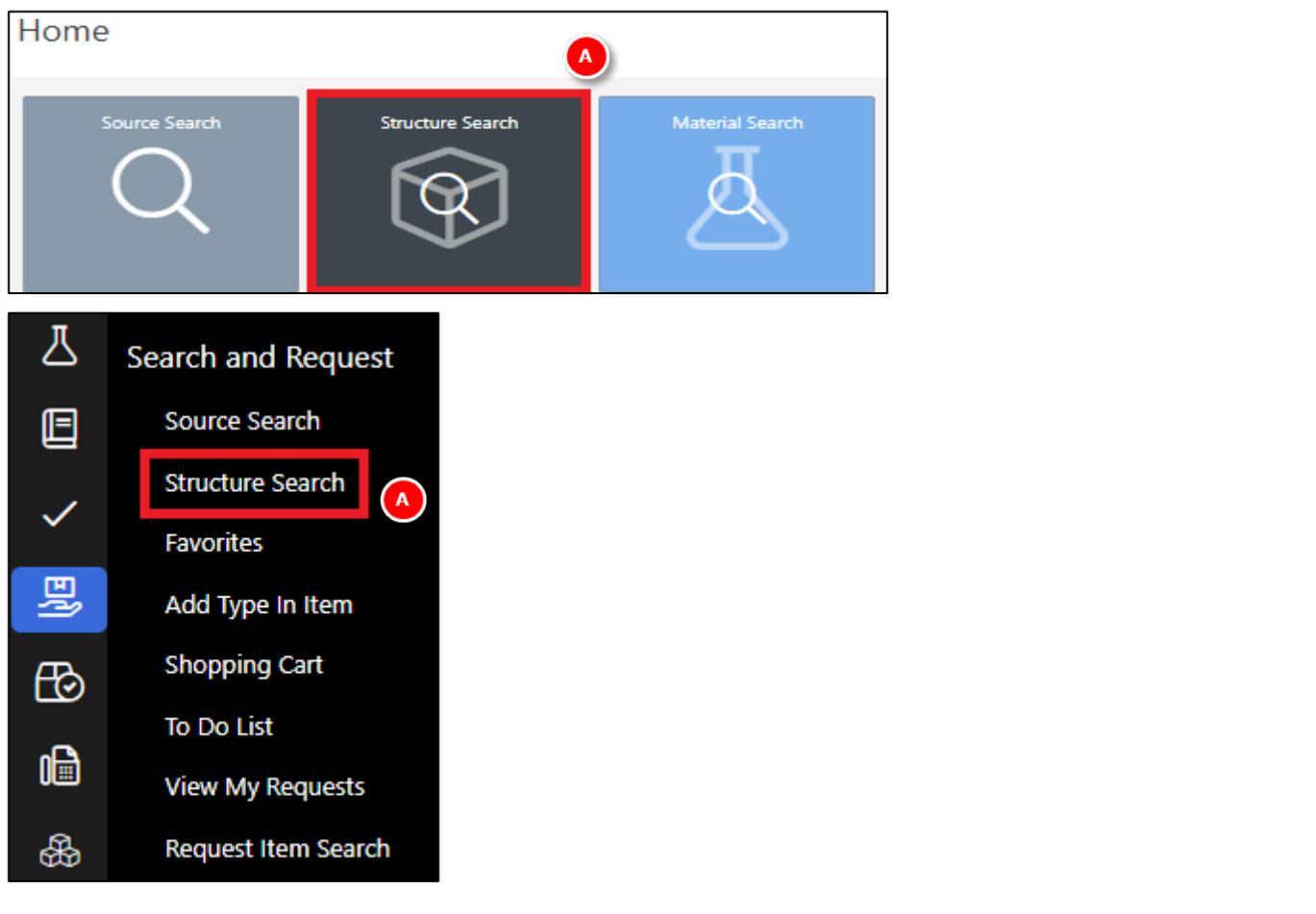


Overview

This quick guide will show you how to complete a Structure Search to find a chemical either in the inventory, or to purchase.

