5. Structure Search Procedure

Overview

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

Steps	Screenshots

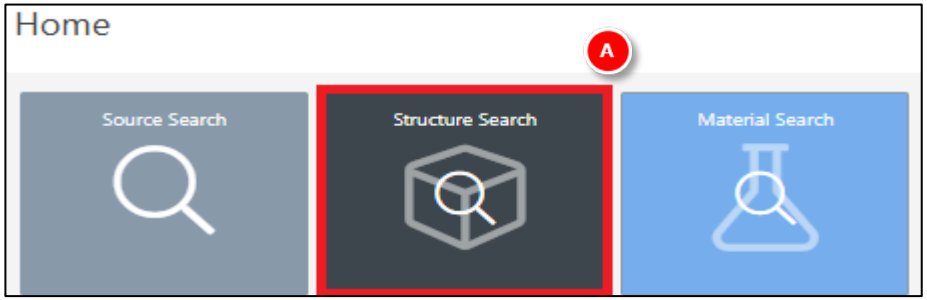
1. Structure Search Window

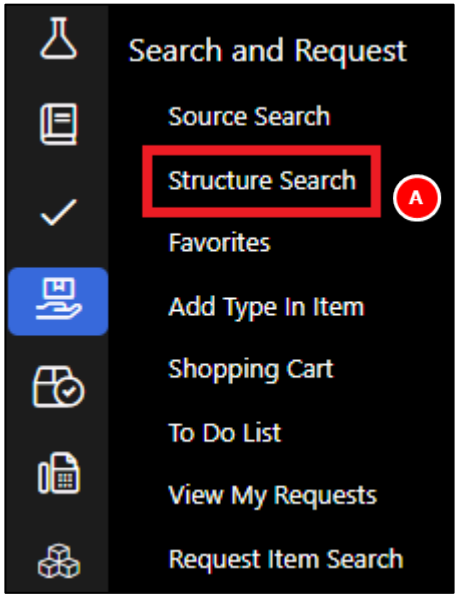
A. Click **Structure Search** or from the Menu go to **Search and Request > Structure Search**.

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:**

   a. Use **Import** or **Paste** to retrieve a structure from a .mol file. You can save .mol files from structures drawn in ChemDraw.

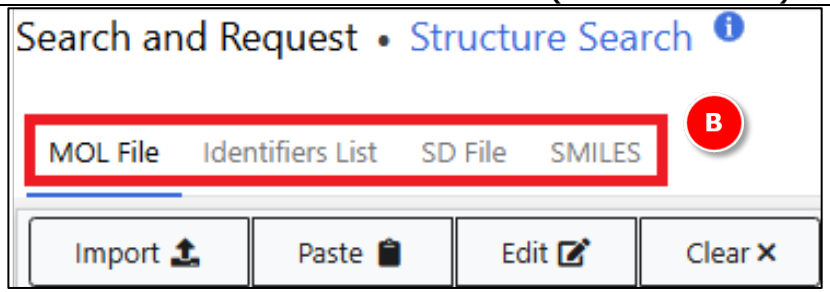
   b. OR Click **Edit** to draw the chemical structure.

