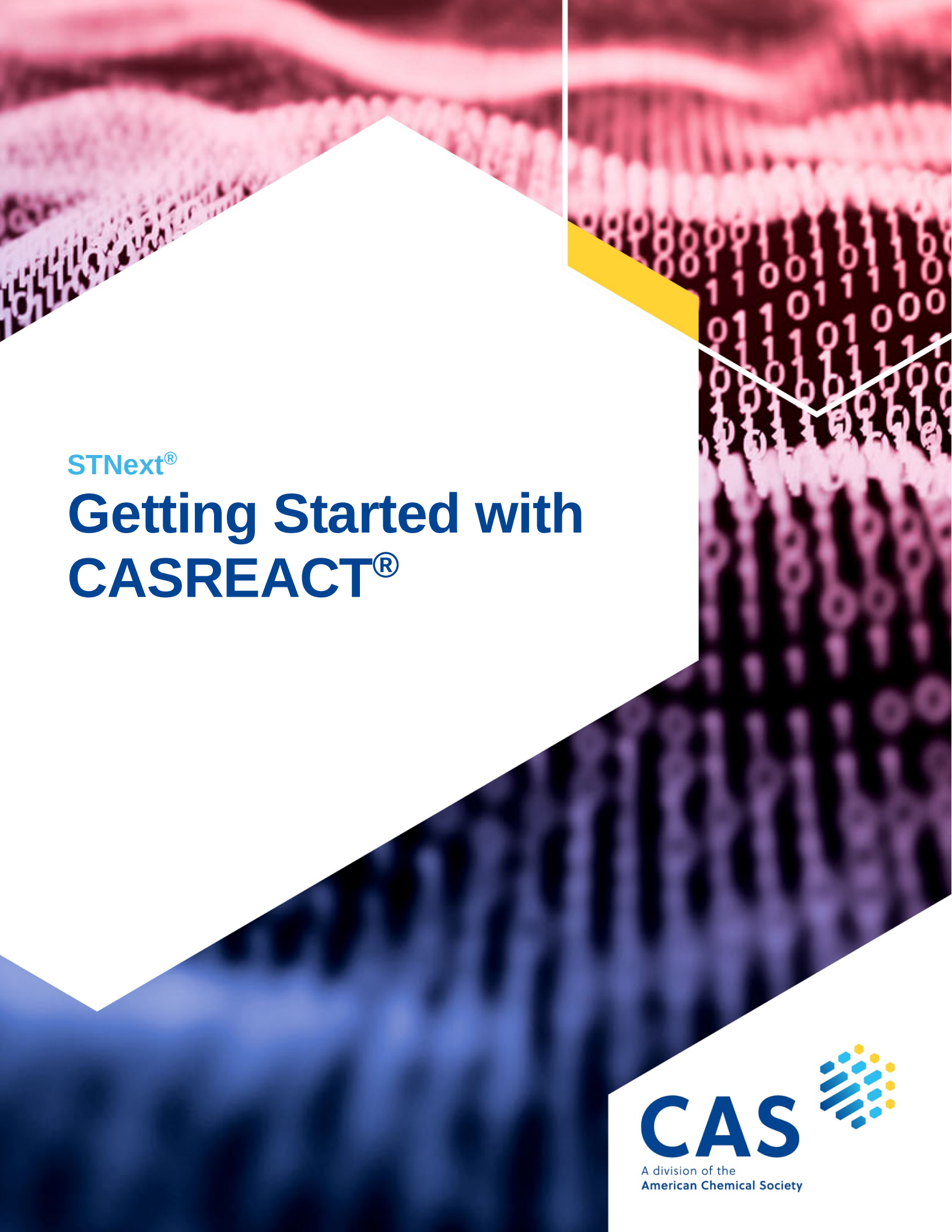


STNext®

Getting Started with CASREACT®

CAS
A division of the
American Chemical Society

Table of Contents

Getting Started with CASREACT

General Information

This getting started guide gives you a brief overview of what is available in CASREACT for answering your reaction questions.

Database Content

CASREACT, the Chemical Abstracts Reaction Search Service, offers you easy access to current reaction information found in literature covering synthetic organic chemistry. The literature includes journals and patents from 1840 to the present. As of end of 2024, the database contained more than 2.3M records. In these records, you will find in-depth reaction and condition information on more than 150 million single- and multi-step reactions. New information is added to the database on a daily basis.

Learning Database

To assist new CASREACT searchers, the LCASREACT^{SM} learning database contains a fixed number of documents with single- and multi-step reactions. All the search and display features found in CASREACT are available in LCASREACT, and there are no search or display fees in LCASREACT. Therefore, LCASREACT is a good place to practice reaction searching techniques and to familiarize yourself with display features.

Search Options

CASREACT offers quick retrieval of answers to your reaction questions with a variety of search options. You can look for reaction information by using:

- Reaction participant structures
- CAS Registry Numbers
- Functional groups
- Functional group class terms
- Special reaction terms such as yields
- Bilbiographic terms
- Search results from other STN databases

Indexes, abstracts, and bibliographic information are also searchable and offer an easy way to refine your search results. For example, you can restrict the answers to work being done by a specific company or to papers published within the past year.

Reaction Queries

In CASREACT, you can specify many things about substances that participate in a reaction:

- Specify the role you want a substance to play in the reaction
- Mark reaction sites
- Indicate atom mapping through the reaction
- Require that a reaction include specific solvents and/or catalysts

STN Interfaces

STN makes it easy to construct a reaction query made up of structures for the reactants and/or products through a structure drawing interface. Consult STNext online help for how to construct strucure reaction search queries.

Looking at Answers

CASREACT offers a variety of ways to look at the answers to your reaction questions. By default, you see a compact display of the first reaction that fits your search query in the most recent document retrieved, i.e., the first hit reaction. The structure diagrams of the reactants and products are shown with reagents, solvents, catalysts, and reaction conditions noted on the reaction arrow. The source and publication year are included in the display.

You can alternatively scan some of the answers to see if your search is on target. Scanning is free, and you can see the title of the paper and the compact display of the first hit reaction.

Complete records with all the bibliographic information, abstracts, indexing, and all the single-step reactions can also be displayed. You can view your answers online or have them delivered to you.

Additional Information

In this getting started guide, we illustrate the various ways of answering your reaction information needs. More information is readily available by referring to:

- *CASREACT User Guide*
- CASREACT Database Summary Sheet

In addition, extensive help messages are available while you are online:

- => HELP DIRECTORY in CASREACT for a list of help messages
- => HELP SFIELD to see the available search fields
- => HELP FORMAT to see the available display formats
- => HELP DFIELD to see the available display fields

STN Help Desks

- You can also get fast and friendly assistance from the experts at your STN Service Center's Help Desk. For contact information, visit: www.cas.org.

Searching in CASREACT

Using CAS REGISTRY Numbers

If you know the CAS Registry Numbers for reaction participants, it is very easy to retrieve reactions. Simply search the CAS Registry Number in the reaction role search fields. The available role search fields are:

- Reactant (/RCT)
- Product (/PRO)
- Reagent (/RGT)
- Reactant or Reagent (/RRT)
- Solvent (/SOL)
- Catalyst (/CAT)
- Nonproduct (/NPRO)
- Basic Index [all roles] (/BI or no qualification)

CAS REGISTRY NUMBER SEARCH OPTIONS

For a single reaction participant:

- Enter SEARCH (S) followed by the CAS Registry Number with /ROLE appended, e.g., => S 50-00-0/RCT.

