNE PI-ALKYNE	
AMINES	AMINE OXIDE AZIRIDINE CHLORAMINE CYANAMIDE ENAMINE	HYDROXYLAMINE IMINE PRIMARY AMINE SECONDARY AMINE TERTIARY AMINE
CARBONATE DERIVATIVES	CARBAMATE CARBONATE GUANIDINE	HALOFORMATE THIOUREA UREA
CARBOXY DERIVATIVES	ACID HALIDE AMIDE AMIDINE ANHYDRIDE CARBOXYLATE CARBOXYLIC HALOFORMATE	IMIDE LACTAM LACTONE PEROXY ACID PEROXY ESTER THIOAMIDE THIOCARBOXY
HALIDES	ACID HALIDE ALKYL HALIDE ALLYL HALIDE ARYL HALIDE CHLORAMINE GEM-DIHALIDE HALOFORMATE	METAL HALIDE SULFENYL HALIDE SULFINYL HALIDE SULFONYL HALIDE TRIHALIDE VIC-DIHALIDE VINYL HALIDE

(continued on next page)

HETEROCYCLES

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

KETONES

ACYCLIC KETONE
CYCLIC KETONE
O-QUINONE
P-QUINONE

ORGANOMETALLICS

ACYLMETAL	METAL NITROSYL
METAL ARENE	METAL PHOSPHINE
METAL CARBENE	METAL SULFUR
METAL CARBONYL	METALLOCARBOCYCLE
METAL CYCLOPENTADIENYL	MU-CARBONYL
METAL HALIDE	ORGANOMETAL
METAL HYDRIDE	PI-ALKENE
METAL METAL BOND	PI-ALKYNE
METAL NITROGEN	PI-ALLYL


Combining Functional Group Terms with OR Logic

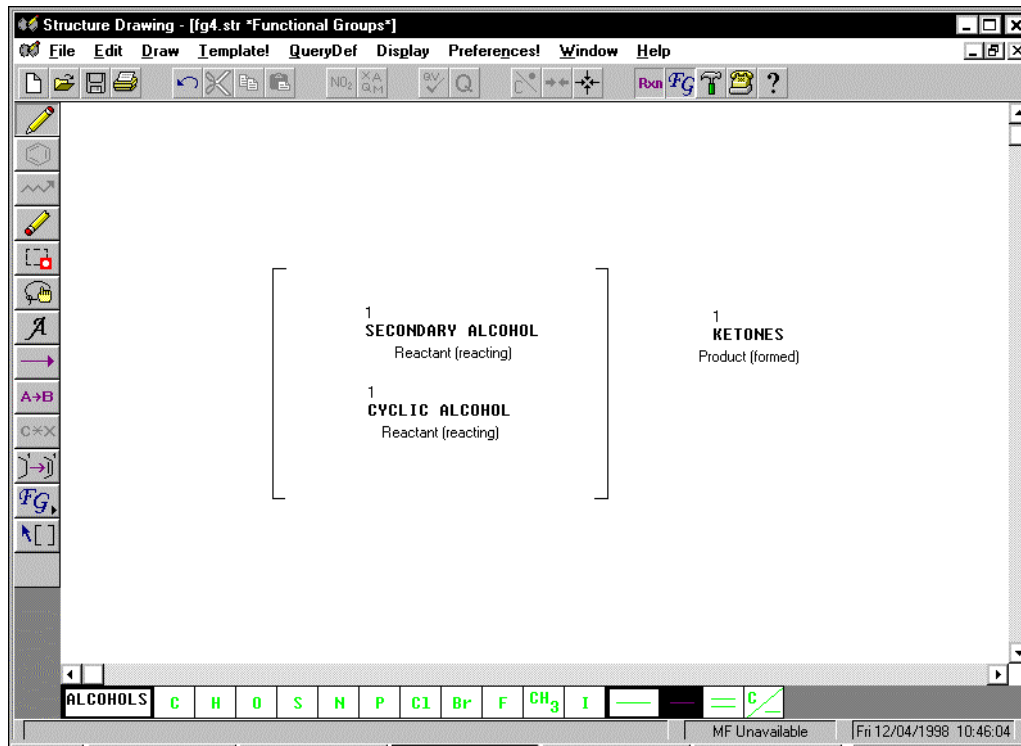
Search Question: Locate methods for converting secondary alcohols or cyclic alcohols to ketones.

To search all relevant functional group terms in one of step, combine the terms using the OR feature.

After

- ◆ Selecting the functional groups
- ◆ Assigning the roles
- ◆ Mapping reactants to the product

Click on the **OR operator** button  and draw a box around the terms to be ORed.



Run the search:

=> FILE CASREACT

=> QUE KETONES/FG.PRO (S) (SECONDARY ALCOHOL/FG.RXN OR CYCLIC ALCOHOL/FG.RXN)

L1 QUE KETONES/FG.PRO (S) (SECONDARY ALCOHOL/FG.RXN OR CYCLIC ALCOHOL/FG.RXN)

=> S L1

62412 KETONES/FG.PRO
51603 SECONDARY ALCOHOL/FG.RXN
4180 CYCLIC ALCOHOL/FG.RXN

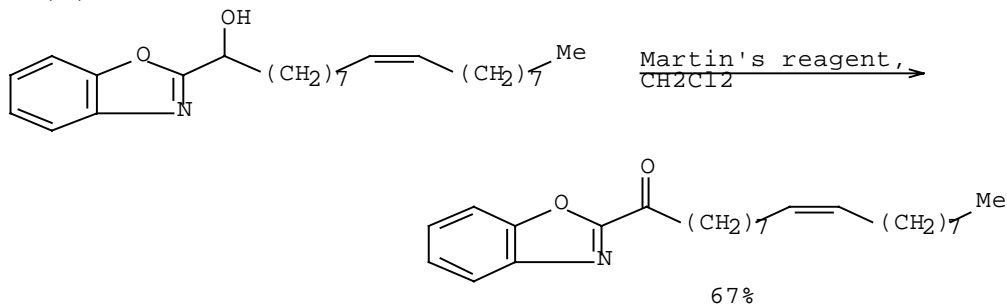
L2 10868 KETONES/FG.PRO (S) (SECONDARY ALCOHOL/FG.RXN OR CYCLIC ALCOHOL/FG.RXN)

=> D SCAN

L2 10868 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Exceptionally potent inhibitors of fatty acid amide hydrolase: the enzyme responsible for degradation of endogenous oleamide and anandamide

RX(4) OF 57



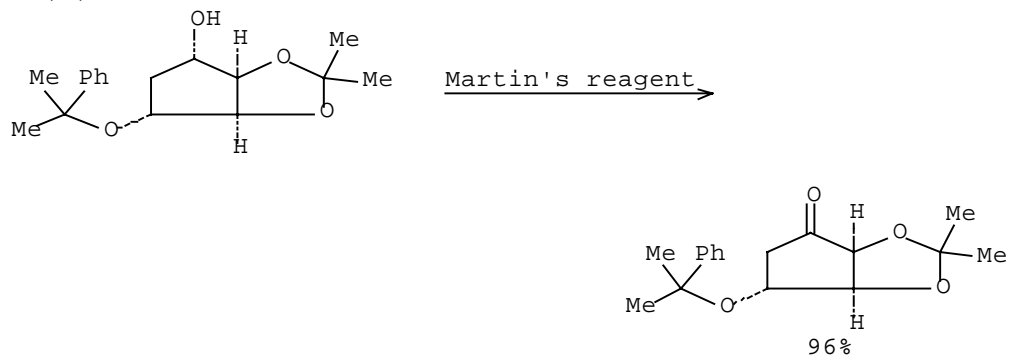
NOTE: STEREOSELECTIVE

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

(continued on next page)

L2 10868 ANSWERS CASREACT COPYRIGHT 2003 ACS
TI An enantiodivergent route to .alpha.-cuparenone utilizing chiral
cyclopentenol having a latent meso structure

RX(5) OF 113



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

Summary

- Functional group terms can be used to search for broadly defined transformations

- Functional groups terms are available for
 - ◆ Reactants
 - ◆ Reagents
 - ◆ Products

- Functional groups are identified as
 - ◆ **Reacting** functionalities
 - ◆ **Formed** functionalities
 - ◆ **Non-reacting** functionalities

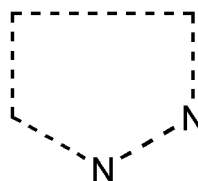
- Functional group queries are easily created in the structure drawing window of STN Express

- "Class terms" can be used to search for broad classes of functional groups

- Search relevant functional group terms in one step by combining them with the OR operator

Skills Practice

1. Locate reactions in which sulfides are converted to sulfones.
2. Locate reactions in which halides are converted to alcohols in the presence of non-reacting primary amines.
3. Locate reactions in which hydrazines are used to prepare the following type of diazoles:



REFINING RESULTS

In this section, you will learn to

- Restrict results to reactions with yields above a given value
- Restrict results to single-step reactions
- Specify that a specific catalyst, reagent, or solvent is or is not present in the reaction
- Include reaction note information in the refinement
- Refine using another reaction structure query (SUBSET searching)

Refining Reaction Results

Several reaction search fields are available for refining reaction search results.

When you want to	Use this search field
Restrict results by yield	/YD
Restrict results by number of steps	/NS
Require/eliminate a specific reaction participant using its	
■ CAS RN and	
■ Reaction role	
◆ Solvent	/SOL
◆ Catalyst	/CAT
◆ Reagent	/RGT
◆ Reactant	/RCT
◆ Reagent or Reactant	/RRT
◆ Product	/PRO
◆ Not a product	/NPRO
Specify terms from the reaction NOTE	Basic Index

Use these fields to refine the reactions in answer sets from

- Structure searches
- Functional group searches

note

Since each answer in CASREACT may contain more than one reaction, use the (L) operator to apply the refinement to the "hit" reactions in the answer set.

Yield

Yields are reported for many, but not all, reactions in CASREACT. Yields are whole number percent values, e.g., 75%. They may be searched as numeric ranges, e.g., YD>80 for yield greater than 80%.

To isolate reactions without yields, use the term NON/YDT.

Helpful HINT

Use (L) to require that one of the products in the hit reaction have the specified yield. In reactions with more than one product, the specified yield may apply to a product other than the "hit" product.

If you retrieved the reactions using a

- Structure search query
- CAS RN for the product

Then use the (A) operator to specify that the yield applies to the hit product.

Number of Steps

The number of steps in a reaction is searched as a numeric range, e.g., 1/NS for single-step reactions.

Helpful HINT

Pot reactions are considered to be single-step reactions.

Individual Reaction Participants

Reaction participants can be specified by a

- CAS RN (solvents and catalysts can *only* be specified with CAS RNs)
- Registry L-number

To specify the role the CAS RN plays in the reaction, use one of these fields:

Use this field	To specify this role
/SOL	Solvent
/CAT	Catalyst
/RGT	Reagent
/RCT	Reactant
/RRT	Reagent or Reactant
/NPRO	Not a Product
/PRO	Product

Examples:

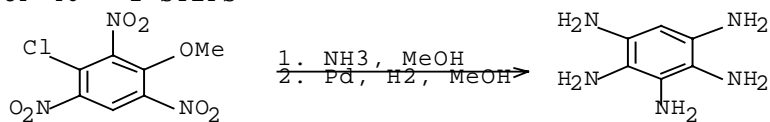
Use this strategy	If you want to
=> S L1 (L) 7440-05-3/CAT	Limit the hit reactions in L1 to those catalyzed by palladium (7440-05-3)
=> S L1 (L) ANY/CAT	Limit the hit reactions in L1 to catalytic reactions
=> S L1 (L) 64-19-7/NPRO	Limit the hit reactions in L1 to those in which acetic acid (64-19-7) is some type of starting material
=> S L1 (NOTL) 108-24-7/RRT	Eliminate the hit reactions from L1 where acetic anhydride (108-24-7) is used as a reactant or reagent

Reaction Note

The NOTE field contains additional information about the reaction that cannot be specified in the reaction diagram via a structure or CAS RN, e.g.,

Safety information:

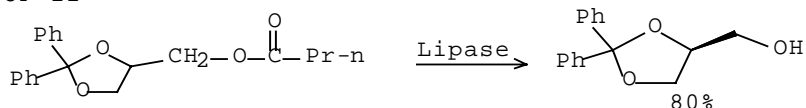
RX(17) OF 46 - 2 STEPS



NOTE: 1) explosive compd.