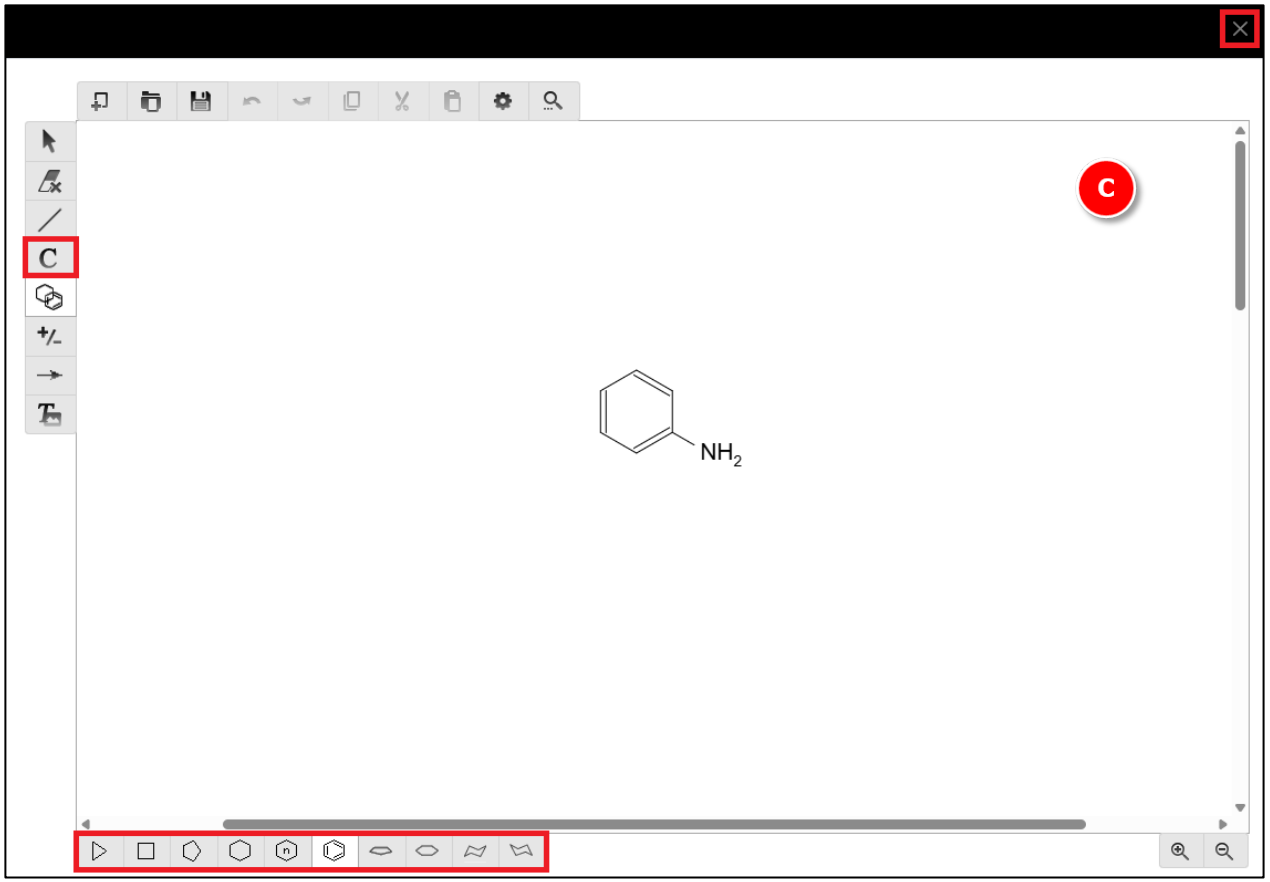




C. If **drawing** a structure:

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:

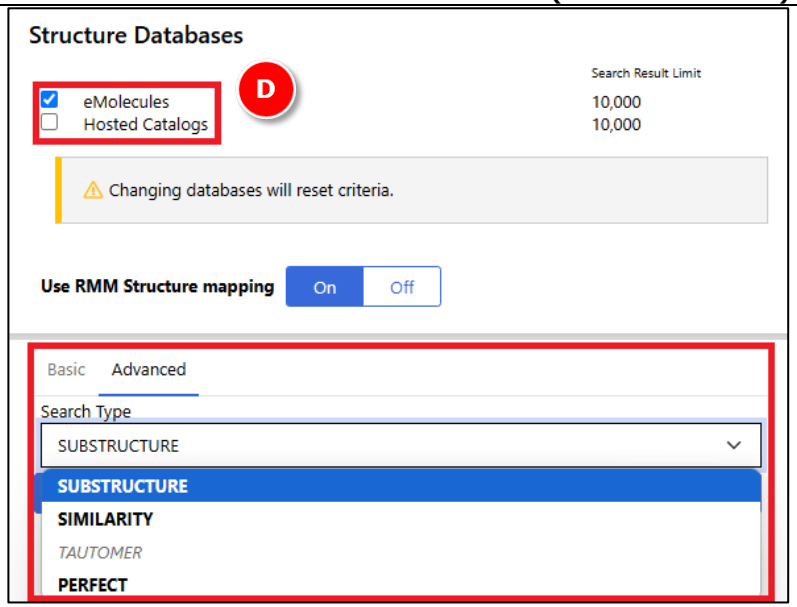
Structure Databases
For maximum results, keep both checked. Some advanced search types may not be compatible with both databases. However, in subsequent steps you will be able to find *results to purchase* from both catalogues regardless of what is selected here.