1. Structure Search Window
2. Retrieving Identifiers
3. Explore Structures & Sources OR
4. Explore Structures
5. Substructure Searches in the Inventory By Keyword

Steps	Screenshots
<p>1. Structure Search Window</p> <p>A. Click Structure Search or from the Menu go to Search and Request > Structure Search.</p> <p>B. Search for a structure using a MOL file (see below), SMILES code, SD (Structured Data) file or through chemical identifiers (like a CAS number). Either import, paste or draw structure:</p> <ol style="list-style-type: none"> a. Use Import or Paste to retrieve a structure from a .mol file. You can save .mol files from structures drawn in ChemDraw. b. OR Click Edit to draw the chemical structure. 	 <p>The screenshot shows the SciTrack interface. At the top, there is a 'Home' header. Below it, there are three main search buttons: 'Source Search' (grey), 'Structure Search' (dark grey with a red border and a red 'A' callout), and 'Material Search' (blue). Below these buttons is a 'Search and Request' menu. The 'Structure Search' option in this menu is also highlighted with a red border and a red 'A' callout. Other options in the menu include 'Source Search', 'Favorites', 'Add Type In Item', 'Shopping Cart', 'To Do List', 'View My Requests', and 'Request Item Search'.</p>

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C. If **drawing** a structure:

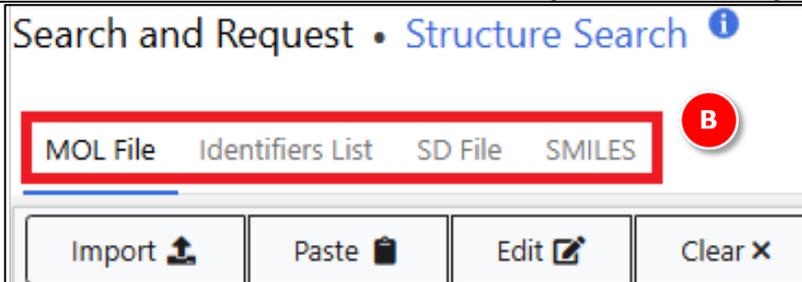
- 1) Draw the backbone of the structure using bonds and/or rings (options are displayed at the bottom of the window).
- 2) To change an atom to something other than carbon, click the **C** icon. Then select the atom you want to change on your structure, type in the new atom or group and press Enter. If you get an A instead of your group, try without Hydrogens.
- 3) When you are finished, click the escape icon on the drawing window to return your structure to the search screen.

D. Select search criteria:

Structure Databases

For maximum results, keep both checked. Some advanced search types may not be compatible with both databases. However, in subsequent steps you will be able to find *results to purchase* from both catalogues regardless of what is selected here.

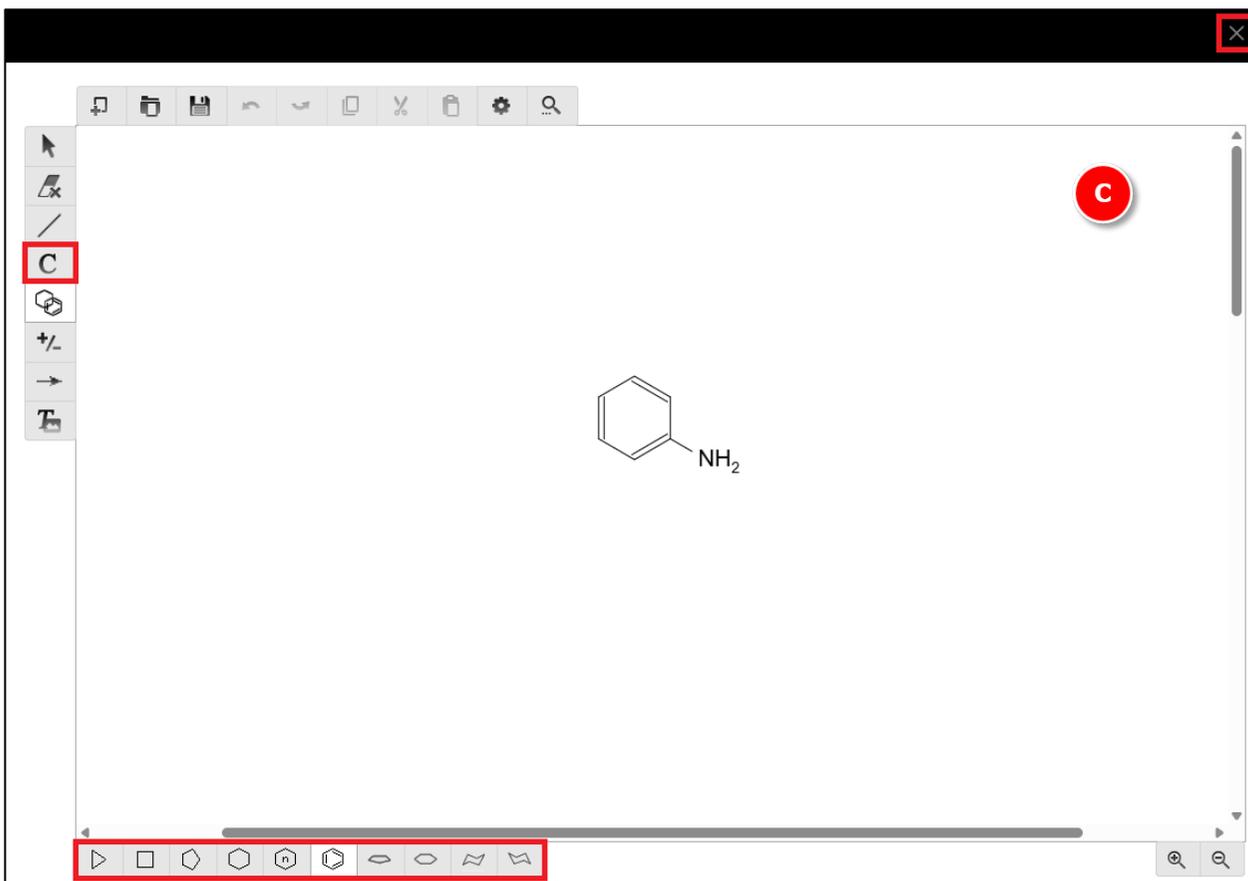
- If a drop-down search type option is not in bold, this means one of the selected catalogues is not compatible with one or more of the search criteria. Please deselect one of the catalogues to make it available.