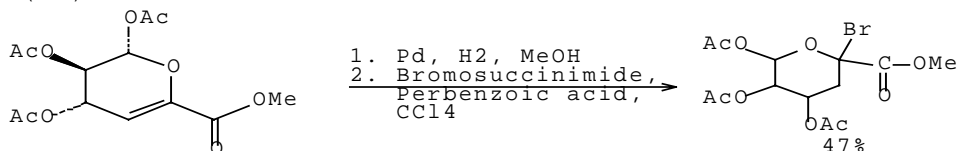
Reaction conditions:

RX(6) OF 12



NOTE: enzymic

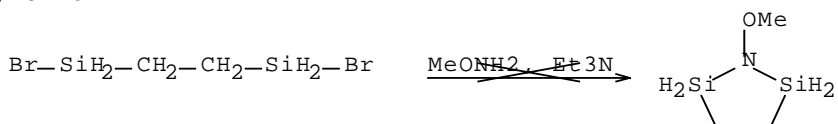
RX(17) OF 19 - 2 STEPS



NOTE: 2) photochem.

Failed reactions:

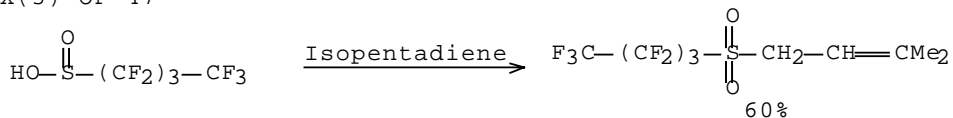
RX(3) OF 5



NOTE: Failed reaction

Participants not indexed via CAS RNs:

RX(3) OF 47



NOTE: Petroleum ether

Helpful HINT

Individual words from the NOTE are in the Basic Index and may be searched. Use truncation and synonyms for best results when searching NOTE words.

Example: => S L1 (L) PHOTOCHEM?

Search Question: *Locate reactions in which sulfides are oxidized to sulfones using sodium perborate in acetic acid with yields >75%.*

Search Strategy

To refine a reaction search with yield and other reaction participants

- Step 1** Locate the CAS RNs for the specific reaction participants.
- Step 2** Use functional group searching to locate reactions.
- Step 3** Refine the reaction search with the other reaction participant and yield requirements.
- Step 4** Display the results.

Step 1: Locate the CAS RNs

```
=> FILE REGISTRY
```

```
=> E SODIUM PERBORATE/CN 5
```

```
E1          1      SODIUM PERACETATE/CN
E2          1      SODIUM PERBENZOATE/CN
E3          2 -->  SODIUM PERBORATE/CN
E4          1      SODIUM PERBORATE (NABO3)/CN
E5          1      SODIUM PERBORATE (NABO3) TETRAHYDRATE/CN
```

```
=> S E3
```

```
L1          2 "SODIUM PERBORATE"/CN
```

You can request just 5 lines of the EXPAND list.

(continued on next page)

=> D L1 1-2 RN IN

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 11138-47-9 REGISTRY
IN Perboric acid, sodium salt (8CI, 9CI)

L1 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS
RN 7632-04-4 REGISTRY
IN Perboric acid (HBO(O2)), sodium salt (9CI)

=> E ACETIC ACID/CN 5

E1 1 ACETIC 6-PROPIONAMIDOHEXANOIC ANHYDRIDE/CN
E2 1 ACETIC ACETOXYACETIC ANHYDRIDE/CN
E3 1 --> ACETIC ACID/CN
E4 1 ACETIC ACID (2,6-DICHLOROBENZYLIDENE)HYDRAZIDE/CN
E5 1 ACETIC ACID (2-AMINOPHENYL)METHYL ESTER/CN

=> S E3

L2 1 "ACETIC ACID"/CN

=> D L2 1 RN IN

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN 64-19-7 REGISTRY
IN Acetic acid (7CI, 8CI, 9CI)

*Use specific display fields
to display pieces of the
REGISTRY answer:*

- ◆ RN = CAS RN
- ◆ IN = CA Index Name

Step 2: Use functional group searching to locate reactions

Since there is a fee for locating reactions using structure search queries and using functional group search queries, do that part of the search separately from the refinement so as to maximize the reactions retrieved for the search fee.

=> FILE CASREACT

=> QUE SULFIDE/FG.RXN (S) SULFONE/FG.FORM

L3 QUE SULFIDE/FG.RXN (S) SULFONE/FG.FORM

=> S L3

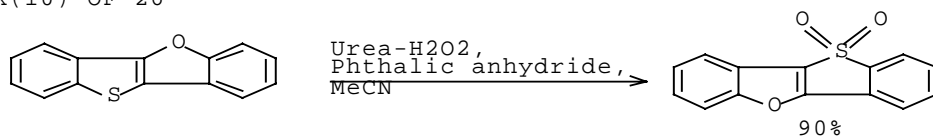
24372 SULFIDE/FG.RXN
5665 SULFONE/FG.FORM
L4 3299 SULFIDE/FG.RXN (S) SULFONE/FG.FORM

(continued on next page)

=> D SCAN

L4 3299 ANSWERS CASREACT COPYRIGHT 2003 ACS
TI Reactivity studies of [1]benzothieno[3,2-b][1]benzofuran

RX(10) OF 26



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

Step 3: Refine the reaction search

=> S L4 (L) (11138-47-9 OR 7632-04-4)/NPRO (L) 64-19-7/SOL (L) YD>75

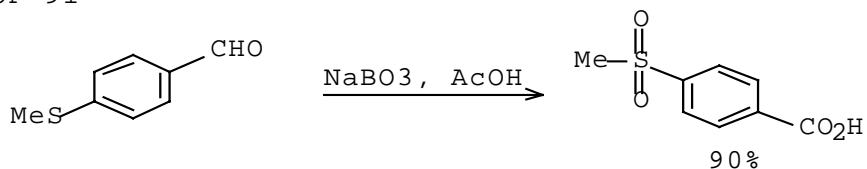
10 11138-47-9/NPRO
128 7632-04-4/NPRO
22473 64-19-7/SOL
219438 YD>75

L5 10 L4 (L) (11138-47-9 OR 7632-04-4)/NPRO (L) 64-19-7/SOL (L)
YD>75

=> D SCAN

L5 10 ANSWERS CASREACT COPYRIGHT 2003 ACS
TI Further functional-group oxidations using sodium perborate

RX(27) OF 91

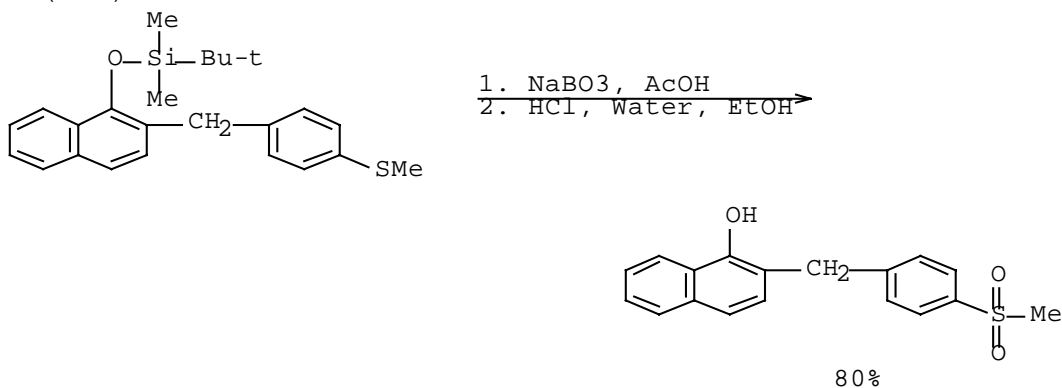


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

(continued on next page)

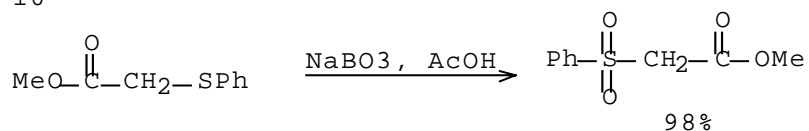
L5 10 ANSWERS CASREACT COPYRIGHT 2003 ACS
TI 2-Substituted-1-naphthols as potent 5-lipoxygenase inhibitors with topical antiinflammatory activity

RX(103) OF 154 - 2 STEPS



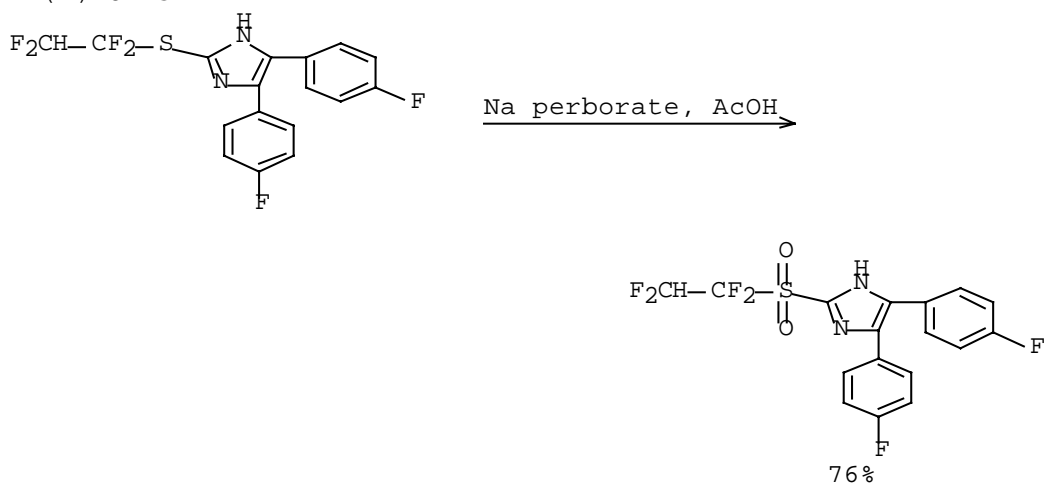
L5 10 ANSWERS CASREACT COPYRIGHT 2003 ACS
TI Chemoselective oxidation of organic sulfides to sulfones with sodium perborate

RX(1) OF 10



L5 10 ANSWERS CASREACT COPYRIGHT 2003 ACS
TI The mild oxidation of some alpha-difluoro sulfides to sulfones with sodium perborate

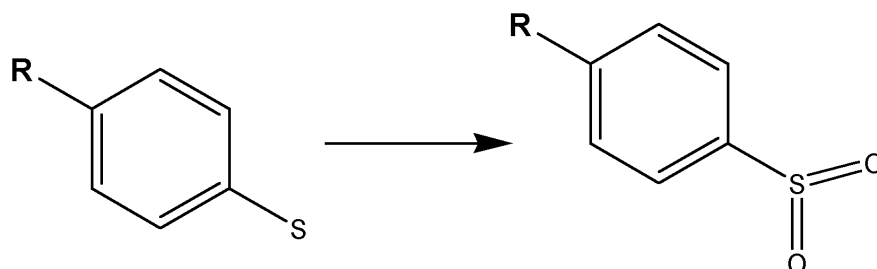
RX(1) OF 3



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

Refining with Reaction Structure Queries

Search Question: Restrict the sulfide → sulfone results to single-step reactions, with yields >80%, and which involve the following types of sulfides and sulfones:



*R = any ring or chain substituent
Any substitution is allowed at all open sites*

Search Strategy

To refine functional group or structure results using a structure query

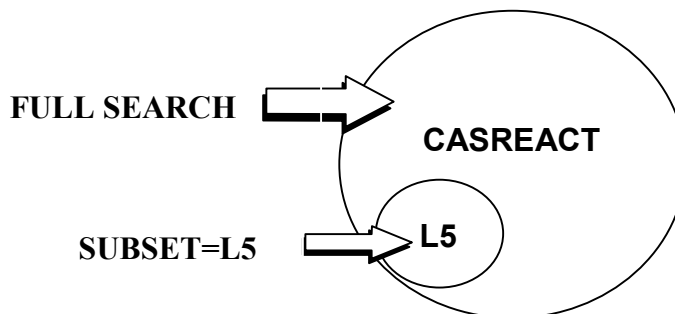
- Step 1** Build the structure reaction query to be used in the refinement.
- Step 2** Enter CASREACT and upload the structure.
- Step 3** Run a 'SUBSET' search using the structure reaction query.
- Step 4 optional** Add additional refinements such as yield and number of steps.
- Step 5** Display the results.