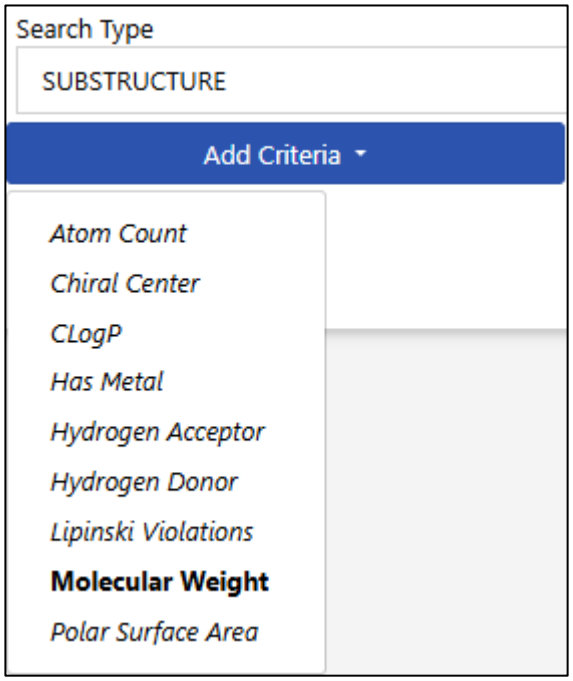
➔ If a drop-down search type option is not in bold, this means one of the selected catalogues is not compatible with one or more of the search criteria. Please deselect one of the catalogues to make it available.

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.

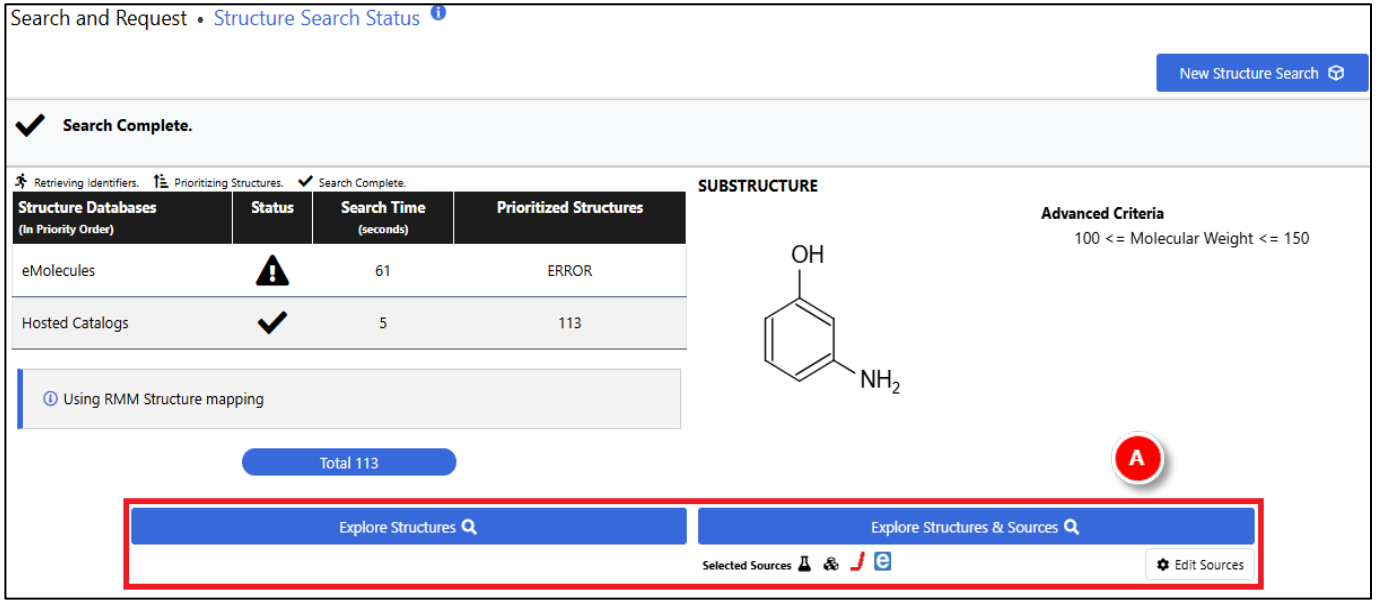




2. Retrieving identifiers

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.