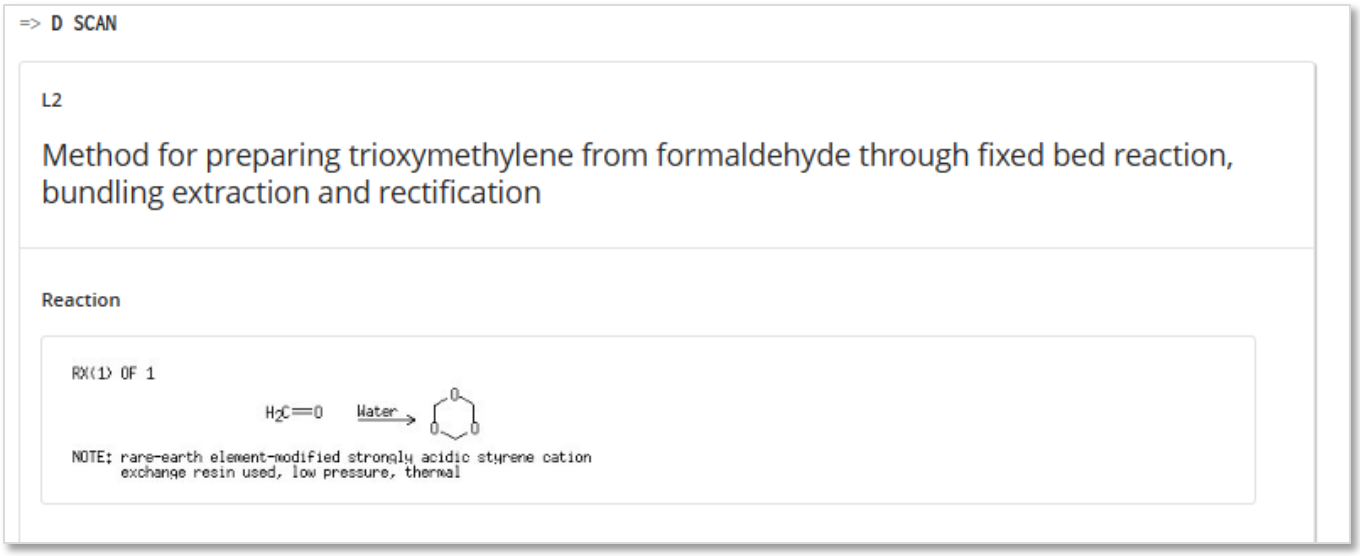
For multiple reaction participants:

- Combine the /ROLE search terms with (L) proximity to search within the same single- or multi-step reaction, e.g., => S 50-00-0/RCT (L) 110-88-3/PRO.

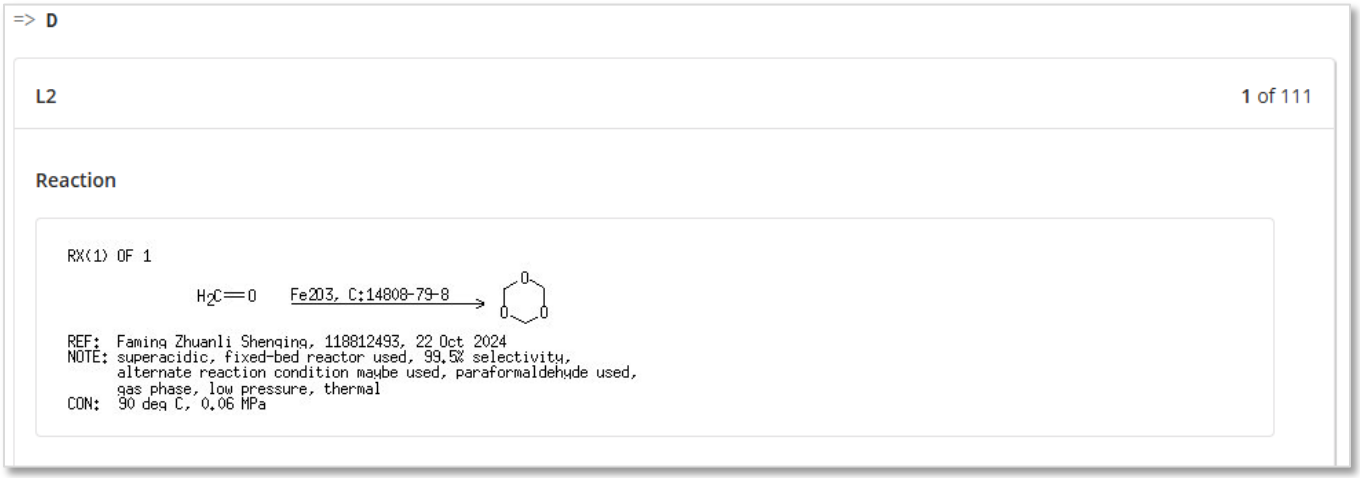
Search Example:
Find reactions that produce trioxane (110-88-3) from formaldehyde (50-00-0).

```
=> s 50-00-0/RCT (L) 110-88-3/PRO

         73426 50-00-0/RCT
           128 110-88-3/PRO
L2         111 50-00-0/RCT (L) 110-88-3/PRO
```

After retrieving answers to your search, you can verify whether they meet your expectations at no charge by using D SCAN.



Once you are satisfied that the results meet with your expectations, you may display more detail by using the default DISPLAY (D) command. Entering simply “D” at a command prompt (=>) shows you the first hit reaction from the most recent retrieved record to enter the database. The default display format (FHIT CRD) shows the compressed form of the reaction with additional detail, including the source information.



The REF field shows the source information. The NOTE field adds detail about the reaction.

Refining Your Answer Set

If you wish to further qualify your answer set, simply use the L-number of the answer set with additional terms.

- Use the (L) operator to limit the search with a single reaction sequence.
- Use the term ANY/CAT to include or exclude catalyzed reactions.
- Use the (NOTL) operator to eliminate specific reaction participants.

- Use 1/NS to limit the search to single-step reactions.
- The /NS field is a numeric field that specifies the number or range of reaction steps desired in your answers.

Search Example:
Sulfuric acid (7664-93-9) is a common catalyst used in the preparation of trioxane from formaldehyde. Find reactions that use other catalysts.

```
=> S L1 (L) ANY/CAT (NOTL) 7664-93-9/CAT

       1263705 ANY/CAT
         26022 7664-93-9/CAT
L2          44 L1 (L) ANY/CAT (NOTL) 7664-93-9/CAT
```

To see the first hit reaction in the most recent retrieved record with highlighted search terms, use the FHIT format. In this display, bonds that are partially or completely broken or formed in the reaction are indicated by an asterisk (*). Letters are used to indicate reactants, reagents, and products.

Using Bibliographic Search Terms

The bibliographic, abstract, and indexing information (apart from the CAS Registry Numbers that are not part of indexed reactions) for a record is also searchable and may be combined with the reaction answer set. The Boolean operators AND, OR, and NOT may be used to combine these document record search terms with a reaction answer set.

Search Example:
Did any of the trioxane synthetic papers come from Hoechst?

```
=> S L1 AND HOECHST/CS

          2500 HOECHST/CS
L3           4 L1 AND HOECHST/CS
```

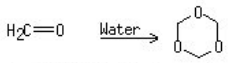
Another option for viewing answers shows the bibliographic information in a compressed format along with the compressed display of the first hit reaction. This is the CBIB FCRD display format.

```
=> D CBIB FCRD
```

L3 1 of 4

Reaction

RX(1) OF 1



NOTE: equilibrium, Amberlyst XN1010 cationic exchange resin
CON: 95 - 100 deg C

129:69105 Process for the production of trioxane from formaldehyde. Steele, Douglas W.; Jawaid, Mahmood N. A.; Allen, William Stewart; Thames, Norwood E., Jr.; Reck, Dwight A. (**Hoechst** Celanese Corporation, USA). (CELANESE CORP). (Celanese). U.S. US 5767294 A 19980616, 12 pp., Cont.-in-part of U.S. Ser. No. 18,688, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1993-162689 19931206. PRIORITY: US 1993-18688 19930217.

Searching with Functional Groups

CASREACT Functional Groups

Common reacting structural entities, called functional groups, may also be searched in CASREACT by using class or ring descriptions. The available search terms are derived from the structures of the reactants, reagents, and products.