Search and Request • Structure Search i

MOL File Identifiers List SD File SMILES B

Import Paste Edit Clear



C

Nc1ccccc1

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Basic > Equal search

This can be used to find an exact match of structure in the hosted catalogues or internal inventory.

Substructure search

You can refine the search to be more applicable. For best results, click the Advanced tab and select Substructure. Then click Add Criteria and select Molecular Weight. A narrower range will maximise the effectiveness of the search.

Advanced Search Criteria

Note: that you will need to deselect the Hosted Catalogs database to access most of the advanced search criteria.

Structure Databases

<input checked="" type="checkbox"/> eMolecules	D	Search Result Limit
<input type="checkbox"/> Hosted Catalogs		10,000
		10,000

⚠ Changing databases will reset criteria.

Use RMM Structure mapping On Off

Basic Advanced

Search Type

SUBSTRUCTURE ▾

SUBSTRUCTURE

SIMILARITY

TAUTOMER

PERFECT

Search Type

SUBSTRUCTURE

Add Criteria ▾

Atom Count

Chiral Center

CLogP

Has Metal

Hydrogen Acceptor

Hydrogen Donor

Lipinski Violations

Molecular Weight

Polar Surface Area

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2. Retrieving identifiers

Allow some time for the search to complete.

- A. To view the results, click either **Explore Structures** or **Explore Structures & Sources**. Details of the next steps are on the following pages.

Search and Request • [Structure Search Status](#)

[New Structure Search](#)

✓ Search Complete.

Retrieving Identifiers. Prioritizing Structures. ✓ Search Complete.

Structure Databases (In Priority Order)	Status	Search Time (seconds)	Prioritized Structures
eMolecules	⚠	61	ERROR
Hosted Catalogs	✓	5	113

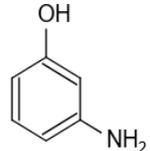
Using RMM Structure mapping

Total 113

Explore Structures
Explore Structures & Sources

Selected Sources [Edit Sources](#)

SUBSTRUCTURE



Advanced Criteria
100 <= Molecular Weight <= 150

A

SciTrack Quick Guide – Structure Search Procedure (Version 3.1)

3. Explore Structures & Sources

- A. Toggle the sources you want to see results for.
- B. Find the structure you are interested in and click the relevant source icon to see the results in the source search page.



shows Hosted Catalogue search results.



shows eMolecules results



shows results in the internal lab inventory

Note that results may be spread across multiple pages. Click the Source Next Page button at the bottom of the page to see the next page.

To purchase an item from the catalogue results, click  to add it to your cart. Complete your cart as per the instructions in SciTrack Quick Guide "3. Hosted Catalogue Purchasing".

Search and Request • [Structure Explorer](#) • Sourcing ?