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.

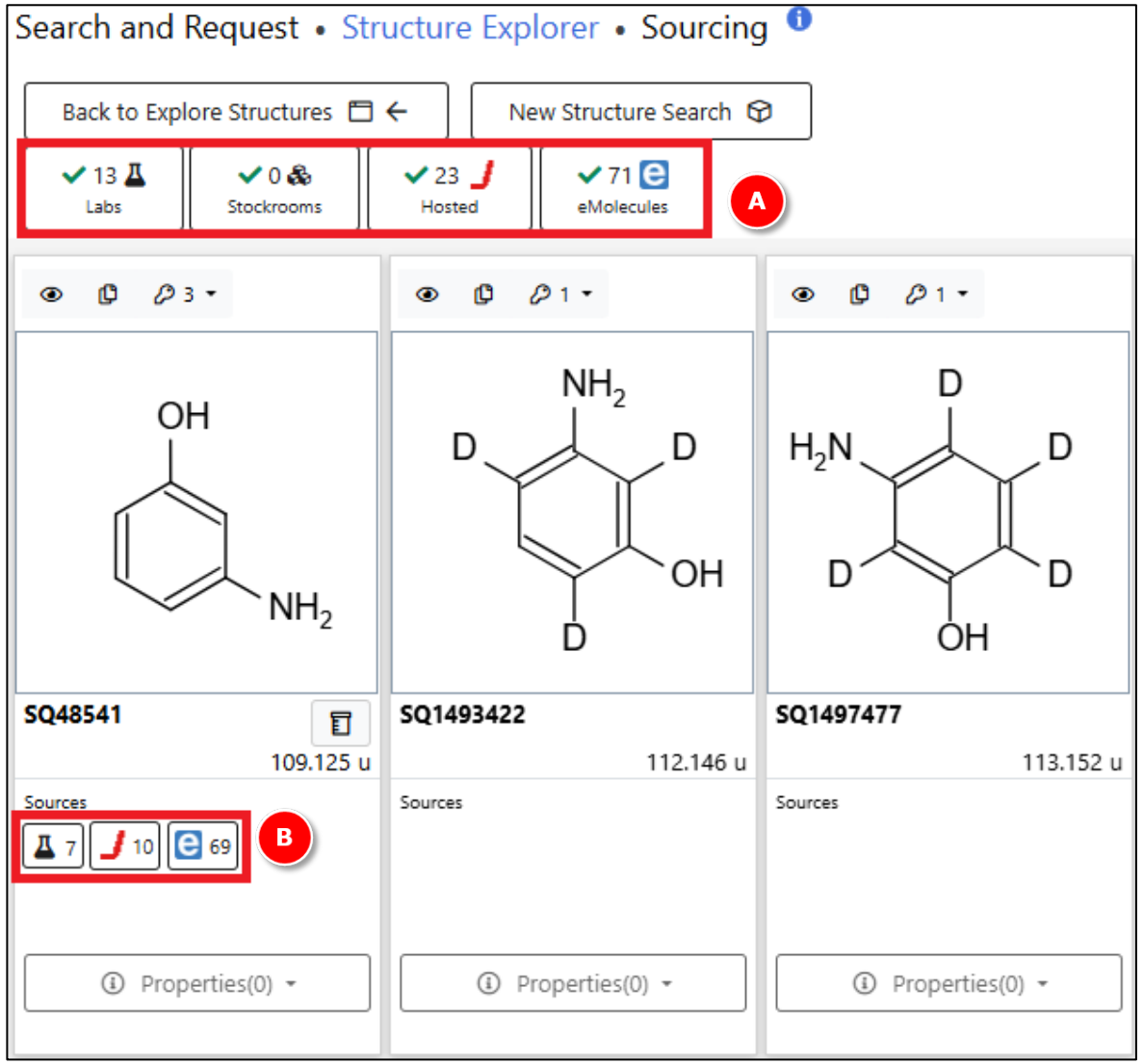
shows Hosted Catalogue search results.