To search using functional groups, enter the functional group term and its qualifying reaction role search field. The search fields allow you to specify not only that the structural feature is present in a reaction participant but also whether it is a reacting, forming, or nonreacting functional group. The available search fields are:

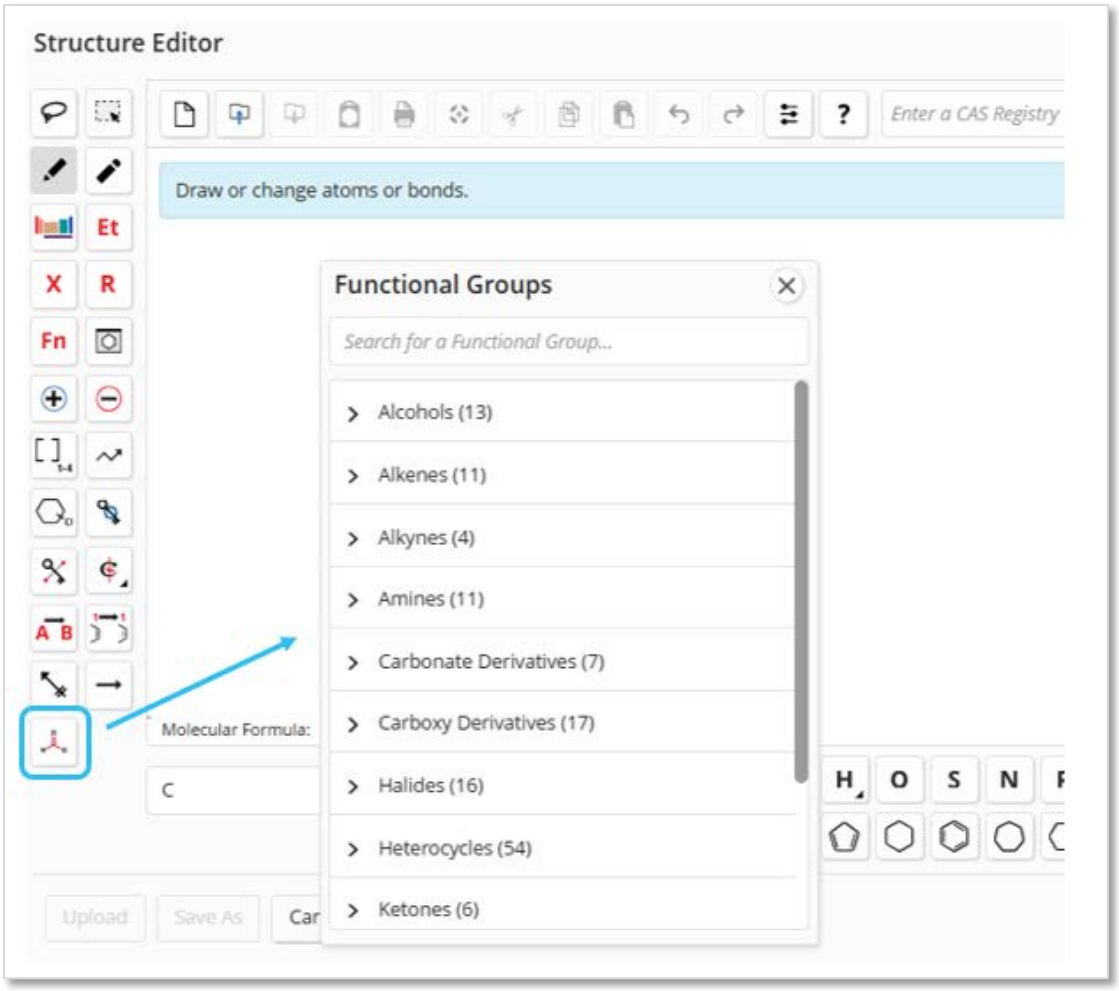
- Functional Group in Reactant (/FG.RCT)
- Functional Group in Product (/FG.PRO)
- Functional Group in Reagent (/FG.RGT)
- Reacting Functional Group (/FG.RXN)
- Forming Functional Group (/FG.FORM)
- Nonreacting Functional Group (/FG.NON)

The first three fields simply indicate that the functional group be present in the specified reaction participant. Use the last three fields to specify that a participant is reacting or forming or present, but not participating in the reaction.

Functional Group List

A list of valid functional group search fields and list of functional group search terms may be displayed online by entering HELP FGA (or HELP FGC for functional group classes) at a command prompt in CASREACT.

The list of valid functional groups can also be found in the structure drawing window of STNext.



Functional Group Search

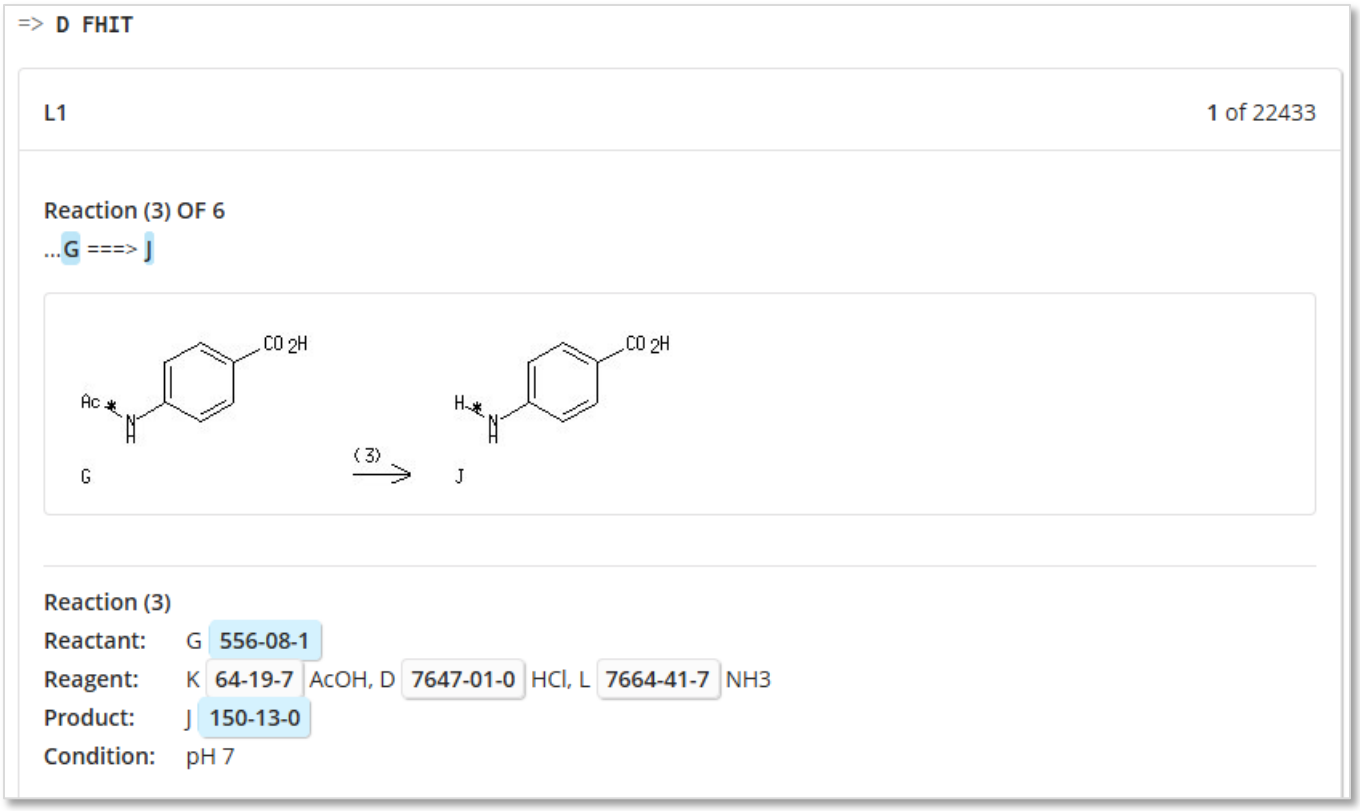
To perform a functional group search, enter the SEARCH command followed by the functional group qualified with the appropriate role, e.g., => S AMIDE/FG.RXN.