SUBSET Structure Searching

A SUBSET search looks for a structure query in the answers from a previous reaction search.

For example:

While a FULL search looks through the entire CASREACT database, a SUBSET search is restricted to an answer subset, e.g., L5.



To run a SUBSET search, add the keyword **SUBSET=L n** to the command line.

For example:

```
=> S L6 SSS FULL SUBSET=L5
```

- ◆ where L5 is the answer set L-number (file subset) to be searched
- ◆ where L6 is the query you want to search as a SSS FULL search in answer set L5

SUBSET searching is useful for:

- Refining results from a structure or functional group reaction search
- Running a broadly defined structure query that will no run in the full database

note

A SUBSET structure search has a lower fee than a full file structure search, when the subset is a

- Functional group answer set
- Structure search answer set

Run a Sample SUBSET search

=> D HIS

•
•
•

FILE 'CASREACT' ENTERED AT ...
 L3 QUE SULFID LFONE/FG.FORM
 L4 3299 S L3 L4 is the subset we want to search.
 L5 10 S L4 (L) 632-04-4)/NPRO (L) 64-19-7/SOL

=>

Uploading sulf.str

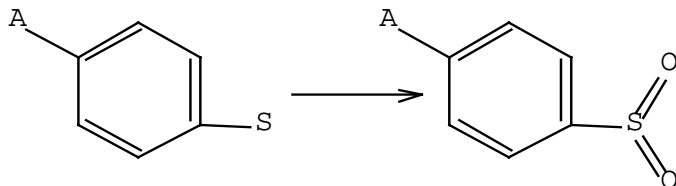
L6 STRUCTURE UPLOADED

=> D L6

L6 HAS NO ANSWERS
 L6 STR

When the structure reaction query was built

- ◆ Node characteristic on the A variable was specified as Ring/Chain
- ◆ The sulfur atom was mapped from reactant to product



=> S L6 SSS SAM SUBSET=L4

SAMPLE SUBSET SEARCH INITIATED 09:58:36 FILE 'CASREACT'
 SCREENING COMPLETE - 204 REACTIONS TO VERIFY FROM 30 DOCUMENTS
 100.0% DONE 204 VERIFIED 72 HIT RXNS 19 DOCS
 SEARCH TIME: 00.00.02

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
 PROJECTED VERIFICATIONS (WITHIN SPECIFIED SUBSET): 3224 TO 4936
 PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 119 TO 641

L7 19 SEA SUB=L4 SSS SAM L6 (72 REACTIONS)

The search is projected to complete in the full subset.

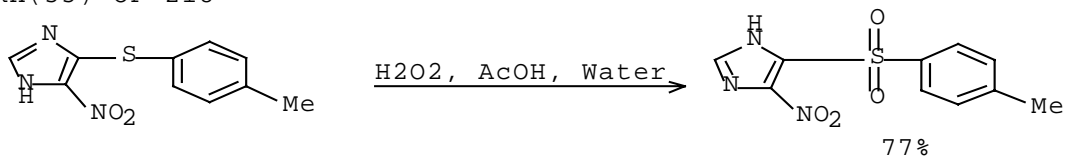
(continued on next page)

=> D SCAN

L7 19 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Nucleophilic displacements of imidazoles. II. Displacements of halogen by S-nucleophiles and displacements of mesyl groups activated by nitro; oxidation of imidazolethiols

RX(55) OF 218



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

Run the Full SUBSET search

=> S L6 SSS FULL SUBSET=L4

FULL SUBSET SEARCH INITIATED 09:59:10 FILE 'CASREACT'

SCREENING COMPLETE - 4671 REACTIONS TO VERIFY FROM 979 DOCUMENTS

100.0% DONE 4671 VERIFIED 3240 HIT RXNS

642 DOCS

SEARCH TIME: 00.00.01

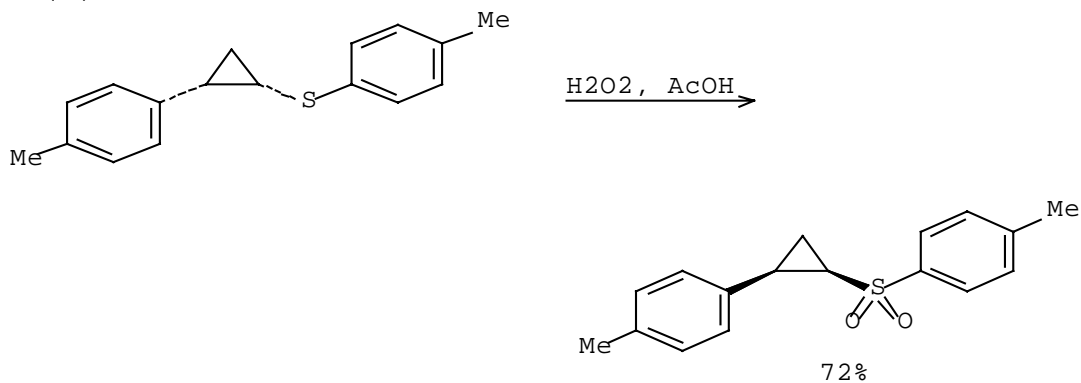
L8 642 SEA SUB=L4 SSS FUL L6 (3240 REACTIONS)

=> D SCAN

L8 642 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Phase transfer catalyzed cyclopropanation of 4-methylstyrene with carbenes and ylides

RX(3) OF 8



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

Add additional refinements

=> S L8 (L) 1/NS (L) YD>80

418671 1/NS

195046 YD>80

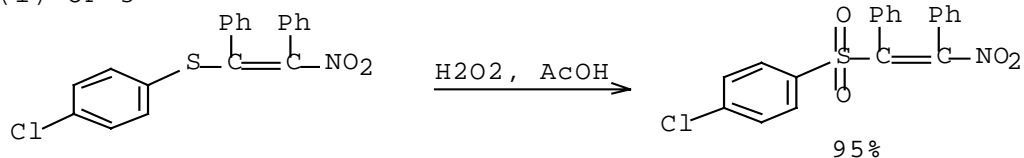
L9 217 L8 (L) 1/NS (L) YD>80

=> D SCAN

L9 217 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Synthesis of 2-(arylsulfonyl)-1-nitro alkenes and
4-(arylsulfonyl)-1,3-alkadienes

RX(1) OF 3

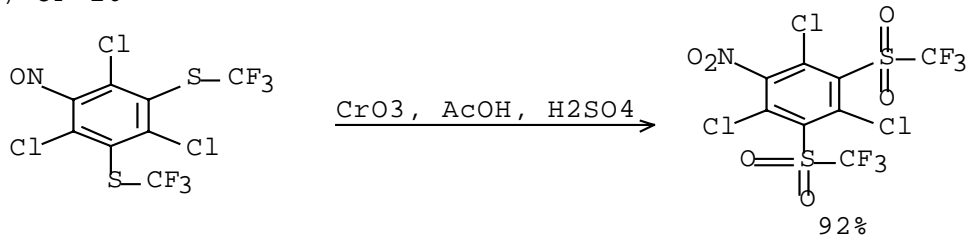


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L9 217 ANSWERS CASREACT COPYRIGHT 2003 ACS

TI Synthesis of 2,6-dichloro- and 2,4,6-trichloro-3,5-bis
[(trifluoromethyl)sulfonyl]nitrobenzenes

RX(7) OF 16



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

Summary

- Structure search results or functional group search results may be further refined

- Results can be refined by
 - ◆ Yield
 - ◆ Number of steps
 - ◆ CAS RNs for reaction participants
 - ◆ Reaction note information

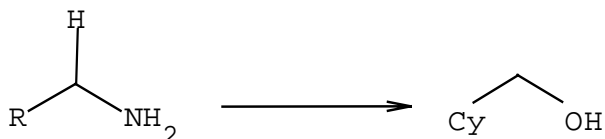
- Use (L) proximity to apply the refinement to the hit reactions in the answer set

- Use SUBSET structure searches to refine structure or functional group search results

- Additional refinements can be added to the hit reactions from the SUBSET search

Skills Practice

1. Locate reactions for carrying out the following transformation:



R = any type of ring system with any type of substitution

2. Restrict the results to single-step reactions not using sodium nitrite (NaNO₂) to accomplish the transformation. What are the reagents and catalysts used in these reactions?
3. Restrict the answers from question 1 to reactions involving a carbocyclic ring instead of any ring system with yields greater than 60%.

REACTION SEARCHING IN CASREACT

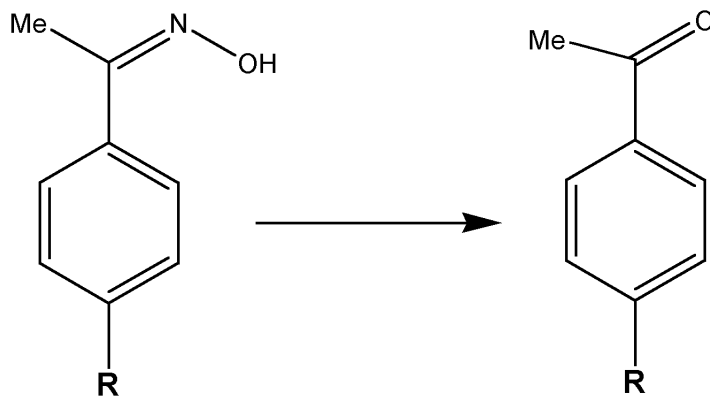
SUGGESTED SOLUTIONS TO SKILLS PRACTICE PROBLEMS

AUGUST 2003

The solutions presented here are solutions that can be attained using techniques and search tools presented in the accompanying workbook.

Skills Practice (page 27):

Question 1: Locate the requested information about the conversion of the following ketoximes to the corresponding ketones:

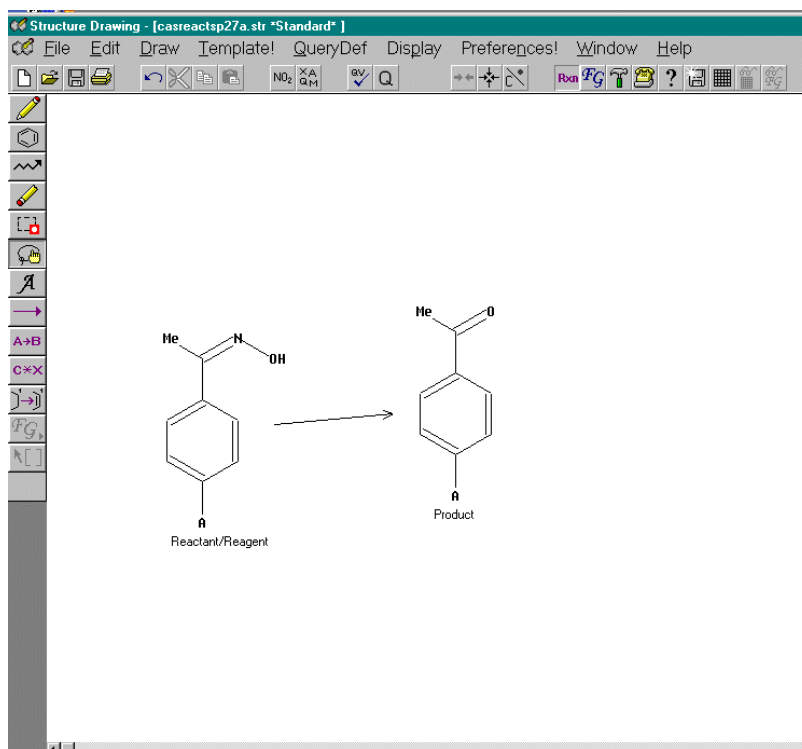


R = any non-hydrogen ring or chain substituent
Rings may have other rings fused to them
Any substitution at all open sites

Suggested Approach:

1. Build the query and upload it to the CASREACT file
2. Test the query with a SAMPLE search
3. Run the FULL reaction search
4. Display the Title (TI) and CRDREF information all answers

Step 1: Build the query and Upload it to CASREACT



Upload the query after logon to STN (see pages 17 ff.)

```
=> FIL CASREACT
```

```
FILE 'CASREACT' ENTERED AT ...
```

```
=>
```

```
Uploading C:\Program Files\stnexp\Queries\casreactsp27a.str
```