[Back to Explore Structures](#) 
[New Structure Search](#) 

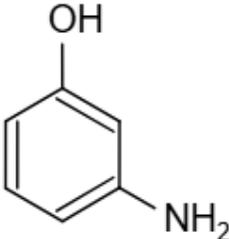
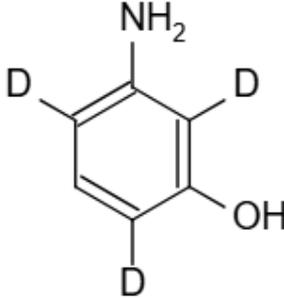
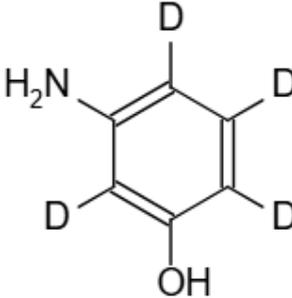
 13 Labs

 0 Stockrooms

 23 Hosted

 71 eMolecules

A

   3	   1	   1
		
SQ48541  109.125 u	SQ1493422 112.146 u	SQ1497477 113.152 u
Sources  7  10  69 B	Sources	Sources
 Properties(0) ▾	 Properties(0) ▾	 Properties(0) ▾

SciTrack Quick Guide – Structure Search Procedure (Version 3.1)

4. Explore Structures

- To find a chemical in the internal inventory, click Yes in the "In Inventory" panel. To search for a chemical to purchase, leave this selection on All.
- Select individual structures using the check boxes or click Select Page on the top left.
- View structures on additional pages by using the navigation aid at the bottom of the screen.
- Click Start Source Search icon.
- Click the relevant icon by the structure you want to see the inventory/purchase details for.



shows Hosted Catalogue search results.



Search and Request • Structure Explorer • Exploring ⚙

New Structure Search ⚙ Edit Sources Start Source Search 🔍

Selected Sources 🧪 🔍 J e

In Inventory Yes(13) No All

Select Page Clear All Selections Remove All Selections Filter 🏠 A ⋮

<div style="border: 1px solid gray; padding: 5px; margin-bottom: 5px;"> <input checked="" type="checkbox"/> B </div> <div style="text-align: center;"> <p>SQ48541</p> <p style="font-size: small;">109.125 u</p> <p style="text-align: center; font-size: x-small;">ⓘ Properties(0) ▾</p> </div>	<div style="text-align: center;"> <p>SQ1493422</p> <p style="font-size: small;">112.146 u</p> <p style="text-align: center; font-size: x-small;">ⓘ Properties(0) ▾</p> </div>	<div style="text-align: center;"> <p>SQ1497477</p> <p style="font-size: small;">113.152 u</p> <p style="text-align: center; font-size: x-small;">ⓘ Properties(0) ▾</p> </div>	<div style="text-align: center;"> <p>SQ11805</p> <p style="font-size: small;">123.152 u</p> <p style="text-align: center; font-size: x-small;">ⓘ Properties(0) ▾</p> </div>
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SQ48541

109.125 u

Sources

🧪 7
J 10
e 69
E

ⓘ Properties(0) ▾

SciTrack Quick Guide – Structure Search Procedure (Version 3.1)

5. Substructure Searches in the Inventory by Keyword

When looking for substructures in the inventory, you may get more complete results by using a keyword search than a structure search.

This is because some chemicals do not have an associated structure to search,

- A. Go to Source Search
- B. Optional: click Preferred next to Labs to only search preferred search locations. See Quick Guide “2. Configure Preferences” for more information.
- C. In the search criteria, enter key words with a wildcard (*) on either side and in-between words as required, and click Search. For example:
 - *amino*phenol*
 - *pyridine*
 - iron*sulfate

The search looks for the key words *in the order specified*, and a wildcard means results will be returned with other words before, between, or after the key words.

e.g. A search for ***boronic acid** will return anything that ends in the exact phrase “boronic acid”.



- D. Click the Labs button
- E. Results may be displayed on multiple pages. Click the info icon to see more container details.

The screenshot shows the SciTrack Source Search interface. At the top left, there is a 'Source Search' button with a magnifying glass icon, highlighted with a red box and labeled 'A'. Below it is a search input field containing '*aniline*', highlighted with a red box and labeled 'C'. To the right of the search field is a 'Reset' button and three filter buttons: 'Internal', 'External', and 'All'. Below these is a 'Labs' button with a checkmark and a flask icon, highlighted with a red box and labeled 'B'. To the right of the 'Labs' button is a 'Preferred (4)' button, also highlighted with a red box and labeled 'B'. Below the search interface, the results for '2,5-Dimethylaniline (1)' are displayed. The chemical structure is shown on the left, and the following information is listed on the right: CAS # 95-78-3, MDL # MFCD00007743, and Cust Compound ID SQ75698. Below the results, there is a table with columns for 'Pre-SciQuest', 'Janssen Chemica', '2,5-Dimethylaniline', 'UOAM000007679', '1466922', 'Created 2/06/2016', and '500 G (500 G) gase'. The table is paginated, with a red box highlighting the page navigation controls (1-10) and labeled 'E'.