To use more than a single reaction participant, combine the terms with (S) proximity to map the reacting atoms to the formed atoms.

Search Example:
Find reactions that convert an amide to a primary amine.

```
=> S AMIDE/FG.RXN (S) PRIMARY AMINE/FG.FORM

        195181 AMIDE/FG.RXN
        226483 PRIMARY AMINE/FG.FORM
L1       22430 AMIDE/FG.RXN (S) PRIMARY AMINE/FG.FORM
```

The functional group terms are not displayable, but if you use a hit display format, the hit designations are highlighted. Examine the structure diagrams of the hit reaction participants for the functional groups that match the search question.

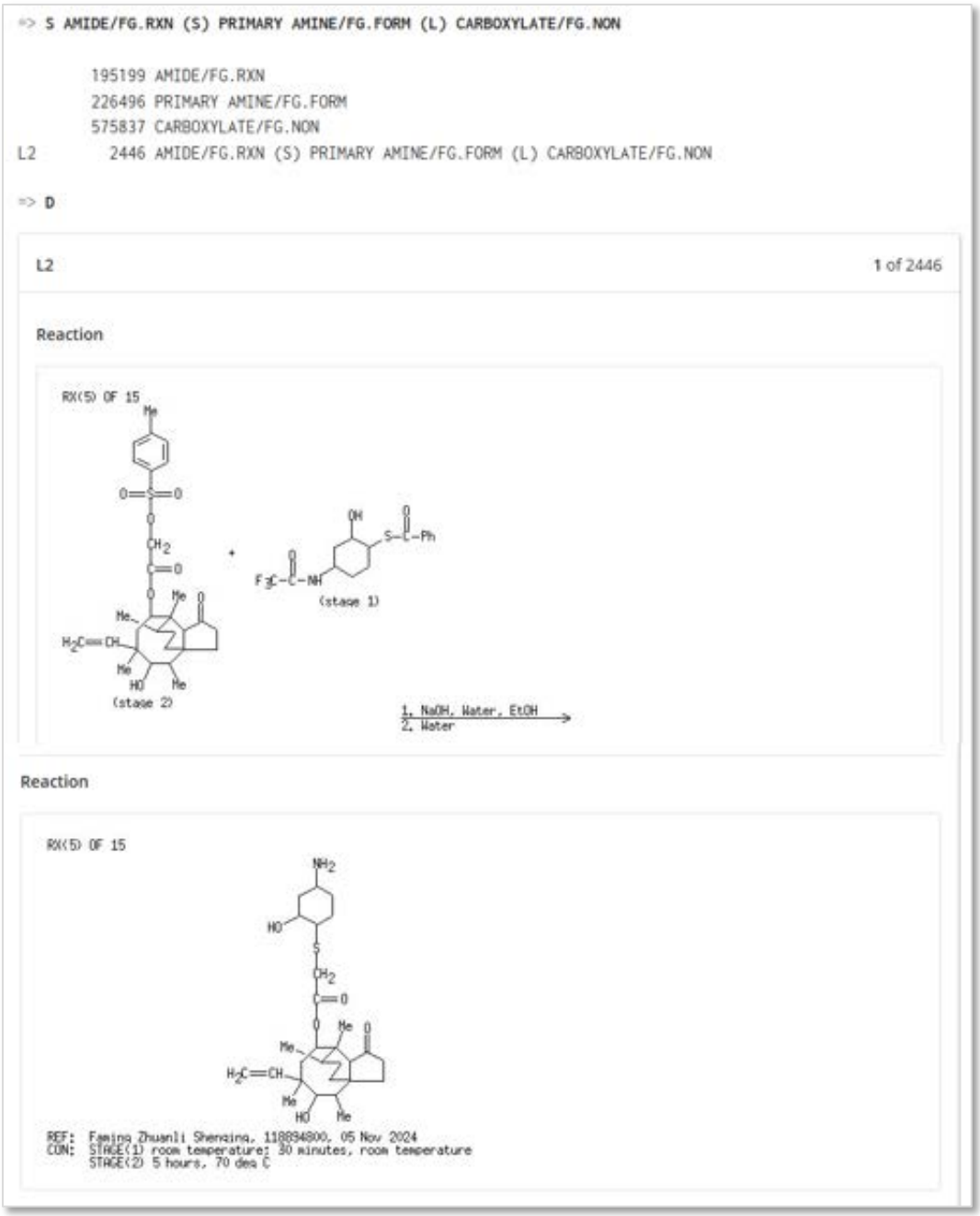


The reaction map (G → J) and the reaction diagram (structures) show the initial reactant and the final product.

Nonreacting Functional Groups

Use (L) proximity to link a nonreacting functional group into the reaction search. The (L) proximity keeps the additional terms within the same reaction sequence.

Search Example:
Find reactions that convert amides to primary amines in the presence of nonreacting carboxylate.



Cost-effective Searching

With functional group searching, plan your strategy so all the functional group terms are included in a single search. You can add functional group search terms to an answer set, but that is billed as an additional functional group search.

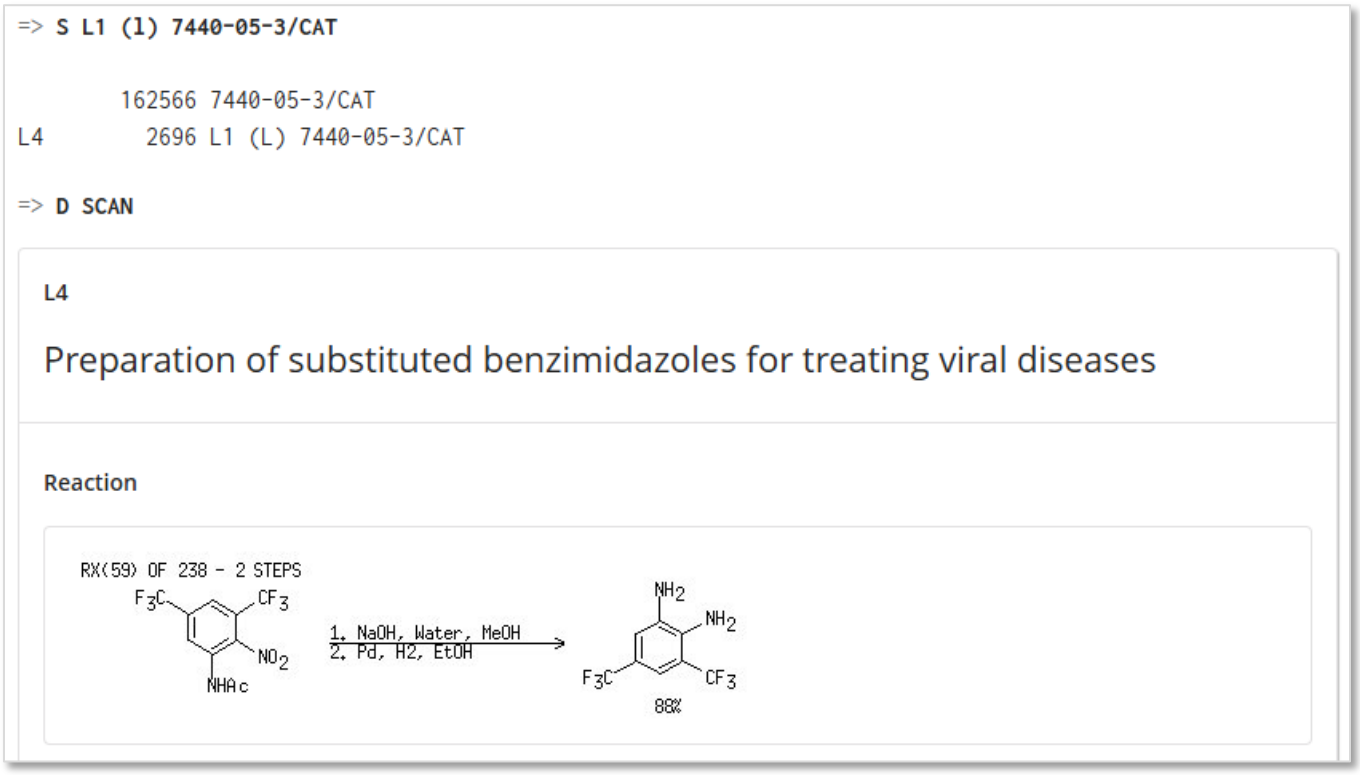
Refining Your Answer Set

You may use a functional group answer set L-number as a search term in further searching. The following illustrates the use of CAS Registry Number and bibliographic terms in combination with a functional group search.