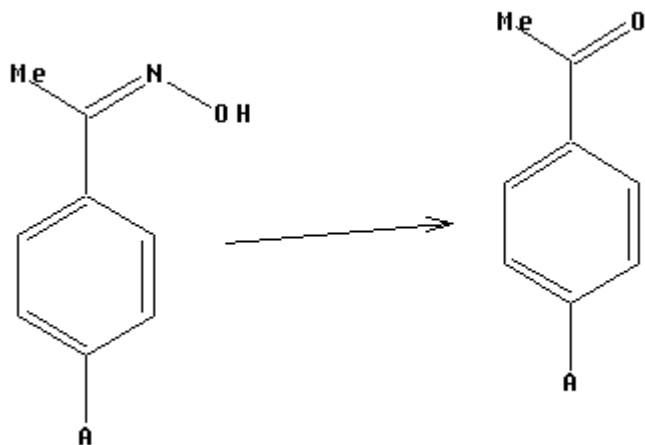
```
L1      STRUCTURE UPLOADED
```

Step 2: Test the query with a SAMPLE search

=> D L1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1 SSS SAM

SAMPLE SEARCH INITIATED 12:53:35

SCREENING COMPLETE - 162 REACTIONS TO VERIFY FROM 33 DOCUMENTS

100.0% DONE 162 VERIFIED 4 HIT RXNS 2 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 2477 TO 4003

PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1 (4 REACTIONS)

Review answers from SAMPLE search using D SCAN command:

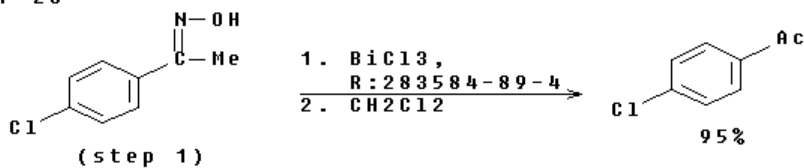
=> D SCAN

L2 2 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI Microwave Assisted Conversion of Oximes and Semicarbazones to Carbonyl Compounds Using Benzyltriphenylphosphonium Peroxymonosulfate

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN?

RX(5) OF 26



NOTE: microwave 2nd step

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

Step 3: Run the FULL reaction search

=> S L1 FUL

FULL SEARCH INITIATED 12:54:24

SCREENING COMPLETE - 3154 REACTIONS TO VERIFY FROM 641 DOCUMENTS

100.0% DONE 3154 VERIFIED 109 HIT RXNS 57 DOCS
SEARCH TIME: 00.00.01

L3 57 SEA SSS FUL L1 (109 REACTIONS)

Step 4: Display the results using TI CRDREF formats

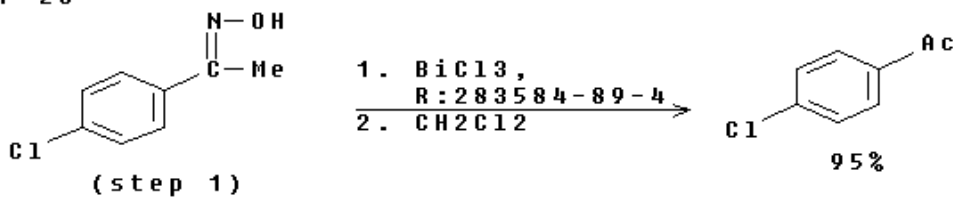
=> D TI CRDREF TOTAL

THE ESTIMATED COST FOR THIS REQUEST IS 210.33 U.S. DO
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

*The Cost Warning for display
has been set to alert users to
display costs above a desired
threshold.*

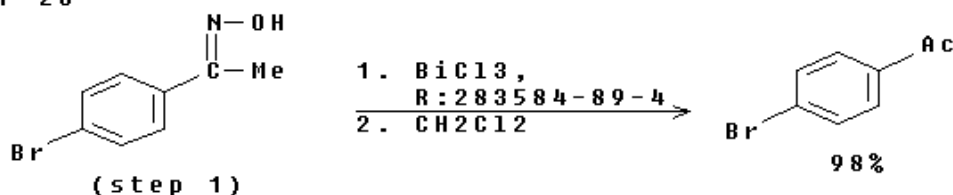
L3 ANSWER 1 OF 57 CASREACT COPYRIGHT 2003 ACS on STN
TI Microwave Assisted Conversion of Oximes and Semicarbazones to
Carbonyl Compounds Using Benzyltriphenylphosphonium
Peroxymonosulfate

RX(5) OF 26



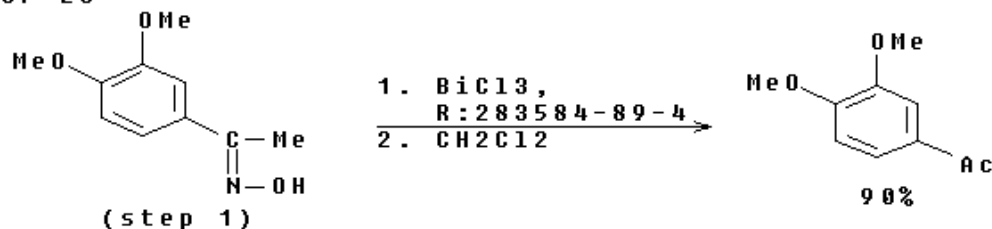
REF: Monatshefte fuer Chemie, 134(1), 45-49; 2003
NOTE: microwave 2nd step

RX(6) OF 26



REF: Monatshefte fuer Chemie, 134(1), 45-49; 2003
NOTE: microwave 2nd step

RX(8) OF 26



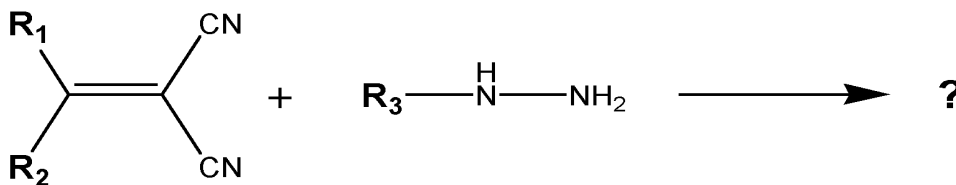
REF: Monatshefte fuer Chemie, 134(1), 45-49; 2003
NOTE: microwave 2nd step

•
•
•

The search retrieved 109 hit reactions in 57 documents.

Skills Practice (page 28):

Question 2: What types of products have been formed from the reaction of the following two starting materials?

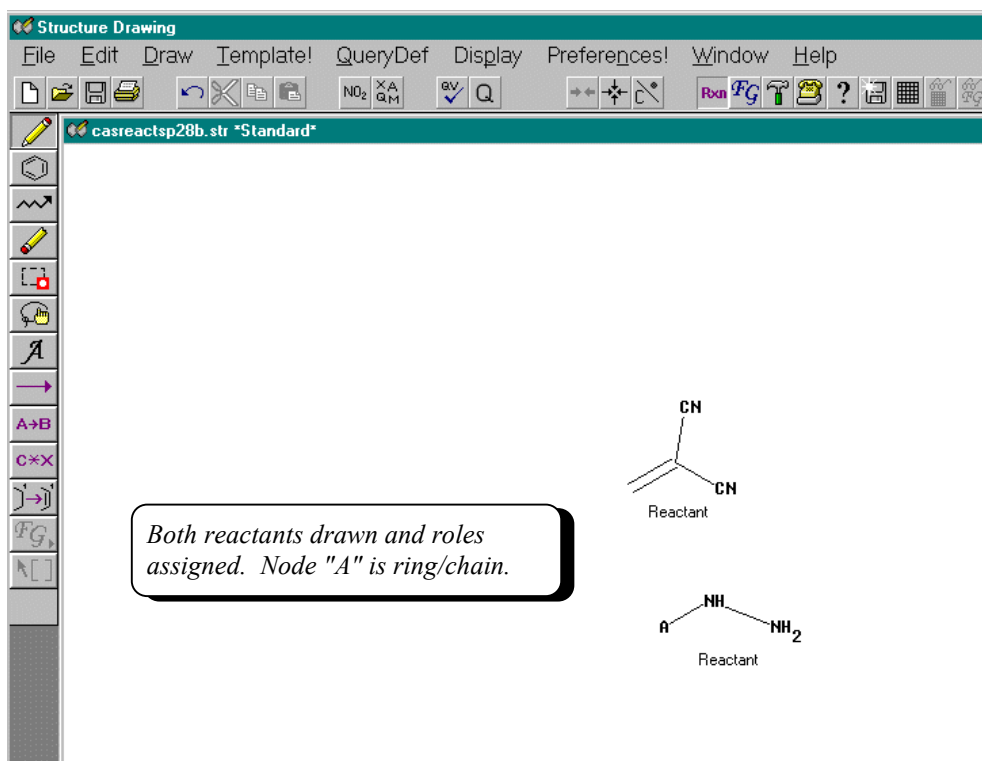


R₁ and R₂ may be any ring or chain atom *including* hydrogen
R₃ may be a ring or chain atom *except* hydrogen

Suggested Approach:

1. Build the query and upload it to the CASREACT file
2. Test the query with a SAMPLE search
3. Run the FULL reaction search
4. Display results

Step 1: Build the query



Step 2: SAMPLE search

```
FILE 'HOME' ENTERED AT 09:11:08 ON ...  
  
=> FIL CASREACT  
  
=>  
Uploading C:\Program Files\stnexp\Queries\casreactsp28b.str  
  
L1          STRUCTURE UPLOADED  
  
=> S L1 SSS SAM  
  
SAMPLE SEARCH INITIATED 09:18:40  
SCREENING COMPLETE -      72 REACTIONS TO VERIFY FROM      15 DOCUMENTS  
  
100.0% DONE      72 VERIFIED      21 HIT RXNS      6 DOCS  
SEARCH TIME: 00.00.01  
  
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**  
                        BATCH   **COMPLETE**  
PROJECTED VERIFICATIONS: 931 TO   1949  
PROJECTED ANSWERS:      6 TO     266  
  
L2          6 SEA SSS SAM L1 (    21 REACTIONS)
```

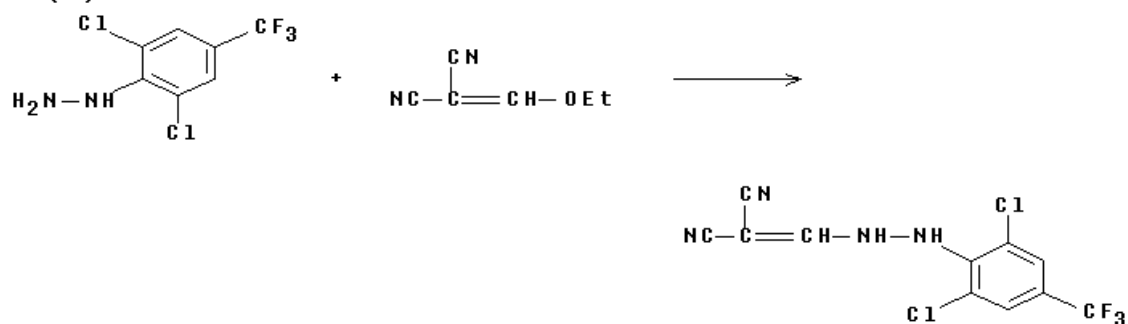
Display the SAMPLE results using D SCAN:

=> D SCAN

L2 6 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI N-Phenylpyrazole derivatives

RX (1) OF 6



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

Step 3: Run the FULL search

=> S L1 SSS FUL

FULL SEARCH INITIATED 09:19:20

SCREENING COMPLETE - 1378 REACTIONS TO VERIFY FROM 289 DOCUMENTS

100.0% DONE 1378 VERIFIED 532 HIT RXNS 138 DOCS

SEARCH TIME: 00.00.01

L3 138 SEA SSS FUL L1 (532 REACTIONS)

The full search retrieved 532 hit reactions in 138 documents.