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".



4. Explore Structures

A. 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.

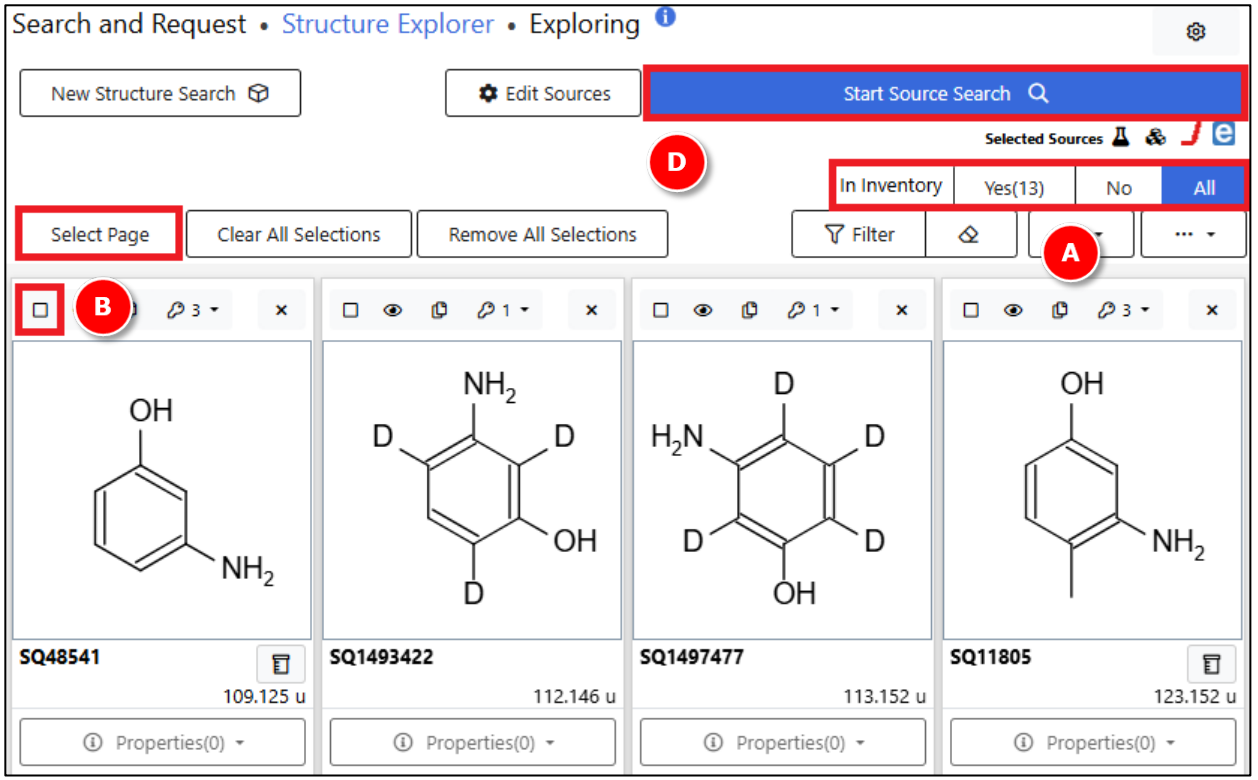
B. Select individual structures using the check boxes or click Select Page on the top left.

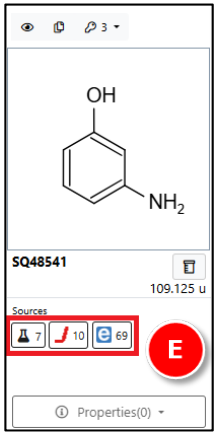
C. View structures on additional pages by using the navigation aid at the bottom of the screen.

D. Click Start Source Search icon.

E. Click the relevant icon by the structure you want to see the inventory/purchase details for.

shows Hosted Catalogue search results.





5. Substructure Searches in the Inventory by Keyword

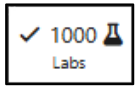
When looking for substructures in the inventory, you may get more complete results by using a keyword search than a structure search.

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.