Using Functional Groups and CAS Registry Number

Functional groups can be combined with CAS Registry Number search terms either in the initial search or in a subsequent refinement step. Use the (L) operator to combine search terms.

Search Example:
Was palladium (7440-05-3) used as a catalyst in any of the reactions found in the amide-primary amine functional group search?



Using Functional Groups and Bibliographic Terms

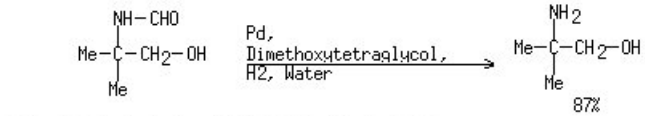
Functional group search terms or answer set L-numbers can be combined with bibliographic search terms or answer set L-numbers by using Boolean operators, AND, OR, or NOT.

Search Example:
Are any of the reactions in L3 found in patents?

```
=> S L3 AND PATENT/DT

        813427 PATENT/DT
L4        1569 L3 AND PATENT/DT

=> D 1
```

L4 **1** of 1569

Reaction



REF: PCT Int. Appl., 2024132621, 27 Jun 2024
NOTE: high pressure, thermal
CON: 220 deg C, 20 bar

Searching with Functional Group Class Terms

Class Terms

Broad classes of functional groups may also be used as search terms. When a class term is used in a search, STN automatically searches the specific functional groups included in the class term definition. For example, the class term KETONES automatically searches ACYCLIC KETONE, CYCLIC KETONE, O-QUINONE, and P-QUINONE.

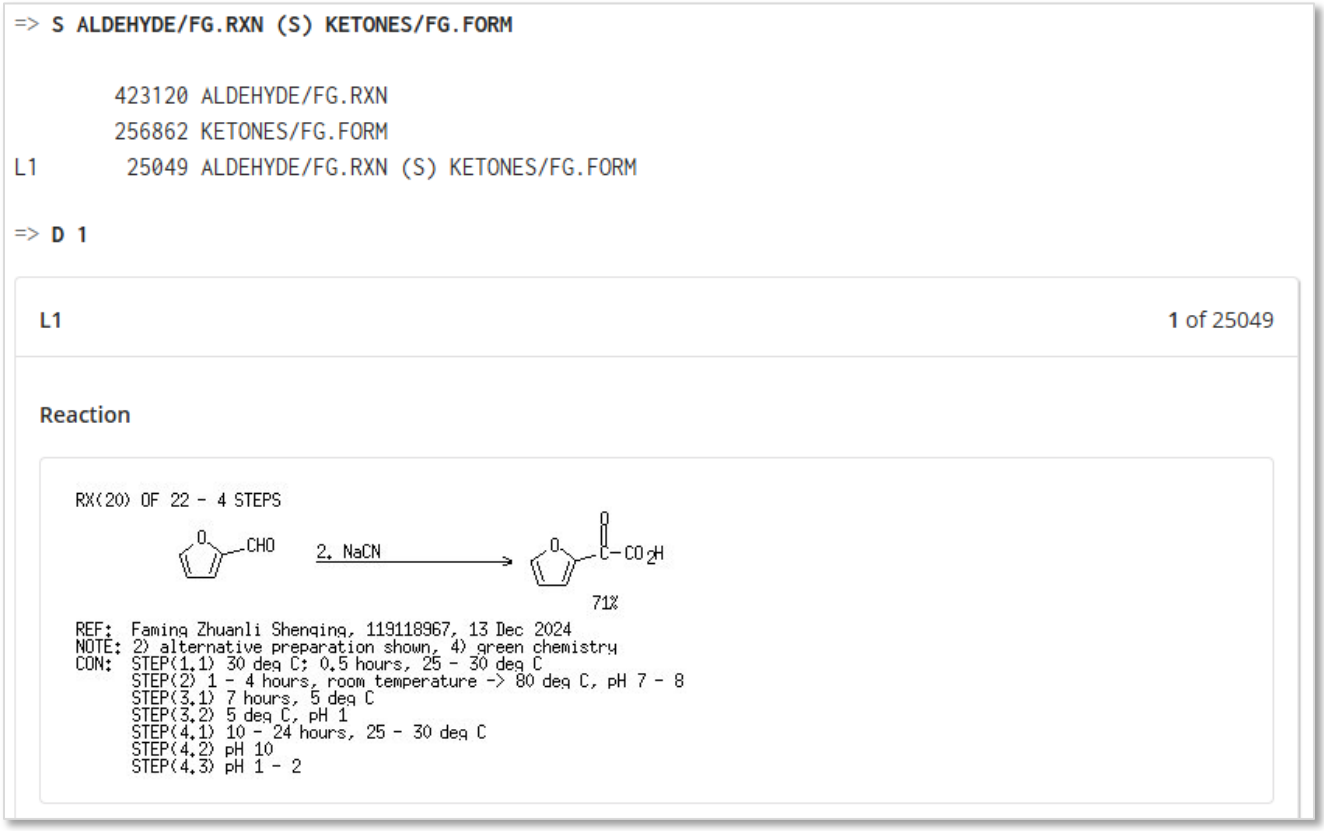
Class Term Definition

A list of valid functional group class terms may be displayed online by entering HELP FGC at a command prompt in CASREACT.

Reaction Roles

Class terms may be searched in the same manner as functional group terms and in the same search fields. When combining more than one class term, use (S) proximity between terms to map the reacting group to the formed group. Use (L) proximity for nonreacting groups to keep all reaction participants within a single reaction sequence.

Search Example:
Find studies that contain reactions that convert aldehydes to ketones.



Refining Your Answer Set

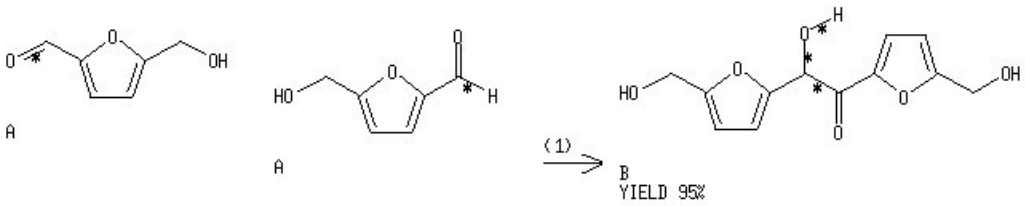
These search results may also be refined with other types of CASREACT search terms.

Search Example:
How many single-step catalyzed reactions were retrieved in L1?

```
=> S L1 (L) ANY/CAT (L) NS=1

       1263767 ANY/CAT
       2410168 NS=1
L2        4421 L1 (L) ANY/CAT (L) NS=1

=> D FHIT
```

L2 **1** of 4421

Reaction (1) OF 10
2 **A** ===> **B**...