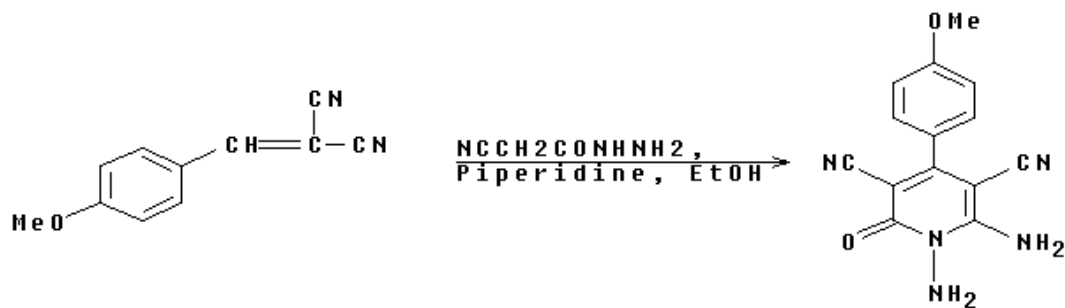
Step 4: Display results

=> D SCAN

L3 138 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI On the reaction of cyanoacetohydrazide with .alpha.-substituted cinnamitriles

RX(1) OF 4



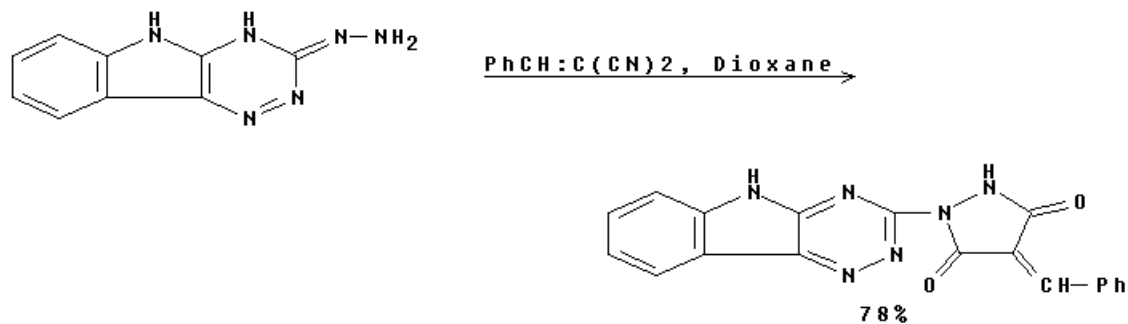
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> D 1

Default display (FCRDREF) of the first answer.

L3 ANSWER 1 OF 138 CASREACT COPYRIGHT 2003

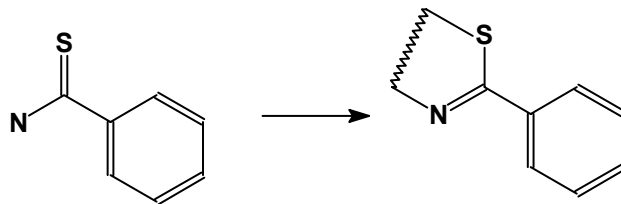
RX(8) OF 11



REF: Chemical Papers, 56(2), 132-137; 2002

Skills Practice (page 44):

Question 1: Locate methods for carrying out the following ring-forming reaction.

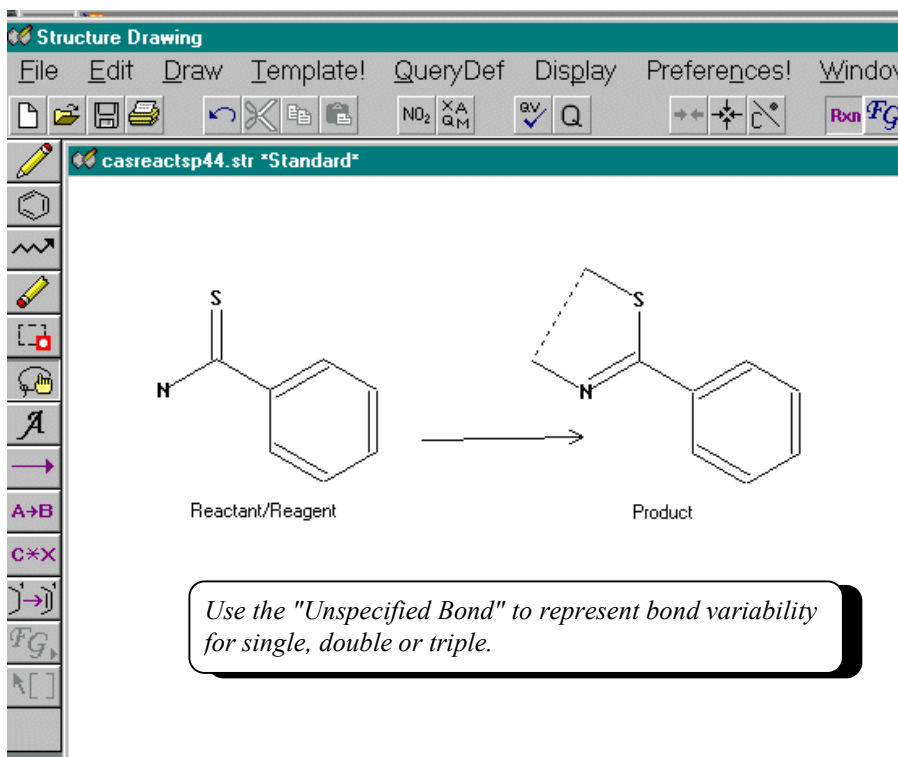


Additional substitution is allowed at all open sites
Additional ring fusion is allowed
The C~C bond may be single, double or triple

Suggested Approach:

1. Build the query and upload it to the CASREACT file.
2. Test the query with a SAMPLE search.
3. Run the FULL reaction search.
4. Display results.

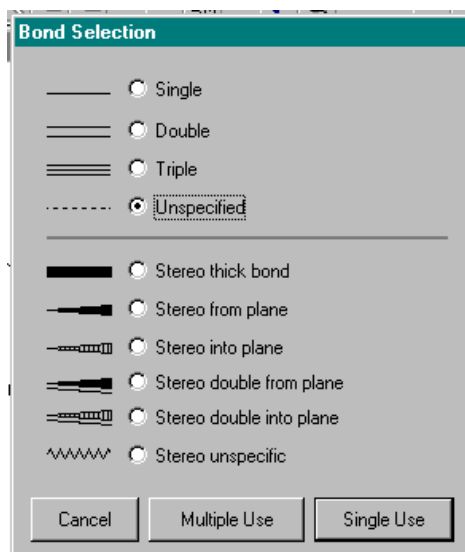
Step 1: Build the query



The "Unspecified Bond" option may be accessed in either of two ways to open the **Bond Selection Menu**.

1. Pull down the **Draw** menu and click on **Bond**.
2. Click in the **Current Bond Box**

In the **Bond Selection Menu**, choose **Unspecified** and click **Single Use**.



Step 2: SAMPLE search

=> FIL CASREACT

FILE 'CASREACT' ENTERED AT ...

=>

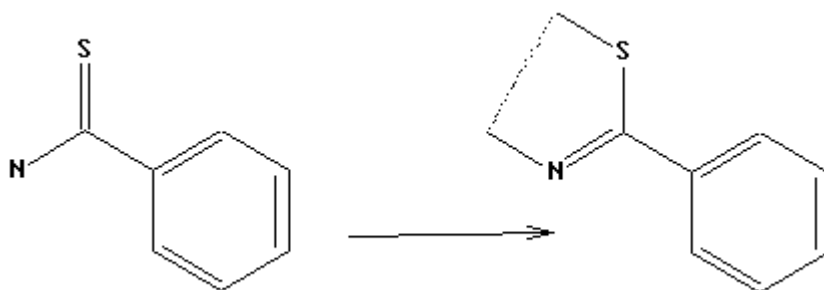
Uploading C:\Program Files\stnexp\Queries\casreactsp44.str

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1 SAM SSS

SAMPLE SEARCH INITIATED 10:25:21

SCREENING COMPLETE - 101 REACTIONS TO VERIFY FROM 19 DOCUMENTS

100.0% DONE 101 VERIFIED 37 HIT RXNS 12 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 1418 TO 2622

PROJECTED ANSWERS: 32 TO 446

L2 12 SEA SSS SAM L1 (37 REACTIONS)

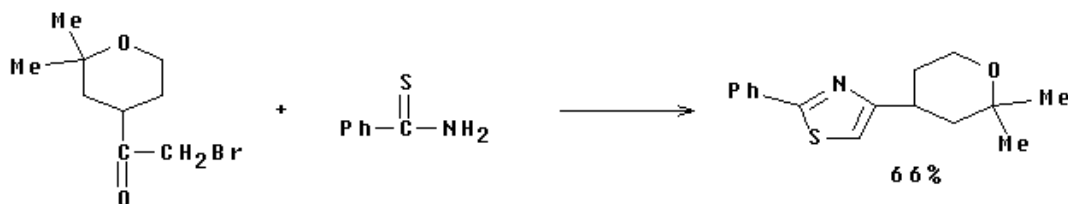
Display SAMPLE search results using D SCAN:

=> D SCAN

L2 12 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI Synthesis and antibacterial properties of thiazoles containing tetrahydropyran rings

RX (40) OF 87



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

Step 3: Run the FULL search

=> S L1 SSS FUL

FULL SEARCH INITIATED 10:26:41

SCREENING COMPLETE - 1935 REACTIONS TO VERIFY FROM 284 DOCUMENTS

100.0% DONE 1935 VERIFIED 1086 HIT RXNS

188 DOCS

SEARCH TIME: 00.00.01

L3 188 SEA SSS FUL L1 (1086 REACTIONS)

The search found 1086 hit reactions in 188 documents.

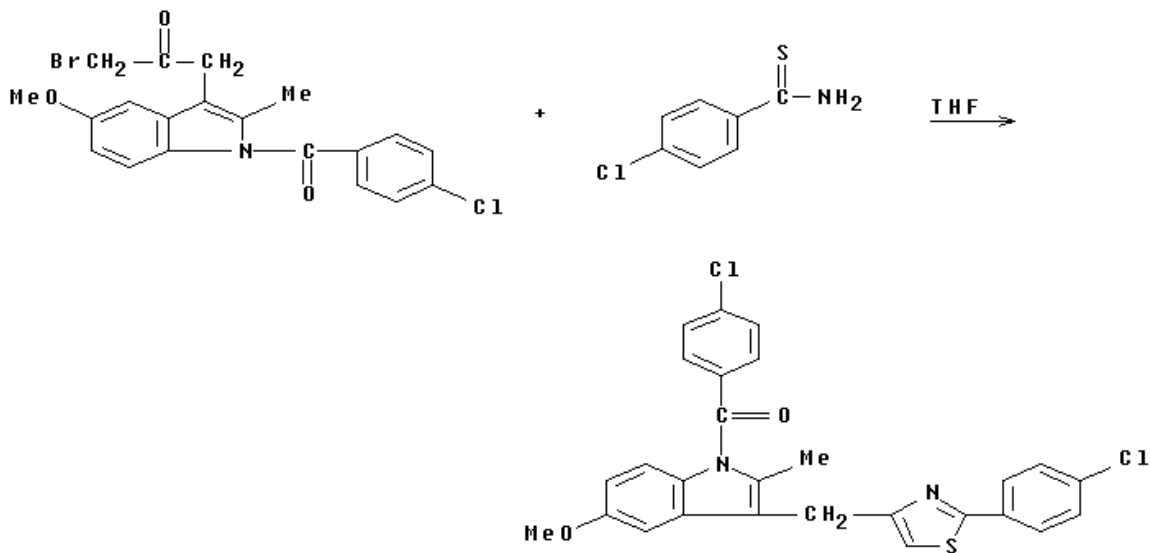
Step 4: Display results

=> D SCAN

L3 188 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI Thiazole analogs of the NSAID indomethacin as selective COX-2 inhibitors

RX(30) OF 67



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

Display an answer using IBIB ABS FHIT formats.

=> D 3 IBIB ABS FHIT

L3 ANSWER 3 OF 188 CASREACT COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 138:55928 CASREACT

TITLE: Synthesis and antimicrobial activity of 3-2 (alkyl/aryl, 4-substituted thiazolo)-6-fluorocinnoline-4-ones

AUTHOR(S): Vingkar, Sharvani K.; Bobade, A. S.; Khadse, B. G.

CORPORATE SOURCE: Dept. of Chemotherapy, Haffkine Institute, Mumbai, 400012, India

SOURCE: Indian Drugs (2001), 38(11), 573-575

CODEN: INDRBA; ISSN: 0019-462X

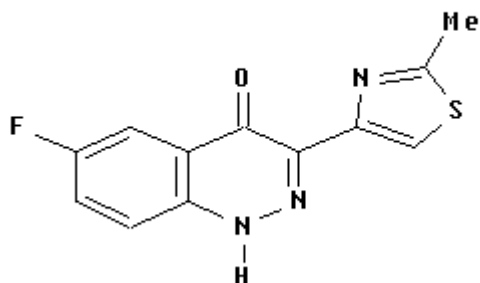
PUBLISHER: Indian Drug Manufacturers' Association

DOCUMENT TYPE: Journal

LANGUAGE: English

(continued on next page)

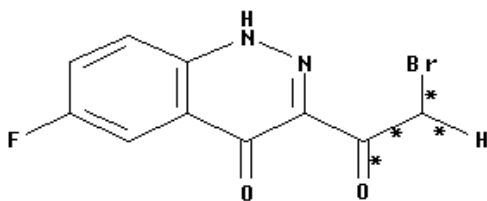
GI



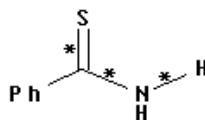
III

AB The new series of title compds. were synthesized by starting with 4-fluoroaniline. Diazotization of 4-fluoroaniline followed by coupling with Et acetoacetate in aq. ethanolic soln. contg. Sodium acetate⁴, afforded the corresponding hydrazone. Intramol. cyclization of the hydrazone with anhyd. $AlCl_3$ in chlorobenzene⁵ resulted in the formation of 3-acetyl-6-fluoro-1H-cinnoline-4-one (I). I was then brominated in the presence of UV light to yield 3-bromoacetyl-6-fluoro-1H-cinnoline-4-one (II). Total of ten various substituted thioamides, derived from different nitriles in pyridine, employing H_2S gas and tri-Et amine, were then combined with compd. II to get the corresponding thiazoles, e.g., III.

RX(6) OF 46 ...L + T ==> U

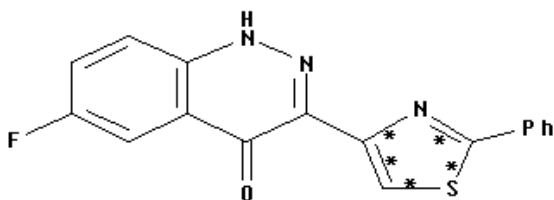


L



T

(6) →



U

RX(6) RCT L 477283-42-4, T 2227-79-4
 PRO U 479415-94-6
 SOL 71-43-2 Benzene

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Skills Practice (page 69):

Question 1: Locate reactions in which sulfides are converted to sulfones.

Suggested Approach:

1. Build the functional group query and upload it to the CASREACT file
2. Run the search
3. Display results

Step 1: Build the query

The screenshot shows the 'Structure Drawing' software interface. The menu bar includes 'File', 'Edit', 'Draw', 'Template!', 'QueryDef', and 'Display'. The toolbar contains icons for file operations, undo, redo, and search. The main window title is 'casreactsp69a.str *Standard*'. A vertical toolbar on the left contains icons for drawing structures, mapping, and functional groups. A callout box contains the text: 'Assign roles of Reactant (reacting) and Product (formed) and use the mapping tool to ensure precision.' Below the callout, the reaction is defined as:

1		1
	SULFIDE	SULFONE
	Reactant (reacting)	Product (formed)

Step 2: Run the search

```
=> FIL CASREACT
FILE 'CASREACT' ENTERED AT ...
=> QUE (SULFIDE/FG.RXN (S) SULFONE/FG.FORM)
L1  QUE (SULFIDE/FG.RXN (S) SULFONE/FG.FORM)
=> S L1
      24610 SULFIDE/FG.RXN
      5729  SULFONE/FG.FORM
L2   3341 (SULFIDE/FG.RXN (S) SULFONE/FG.FORM)
```

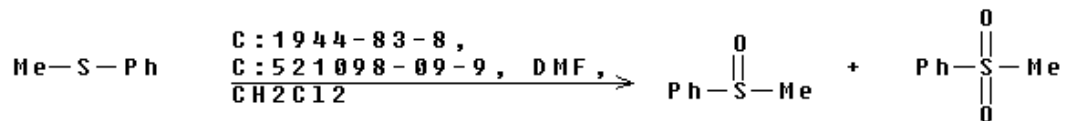
The uploaded functional group query is automatically shown as a QUE in L1. The (S) operator indicates mapping.

Step 3: Display results

```
=> D 10 CBIB CRD
```

```
L2  ANSWER 10 OF 3341 CASREACT COPYRIGHT 2003 ACS on STN
138:368439 Fe2+-Catalyzed Heterolytic RO-OH Bond Cleavage and Substrate
Oxidation: A Functional Synthetic Non-Heme Iron Monooxygenase
System. Foster, Trina L.; Caradonna, John P. (Department of
Chemistry, Boston University, Boston, MA, 02215, USA). Journal of
the American Chemical Society, 125(13), 3678-3679 (English) 2003.
CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.
```

```
RX(2) OF 3
```



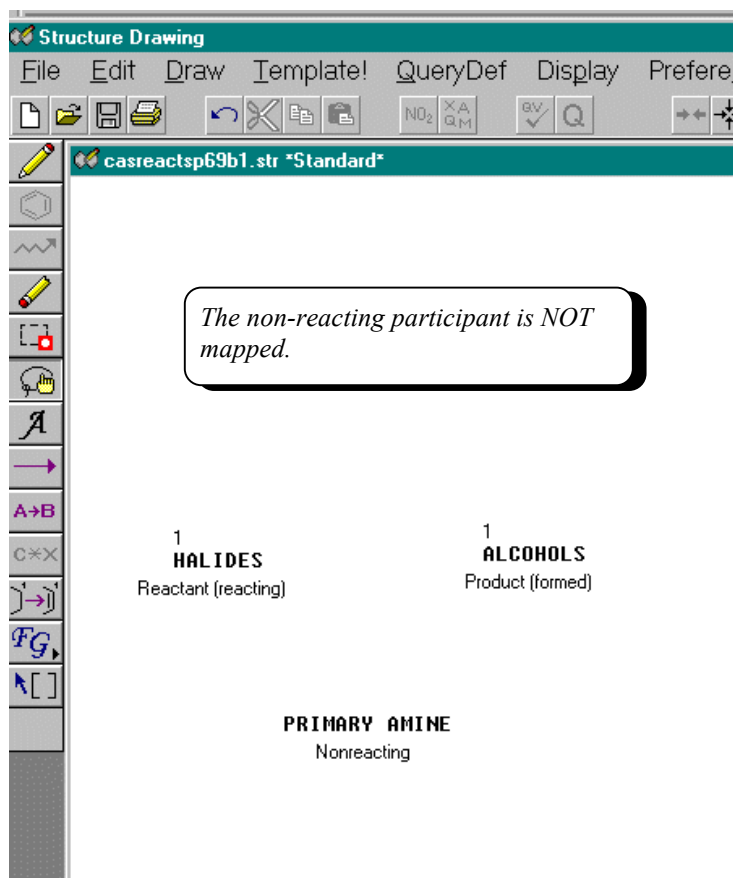
Skills Practice (page 69):

Question 2: Locate reactions in which halides are converted to alcohols in the presence of non-reacting primary amines.

Suggested Approach:

1. Build the functional group query and upload it to the CASREACT file
2. Run the search
3. Display results

Step 1: Build the query



Step 2: Run the search

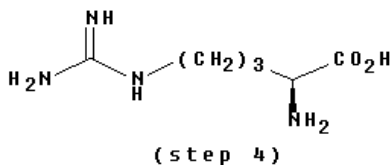
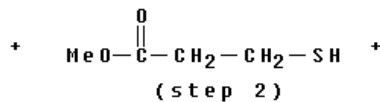
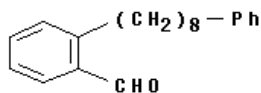
```
=> FIL CASREACT  
FILE 'CASREACT' ENTERED AT ...  
=> QUE PRIMARY AMINE/FG.NON (L) (ALCOHOLS/FG.FORM (S) HALIDES/FG.RXN)  
L1  QUE PRIMARY AMINE/FG.NON (L) (ALCOHOLS/FG.FORM (S) HALIDES/FG.RXN)  
=> S L1  
    13167 PRIMARY AMINE/FG.NON  
    114018 ALCOHOLS/FG.FORM  
    182850 HALIDES/FG.RXN  
L2      60 PRIMARY AMINE/FG.NON (L) (ALCOHOLS/FG.FORM (S) HALIDES/FG.RXN)
```

The non-reacting functional group is connected by an (L) operator since it is not mapped.

Step 3: View results

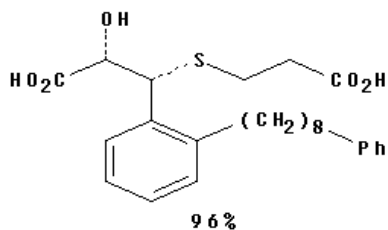
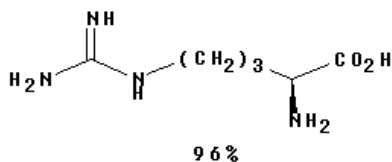
```
=> D SCAN  
L2  60 ANSWERS  CASREACT  COPYRIGHT 2003 ACS on STN  
TI  Benzyl mercaptan derivatives as leukotriene antagonists
```

RX(212) OF 341 - 4 STEPS



1. C1CH2CO2Me →

RX(212) OF 341 - 4 STEPS



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

Locate the record highlighted by D SCAN:

=> S L2 AND BENZYL MERCAPTAN/TI

2613 BENZYL/TI
 74 MERCAPTAN/TI
 156 MERCAPTANS/TI
 230 MERCAPTAN/TI
 ((MERCAPTAN OR MERCAPTANS)/TI)
 10 BENZYL MERCAPTAN/TI
 ((BENZYL(W)MERCAPTAN)/TI)
 L3 1 L2 AND BENZYL MERCAPTAN/TI

=> D BIB FHIT

L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2003 ACS on STN
 AN 106:213567 CASREACT
 TI Benzyl mercaptan derivatives as leukotriene
 antagonists
 PA SmithKline Beckman Corp., USA
 SO Jpn. Kokai Tokkyo Koho, 44 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	JP 61249958	A2	19861107	JP 1986-91151	19860418
	JP 04074348	B4	19921126		
	AU 8656050	A1	19861023	AU 1986-56050	19860414
	AU 595193	B2	19900329		
	EP 202759	A2	19861126	EP 1986-302752	19860414
	EP 202759	A3	19880907		
	EP 202759	B1	19900620		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	EP 358240	A2	19900314	EP 1989-118801	19860414
	EP 358240	A3	19900620		
	EP 358240	B1	19930609		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	AT 53991	E	19900715	AT 1986-302752	19860414
	CA 1276937	A1	19901127	CA 1986-506607	19860414
	AT 90330	E	19930615	AT 1989-118801	19860414
	ZA 8602794	A	19870624	ZA 1986-2794	19860415
	IL 78495	A1	19930114	IL 1986-78495	19860415
	IL 91349	A1	19940412	IL 1986-91349	19860415
	FI 8601635	A	19861020	FI 1986-1635	19860417
	FI 88293	B	19930115		
	FI 88293	C	19930426		
	DK 8601765	A	19861020	DK 1986-1765	19860417
PRAI	US 1985-725264		19850419		
	US 1986-848608		19860407		
	US 1986-884608		19860407		
	CA 1986-506607		19860414		
	EP 1986-302752		19860414		
	EP 1989-118801		19860414		

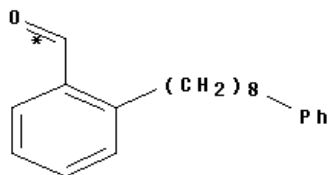
(continued on next page)

IL 1986-78495 19860415
 US 1986-926314 19861031
 US 1988-195355 19880516
 US 1988-248770 19880923

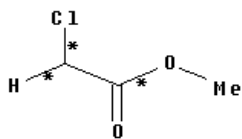


RX(212) OF 341 COMPOSED OF RX(51), RX(52), RX(54), RX(55)