Reaction (1)
Reactant: A **67-47-0**
Product: B **1403335-29-4**
Catalyst: **154643-41-1** 1H-1,2,4-Triazole, 4,5-dihydro-5-methoxy-1,3,4-triphenyl-
Solvent: **616-38-6** Me2CO3
Condition: 1 hour, 60 deg C
Note: green chemistry-solvent

Searching with Special Reaction Terms

Special Terms

There are several CASREACT reaction search fields that may be used for special searches or used to refine broad-based CAS Registry Number or structure searches in CASREACT.

- Number of Steps in a Reaction
- Yield Information
- Words in Reaction Notes

Reaction Steps

You can specify a specific number of reaction steps or a range of reaction steps by using the Number of Steps (/NS) field. /NS is a numeric field and may be searched by using the spectrum of numeric operators. You can easily limit an answer set to single-step reactions by using NS=1 or 1/NS in your search logic. Use (L) proximity to combine the number of steps with other reaction search terms to restrict results to a single reaction sequence.

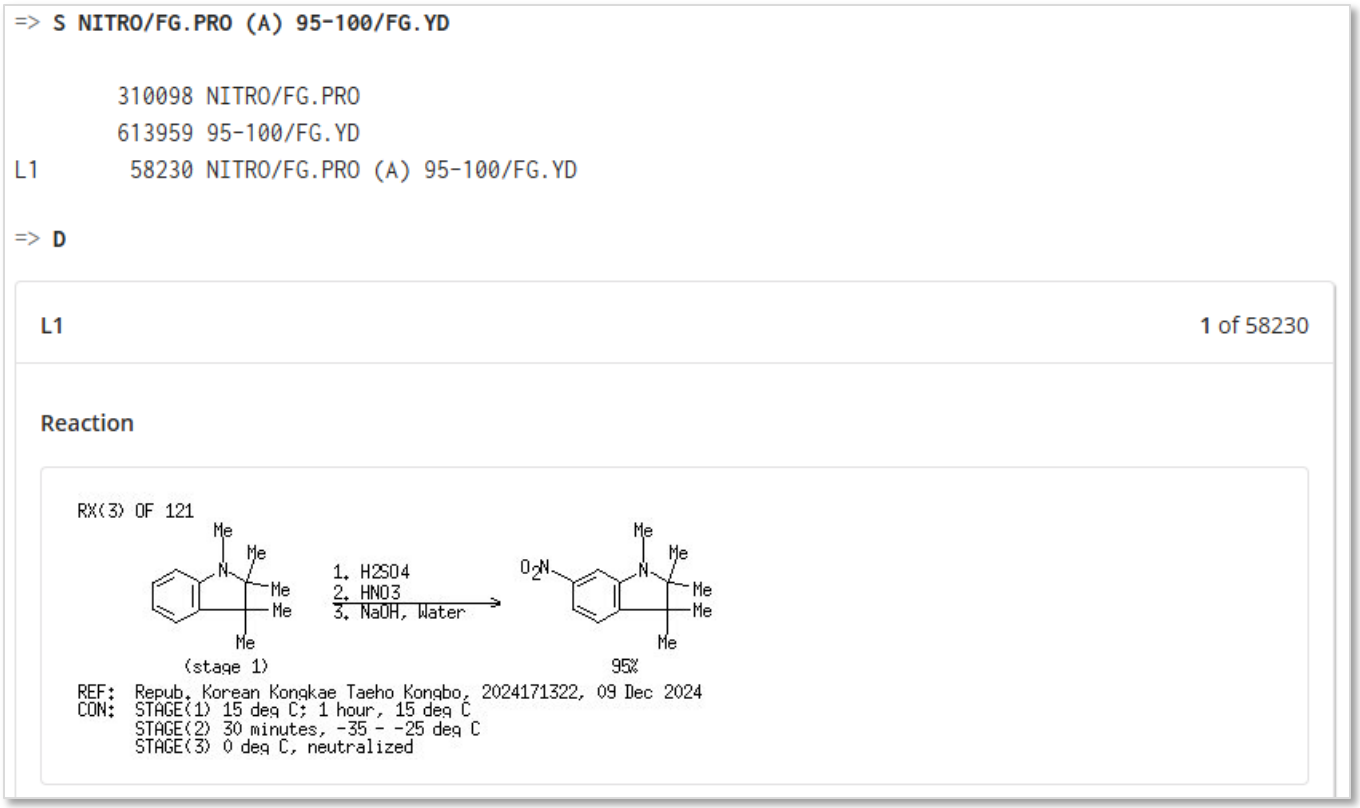
Yield Information

Yield information may also be used as a search term. When the original document gives the yield for the product, it is included in the reaction information in the CASREACT record. The Yield (/YD) field is numeric and may be searched by using numeric operators. For further information, enter HELP YIELD at a command prompt in CASREACT.

Use (A) proximity to combine the yield information with a specific product, e.g., => S 138687-69-1/PRO (A) YD>=50.

If you are searching with a functional group, enter the desired yield in the Functional Group Yield (/FG.YD) field. Use (A) proximity here as well, e.g., => S NITRO/FG.FORM (A) 95-100/FG.YD.

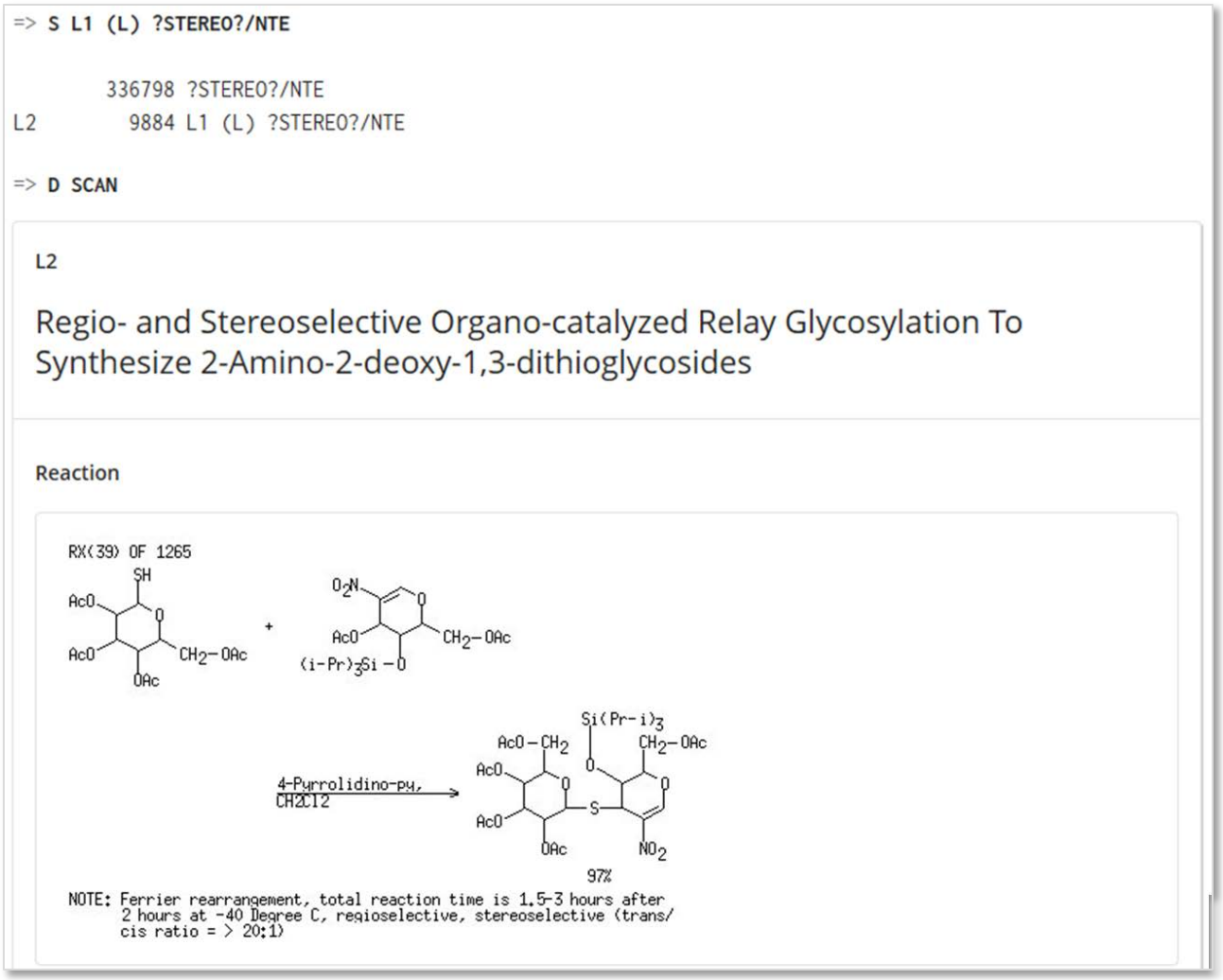
Search Example:
Find high-yield (95-100%) preparations of products containing a nitro group.