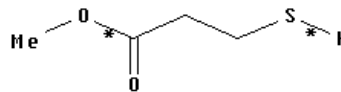
RX(212) AI + BY + R + CD ==> CE



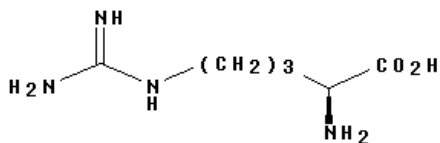
AI



BY

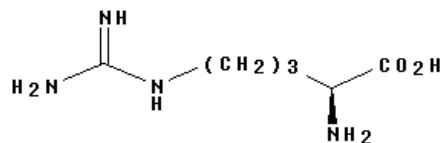


R

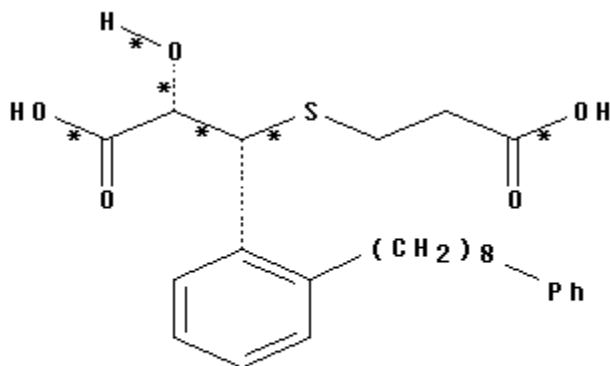


CD

4
STEPS
→



CE: CM 1
YIELD 96%

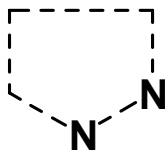


CE: CM 2
YIELD 96%

RX(51) RCT AI 96964-45-3, BY 96-34-4
 PRO BZ 120379-10-4
 RX(52) RCT R 2935-90-2, BZ 120379-10-4
 PRO CA 120427-74-9
 RX(54) RCT CA 120427-74-9
 PRO CC 120521-74-6
 RX(55) RCT CC 120521-74-6, CD 74-79-3
 PRO CE 107041-36-1

Skills Practice (page 69):

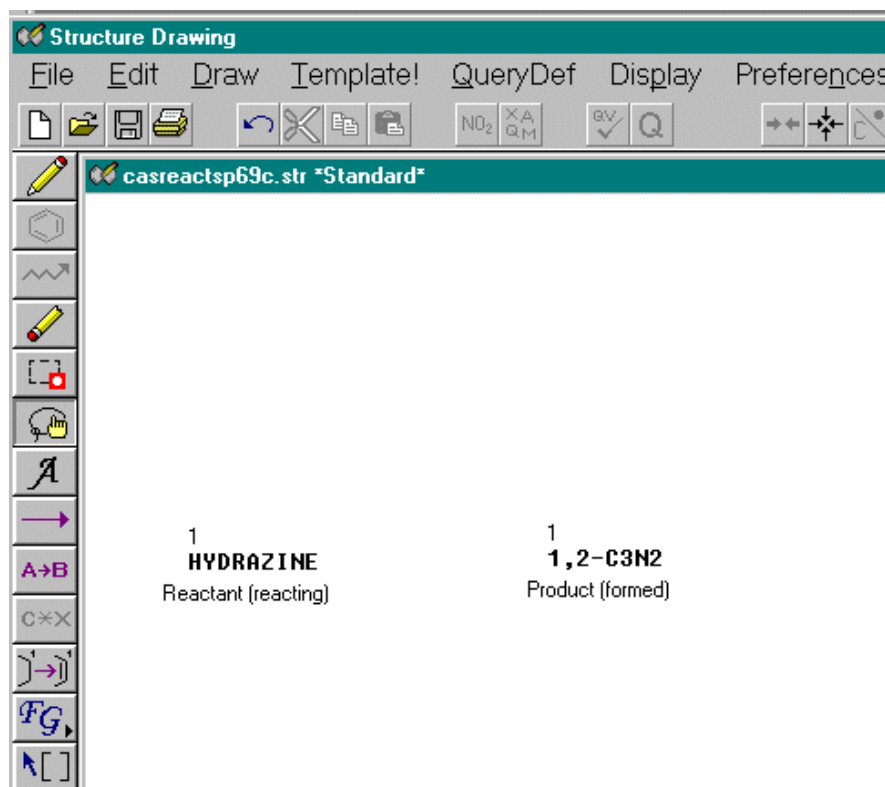
Question 3: Locate reactions in which hydrazines are used to prepare the following type of diazoles.



Suggested Approach:

1. Build the functional group query and upload it to the CASREACT file
2. Run the search
3. Display results

Step 1: Build the query



Structure Drawing

File Edit Draw Template! QueryDef Display Preferences

casreactsp69c.str *Standard*

1
HYDRAZINE
Reactant (reacting)

1
1,2-C3N2
Product (formed)

Step 2: Run the search

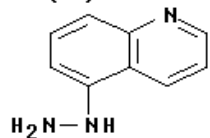
```
=> FIL CASREACT  
FILE 'CASREACT' ENTERED AT ...  
=> QUE (HYDRAZINE/FG.RXN (S) 1,2-C3N2/FG.FORM)  
L1 QUE (HYDRAZINE/FG.RXN (S) 1,2-C3N2/FG.FORM)  
=> S L1  
  
11490 HYDRAZINE/FG.RXN  
6193 1,2-C3N2/FG.FORM  
L2 2477 (HYDRAZINE/FG.RXN (S) 1,2-C3N2/FG.FORM)
```

The search retrieved 2477 documents; each with at least one hit reaction.

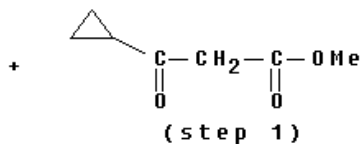
Step 3: Display results

```
=> D FCRDREF 1 1000 2477  
L2 ANSWER 1 OF 2477 CASREACT COPYRIGHT 2003 ACS on STN
```

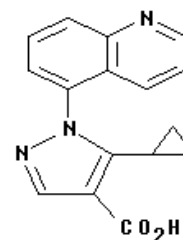
RX(2) OF 10



2 HCl
(step 2)



1. (MeO)₂CHNMe₂,
AcOEt
2. Et₃N

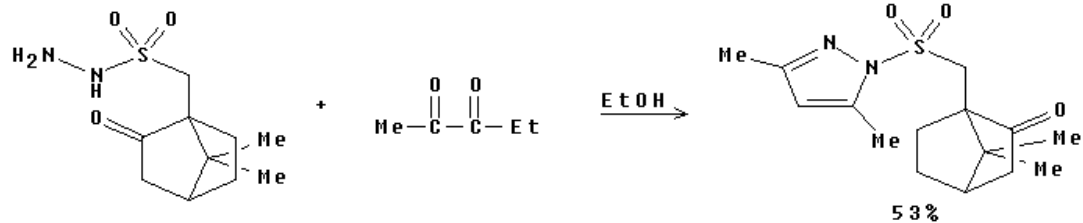


REF: PCT Int. Appl., 2003051845, 26 Jun 2003

(continued on next page)

L2 ANSWER 1000 OF 2477 CASREACT COPYRIGHT 2003 ACS on STN

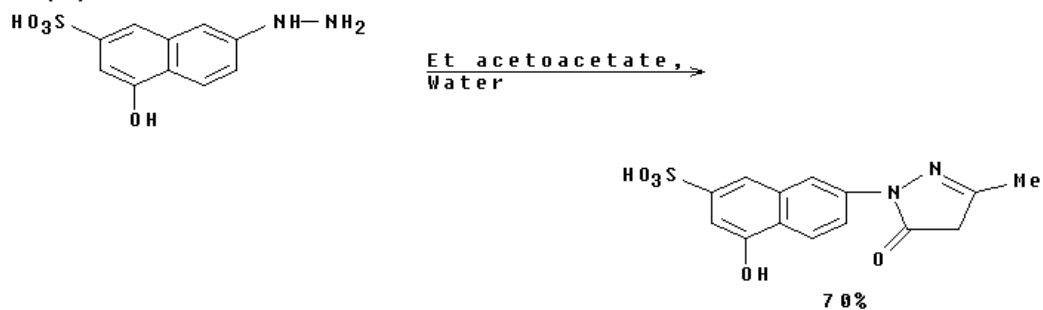
RX(9) OF 68



REF: Phosphorus and Sulfur and the Related Elements, 40(1-2), 91-7; 1988

L2 ANSWER 2477 OF 2477 CASREACT COPYRIGHT 2003 ACS on STN

RX(1) OF 1

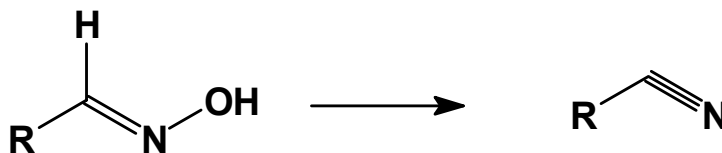


REF: Bull. soc. chim., 33,, 1481-510; 1923

NOTE: Classification: Heterocycle formation; Condensation; Hydrazination; N-Acylation; # Conditions: NaOH H₂O; water bath 1h30mn

Skills Practice (page 88):

Question 1: Locate reactions for carrying out the following transformation:



R = any type ring system with any type of substitution.

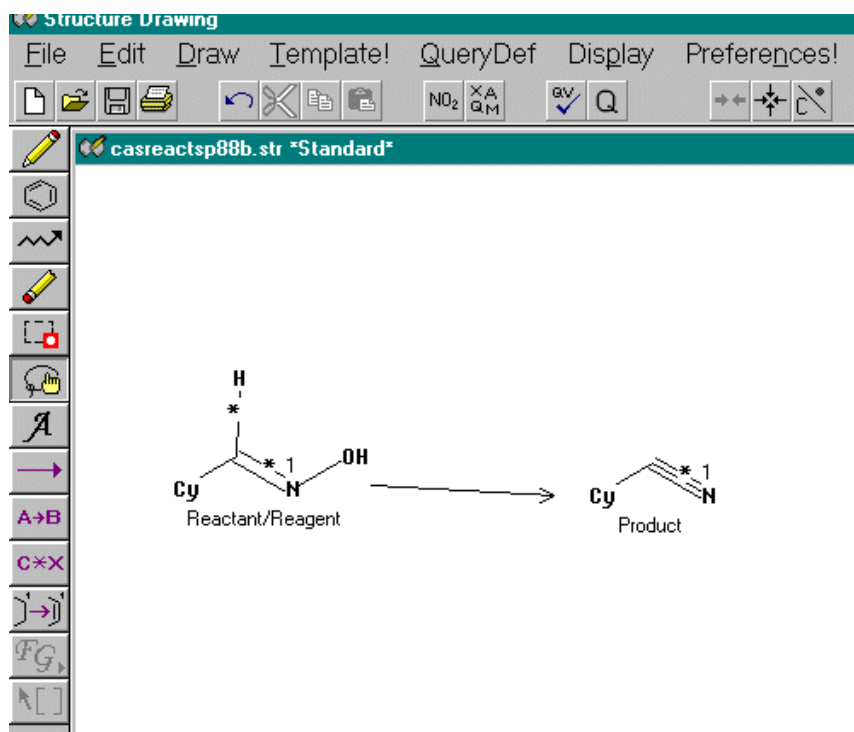
Question 2: Restrict the results to single step reactions not using sodium nitrite (NaNO_2) to accomplish the transformation. What are the reagents and catalysts used in these reactions?

Question 3: Restrict the answers from question 1 to reactions involving a carbocyclic ring instead of any ring system with yields greater than 60%.