Words in Reaction Notes

The text displayed in the Reaction Notes (/NTE) field is searchable. You may even use left truncation and simultaneous left and right truncation on the search terms in the NTE field. Search terms in this field are combined with other reaction search terms by using (L) proximity to limit the results to a single reaction in the document record.

Search Example:
Were any of the high-yield nitro preparations in L1 stereoselective?



Searching with Bibliographic Search Terms

Document-Based Database

CASREACT also includes many types of bibliographic search terms for creating and refining reaction answer sets. If you do not qualify a search term, it is searched in the Basic Index, which contains single words from the title, abstract, supplementary terms, indexing terms, and reaction notes in the document record. The CAS Registry Numbers indexed for the document record are not searchable unless they are for an indexed reaction participant. Left truncation and simultaneous left and right truncation are available in the Basic Index.

Bibliographic Terms

The bibliographic terms offer a way to create an answer set that contains document information relevant to your reaction search.

Search Example:
Find papers dealing with a Claisen rearrangement.

```
=> S CLAISEN REARRANG?

         13577 CLAISEN
             2 CLAISENS
         13578 CLAISEN
                 (CLAISEN OR CLAISENS)
         73004 REARRANG?
L1        5635 CLAISEN REARRANG?
                 (CLAISEN(W)REARRANG?)
```

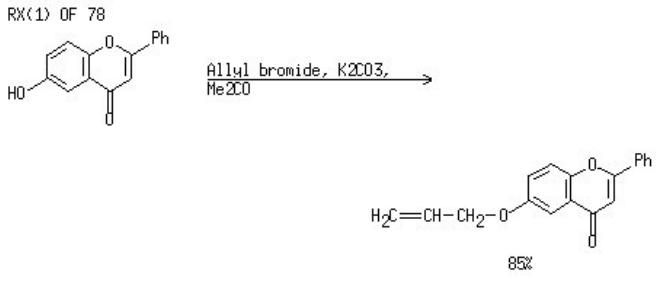
Searches of this type can be used to create a small answer set to be combined with reaction search terms or to narrow the reaction search result. Use Boolean operators to combine bibliographic search results with reaction search results.

```
=> S L1 AND HETEROCYCLES/FG.RCT

       1403821 HETEROCYCLES/FG.RCT
L2        3857 L1 AND HETEROCYCLES/FG.RCT

=> D SCAN
```

L2

Synthesis of novel oxa-carbocycle annulated flavones and bis-flavones by ring closing/cross metathesis

Reaction



Range Searches

Searches in CASREACT may be restricted to a Collective Index Period, a CA Volume, a CA Publication Year, an Accession Number, or a collection of these parameters by using SEARCH RANGE.

Search Example
For the Claisen Rearrangement search that included heterocycles as a functional group, how many were entered into CASREACT in 2024?

```
=> S L2 RANGE=(2024)

         52746 HETEROCYCLES/FG.RCT
L3          46 L1 AND HETEROCYCLES/FG.RCT
```

Searching with Answer Sets from Other STN Databases

Crossover Searches

An answer set created in another STN database may be used as a search term in CASREACT. Simply create an answer set in an STN database, enter CASREACT, and search the answer set L-number from the initial search. The query from the initial search is automatically searched in CASREACT. A crossover answer set may be combined with a reaction search just like any other L-number.

For further information, enter HELP CROSSOVER at a command prompt.

Special Type of Crossover

There are two special types of crossover into CASREACT:

- Crossover from CA/CAplus (also HCA/HCAplus or ZCA/ZCAplus)
- Crossover from CAS REGISTRY

CA/CAplus Crossover

If you search an L-number from CA/CAplus in CASREACT, the Accession Numbers from the database are searched in CASREACT. For further details, enter HELP CACROSSOVER at a command prompt in CASREACT.

REGISTRY Crossover

If you search a REGISTRY L-number answer set in CASREACT, the CAS Registry Numbers contained in the answer set are searched. The L-number may be qualified with any of the reaction role search fields. This is a convenient way to search broad groups of compounds in the reaction search fields such as /CAT.

The term CASREACT appears in the Locator field (/LC) of every CASREACT substance found in REGISTRY. This term may be used to restrict the answer set to only those substances found in CASREACT prior to the actual crossover. Enter HELP RNCROSSOVER at a command prompt in CASREACT for further details.

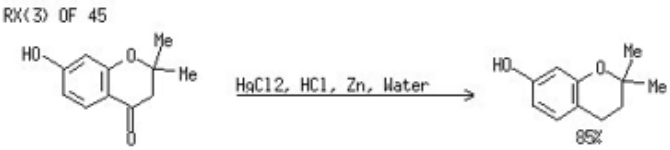
Search Example:
Find mercury-containing catalysts used in phenolic reactions.

```
=> FILE REG
=> S HG/ELS AND CASREACT/LC

         68233 HG/ELS
      25719506 CASREACT/LC
L1       13050 HG/ELS AND CASREACT/LC

=> FILE CASREACT
=> S L1/CAT (L) PHENOL/FG.RCT

          2251 L1/CAT
        444758 PHENOL/FG.RCT
L2         239 L1/CAT (L) PHENOL/FG.RCT

=> D SCAN
```

L2

Efficient total synthesis of naturally occurring anti-TMV compound gramniphenol G