Suggested Approach:

1. Build the structure query and upload it to the CASREACT file
2. Run the search and display results using D SCAN
3. Enter the REGISTRY file and obtain the CAS RN for sodium nitrite
4. Renter CASREACT and limit the results using 1/NS (single step reactions) and eliminating reactions which use sodium nitrite (NOTL)
5. View results
6. Build query with CB (carbocyclic ring) instead of Cy (any ring) and upload query
7. Run SUBSET search on original answer set.
8. Restrict results to those with yield greater than 60% or those with no yield data
9. View results

Step 1: Build the query



Step 2: SAMPLE and FULL searches; DISPLAY results

```
=> FIL CASREACT
```

```
FILE CASREACT ENTERED AT ...
```

```
=>
```

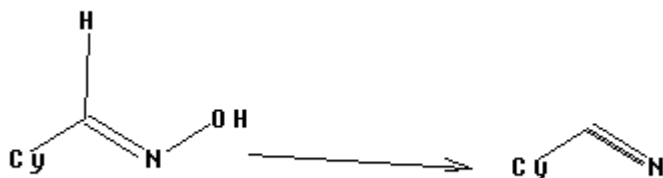
```
Uploading C:\Program Files\stnexp\Queries\casreactsp88b.str
```

```
L1 STRUCTURE UPLOADED
```

```
=> D L1
```

```
L1 HAS NO ANSWERS
```

```
L1 STR
```



SAMPLE search:

=> S L1

SAMPLE SEARCH INITIATED 09:22:09

SCREENING COMPLETE - 903 REACTIONS TO VERIFY FROM 224 DOCUMENTS

100.0% DONE 903 VERIFIED 63 HIT RXNS 19 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 16260 TO 19860

PROJECTED ANSWERS: 119 TO 641

L2 19 SEA SSS SAM L1 (63 REACTIONS)

=> D SCAN

L2 19 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI Polyhaloaromatic compounds. Part 45. Synthesis and cycloaddition reactions of pentabromobenzonitrile N-oxide

RX(5) OF 38



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

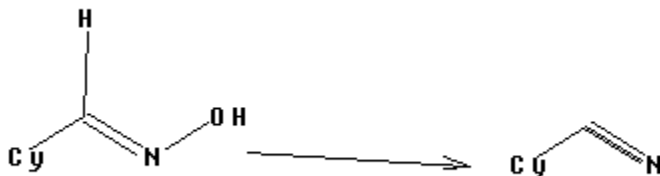
CNO answers (see product above) are not desired. Revise query to eliminate (Non-H attachments = Exactly 1 for the N atom of the nitrile). Upload revised query.

L3 STRUCTURE UPLOADED

=> D L3

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L3

SAMPLE SEARCH INITIATED 09:24:10

SCREENING COMPLETE - 903 REACTIONS TO VERIFY FROM 224 DOCUMENTS

100.0% DONE 903 VERIFIED 39 HIT RXNS 12 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 16260 TO 19860
PROJECTED ANSWERS: 33 TO 447

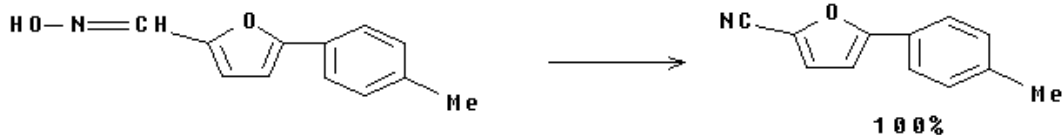
L4 12 SEA SSS SAM L3 (39 REACTIONS)

=> D SCAN

L4 12 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI Preparation and testing of 2-(5-phenyl-2-furanyl)imidazoles useful
as cardiotoxic agents

RX(2) OF 8



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

FULL SEARCH:

=> S L3 FUL

FULL SEARCH INITIATED 09:24:31

SCREENING COMPLETE - 23894 REACTIONS TO VERIFY FROM 4964 DOCUMENTS

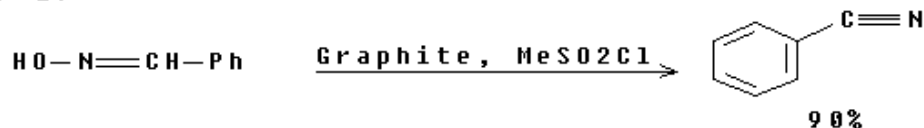
100.0% DONE 23894 VERIFIED 950 HIT RXNS 348 DOCS
SEARCH TIME: 00.00.02

L5 348 SEA SSS FUL L3 (950 REACTIONS)

=> D

L5 ANSWER 1 OF 348 CASREACT COPYRIGHT 2003 ACS on STN

RX(17) OF 27



REF: Synthesis, (2), 243-246; 2003
NOTE: no solvent

Step 3: Obtain CAS RN for sodium nitrite

```
=> FIL REG
FILE 'REGISTRY' ENTERED AT ...

=> E SODIUM NITRITE/CN 5
E1          1      SODIUM NITRILOTRIACETATE N-OXIDE/CN
E2          1      SODIUM NITRILOTRISULFONATE/CN
E3          1 --> SODIUM NITRITE/CN
E4          1      SODIUM NITRITE (NaNO2)/CN
E5          1      SODIUM NITRITE OXIDE (Na3(NO2)O)/CN

=> S E3
L6          1      "SODIUM NITRITE"/CN

=> D CN
L6  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS on STN
CN  Nitrous acid, sodium salt (8CI, 9CI)  (CA INDEX NAME)
OTHER NAMES:
CN  Anti-Rust
CN  E 250
CN  Erinirit
CN  Filmerine
CN  M 138C
CN  Nitrous acid sodium salt (1:1)
CN  Sodium nitrite
CN  Sodium nitrite (NaNO2)
CN  Synfat 1004
```

Step 4: Single Step Reactions without NaNO₂

```
=> FIL CASREACT
FILE 'CASREACT' ENTERED AT ...

=> D HIS
      (FILE 'CASREACT' ENTERED AT ...
              DEL HIS Y
L1          STRUCTURE UPLOADED
L2          19 S L1
L3          STRUCTURE UPLOADED
L4          12 S L3
L5          348 S L3 FUL

      FILE 'REGISTRY' ENTERED AT ...
              E SODIUM NITRITE/CN
L6          1 S E3

      FILE 'CASREACT' ENTERED AT ...
```

=> S L5 (L) 1/NS (NOTL) L6/NPRO

423501 1/NS

6445 L6/NPRO

L7

346 L5 (L) 1/NS (NOTL) L6/NPRO

*1/NS = single step reactions
L6/NPRO = sodium nitrite in any role except product
(L) = link only to hit reactions*

Step 5: View results

=> D 1 150 346 FCRDREF

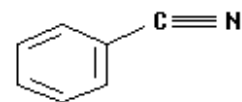
Display the first, last and a middle answer in the default FCRDREF format.

L7 ANSWER 1 OF 346 CASREACT COPYRIGHT 2003 ACS on STN

RX(17) OF 27

HO-N=CH-Ph

Graphite, MeSO₂Cl



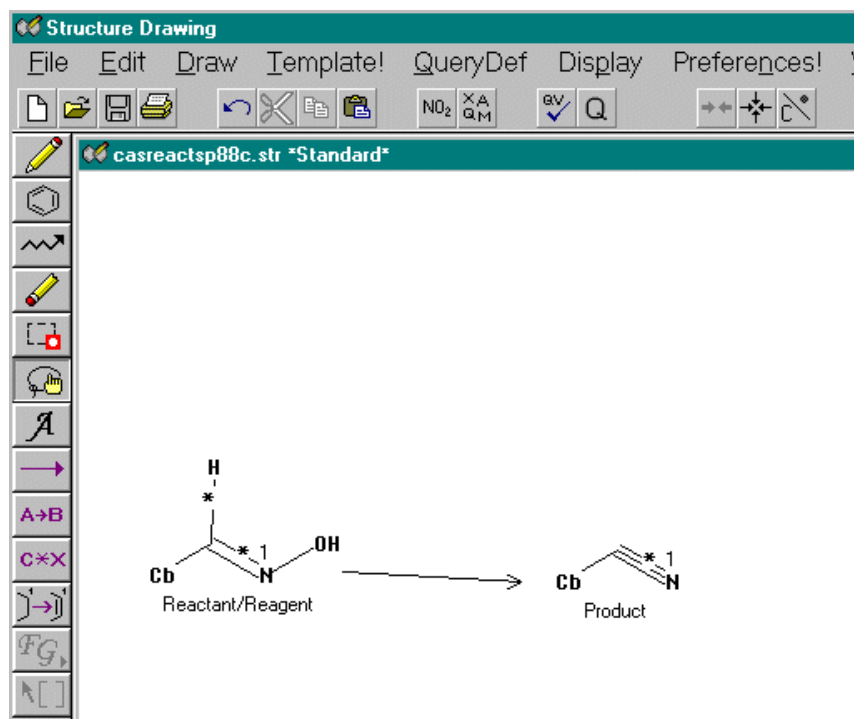
90%

REF: Synthesis, (2), 243-246; 2003

NOTE: no solvent

•
•
•

Step 6: Carbocyclic ring query



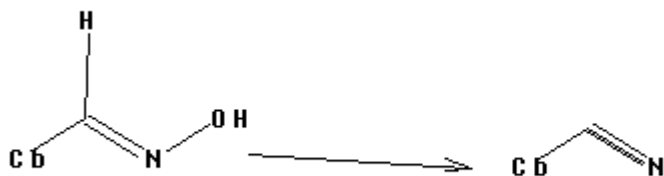
Step 7: SUBSET search

L8 STRUCTURE UPLOADED

=> D L8

L8 HAS NO ANSWERS

L8 STR



=> D HIS 5

(FILE 'CASREACT' ENTERED AT 09:16:56 ON 05 AUG 2003)

DEL HIS Y

L4 12 S L3
L5 348 S L3 FUL

FILE 'REGISTRY' ENTERED AT 09:25:05 ON 05 AUG 2003

E SODIUM NITRITE/CN

L6 1 S E3

FILE 'CASREACT' ENTERED AT 09:26:26 ON 05 AUG 2003

L7 346 S L5 (L) 1/NS (NOTL) L6/NPRO
L8 STRUCTURE UPLOADED

=> S L8 SUB=L5 SSS SAM

SAMPLE SUBSET SEARCH INITIATED 09:30:18

SCREENING COMPLETE - 39 REACTIONS TO VERIFY FROM 12 DOCUMENTS

100.0% DONE 39 VERIFIED 12 HIT RXNS 4 DOCS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET): ONLINE **COMPLETE**
PROJECTED VERIFICATIONS (WITHIN SPECIFIED SUBSET): 406 TO 1154
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 4 TO 199

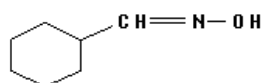
L9 4 SEA SUB=L5 SSS SAM L8 (12 REACTIONS)

=> D SCAN

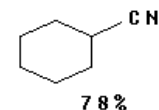
L9 4 ANSWERS CASREACT COPYRIGHT 2003 ACS on STN

TI A convenient method for the preparation of nitriles and carbodiimides using N-methyl-2-pyridinecarbamoyl chloride

RX(2) OF 6



R: 13980-56-8, Et3N,
4-DMAP, CH2Cl2



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

=> S L8 SUB=L5 SSS FUL

FULL SUBSET SEARCH INITIATED 09:30:38

SCREENING COMPLETE - 950 REACTIONS TO VERIFY FROM 348 DOCUMENTS

100.0% DONE 950 VERIFIED 435 HIT RXNS 151 DOCS
SEARCH TIME: 00.00.01

L10 151 SEA SUB=L5 SSS FUL L8 (435 REACTIONS)

Step 8: Restrict Results by Yield

Use the /YD field (numeric) to limit answers to those with greater than 60% yield. The (A) operator links to the yield in the final step of a multistep reaction. NONE/YDT includes reactions where no yield is reported.

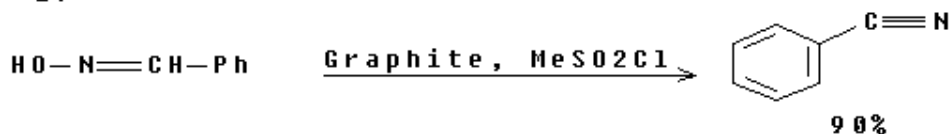
```
=> S L10 (A) (YD>60 OR NONE/YDT)
      267174 YD>60
      225665 NONE/YDT
L11   145 L10 (A) (YD>60 OR NONE/YDT)
```

Step 9: View Results

```
=> D 1 75 145
```

```
L11 ANSWER 1 OF 145 CASREACT COPYRIGHT 2003 ACS on STN
```

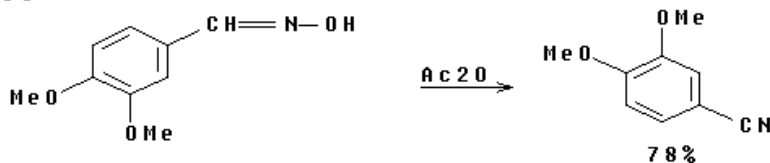
```
RX(17) OF 27
```



```
REF: Synthesis, (2), 243-246; 2003
NOTE: no solvent
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L11 ANSWER 75 OF 145 CASREACT COPYRIGHT 2003 ACS on STN
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REF: Indian Journal of Chemistry, Section B: Organic Chemistry
Including Medicinal Chemistry, 26B(9), 856-60; 1987
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