Reaction

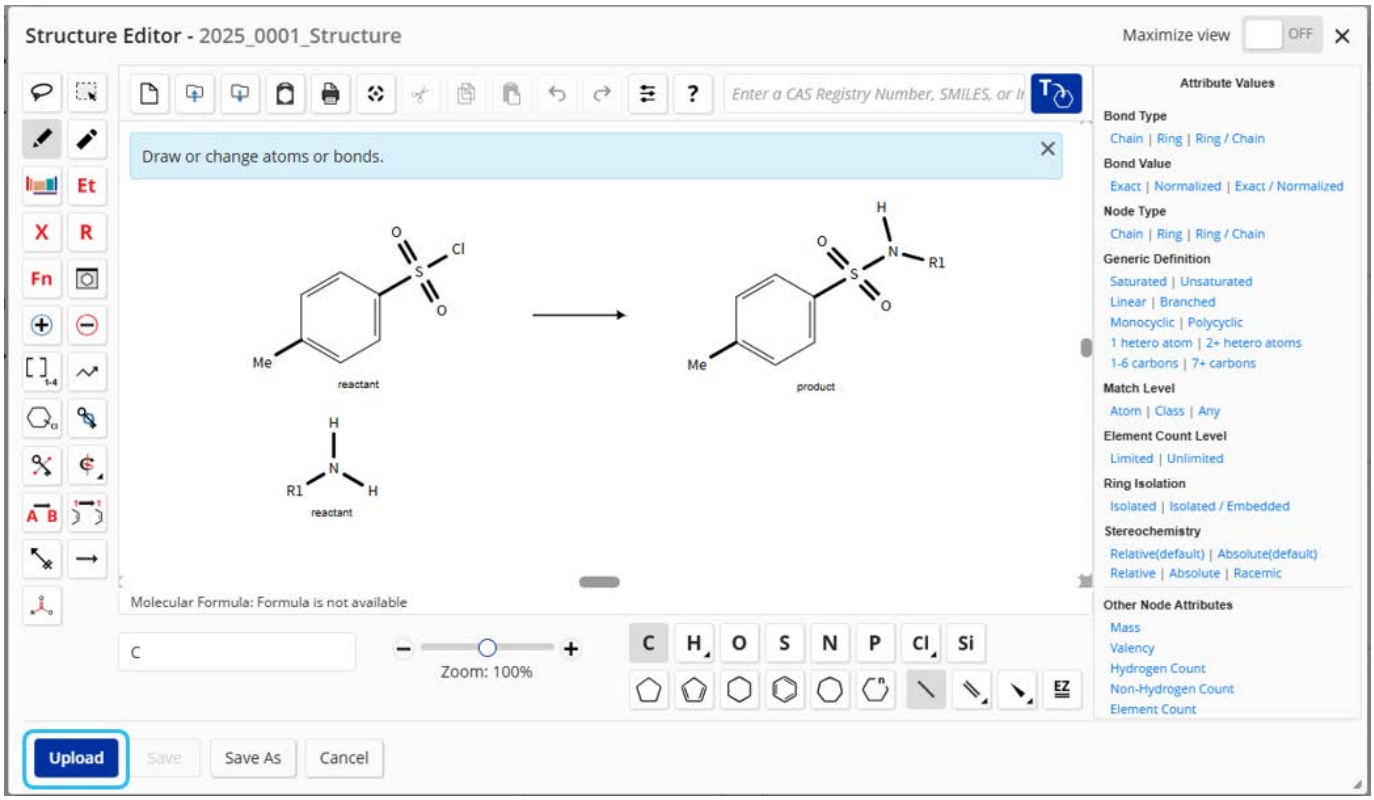


Reaction Structure Searching

All reactants, reagents, and products indexed in CASREACT are structure searchable.

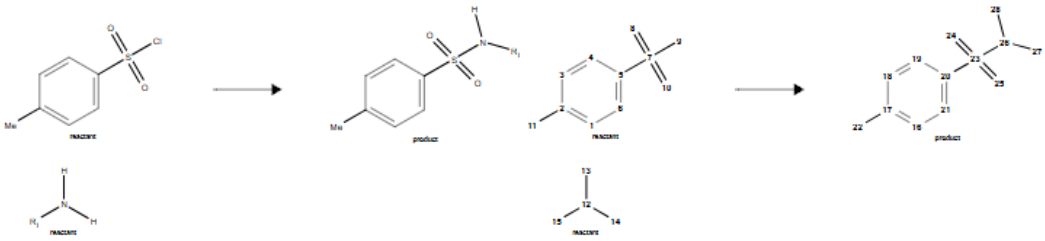
Consult STNext online help for how to construct strucure reaction search queries.

With a structure reaction created, the next step is to upload the reaction.



Upon uploading, review the reaction displayed to verify it uploaded properly.

```
=>
Uploading structure file: 2025_0001_Structure
```



```
R-Group Definitions
R1: Cy,Hy
Node Attributes
Ring Nodes : 1  2  3  4  5  6  16  17  18  19  20  21
Chain Nodes : 7  8  9  10  12  13  14  23  24  25  26  28
Bond Attributes
Ring Bonds : 1-2  2-3  3-4  4-5  5-6  6-1  16-17  17-18  18-19  19-20  20-21  21-16
Chain Bonds : 2-11  5-7  7-8  7-9  7-10  12-13  12-14  12-15  17-22  20-23  23-24  23-25  23-26  26-27  26-28
Exact Bonds : 2-11
Normalized Bonds : 1-2  2-3  3-4  4-5  5-6  6-1  16-17  17-18  18-19  19-20  20-21  21-16
Exact/Normalized Bonds : 5-7  7-8  7-9  7-10  12-13  12-14  12-15  17-22  20-23  23-24  23-25  23-26  26-27  26-28
Markush Attributes
Match Level (ATOM) : 1  2  3  4  5  6  16  17  18  19  20  21
Match Level (CLASS) : 7  8  9  10  11  12  13  14  22  23  24  25  26  28
Element Count Level (LIMITED) : 1  2  3  4  5  6  7  8  9  10  11  12  13  14  16  17  18  19  20  21  22  23  24  25  26
28


L1      STRUCTURE UPLOADED
```

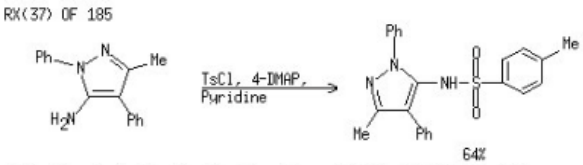
Once verified, run a sample search.

```
=> S L1

SAMPLE SEARCH INITIATED 13:36:31 FILE 'CASREACT'
SCREENING COMPLETE -    38016 REACTIONS TO VERIFY FROM     1150 DOCUMENTS

 13.5% DONE      5126 VERIFIED        54 HIT RXNS                        12 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:    748652 TO   771988
PROJECTED ANSWERS:            3153 TO     4847

L2           12 SEA SSS SAM L1 (       54 REACTIONS)
```

```
=> D L2
```

L2 1 of 12

Reaction



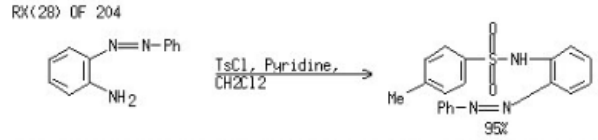
REF: Organic & Biomolecular Chemistry, 22(31), 6288-6293; 2024
CON: 12 hours, room temperature

After sampling, run the full reaction search.

```
=> S L1 FULL

FULL SEARCH INITIATED 13:39:37 FILE 'CASREACT'
SCREENING COMPLETE -   837233 REACTIONS TO VERIFY FROM    23197 DOCUMENTS

100.0% DONE    837233 VERIFIED     30078 HIT RXNS                    3998 DOCS
SEARCH TIME: 00.00.02

L3         3998 SEA SSS FUL L1 (    30078 REACTIONS)

=> D
```

L3 1 of 3998

Reaction



REF: European Journal of Organic Chemistry, 27(46), e202400854; 2024
CON: STAGE(1) 0 deg C; 8 - 9 hours, room temperature

Results may be refined in the same way that other reaction searches are refined. For example, we can limit the search to single-step reactions.

```
=> S L3 (L) NS=1

       2410168 NS=1
L4        3894 L3 (L) NS=1
```

The majority of the full reactions retrieved were single step reactions.

Conclusion

CASREACT offers you a wide variety of search methods that allow you to find the answers to your reaction questions by the means best suited to the question. Since CASREACT is a document-based database, you have access to bibliographic information as well as the synthesis information found in literature covering organic chemistry.

Once the answers have been obtained, you may view them by using any of the several available display formats that graphically display the reaction information, as well as the bibliographic, abstract, and indexing information.

CASREACT works very well in tandem with other STN databases, making your searches for reaction information efficient and cost effective.

Solution images are included for illustrative purposes only. Your experience may vary based on recent enhancements or product license.

CAS is a leader in scientific information solutions, partnering with innovators around the world to accelerate scientific breakthroughs. CAS employs over 1,400 experts who curate, connect, and analyze scientific knowledge to reveal unseen connections. For over 100 years, scientists, patent professionals, and business leaders have relied on CAS solutions and expertise to provide the hindsight, insight, and foresight they need so they can build upon the learnings of the past to discover a better future.
CAS is a division of the American Chemical Society.

Connect with us at cas.org

CAS
A division of the
American Chemical Society