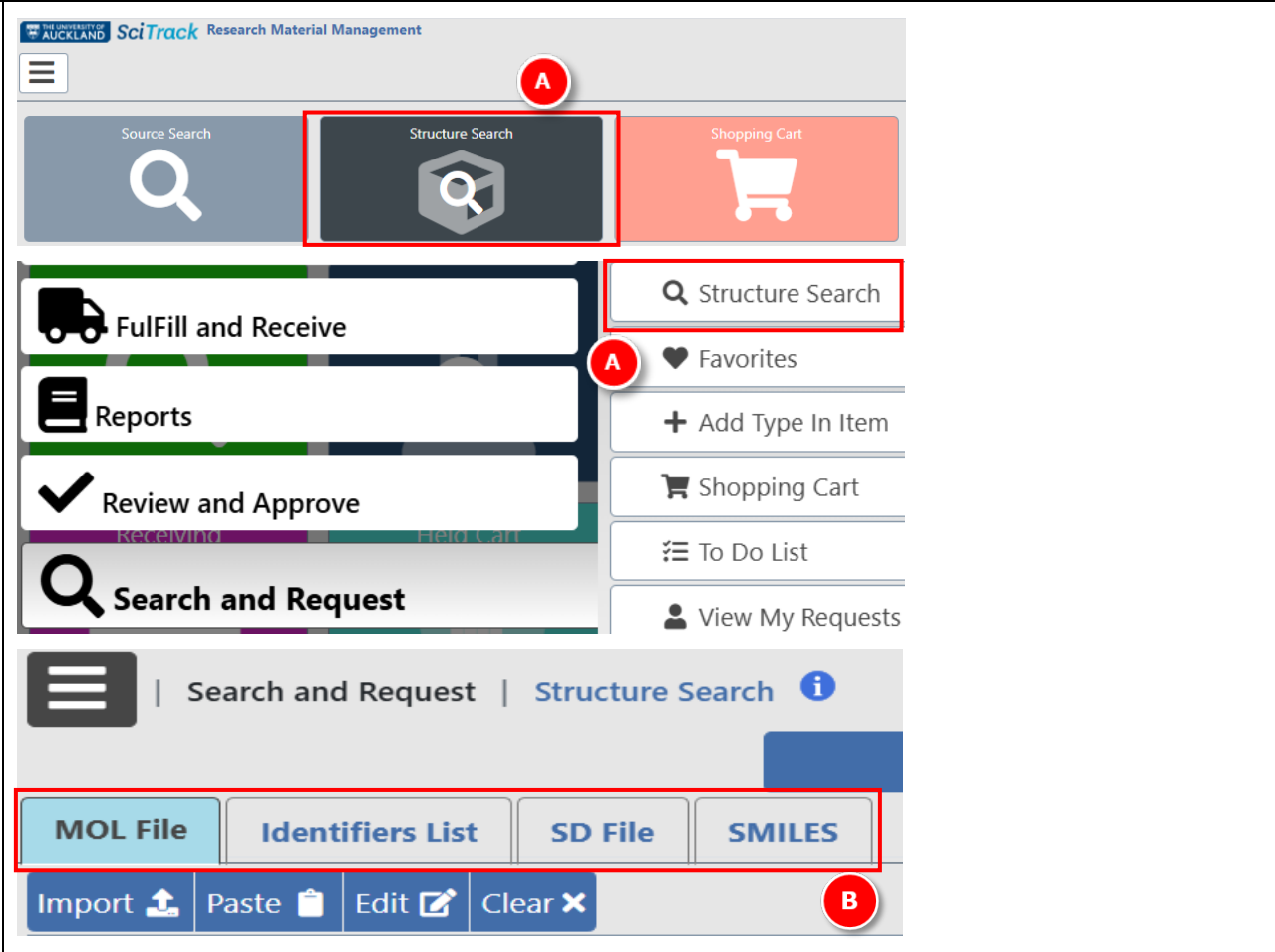


5. Structure Search Procedure

Overview

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

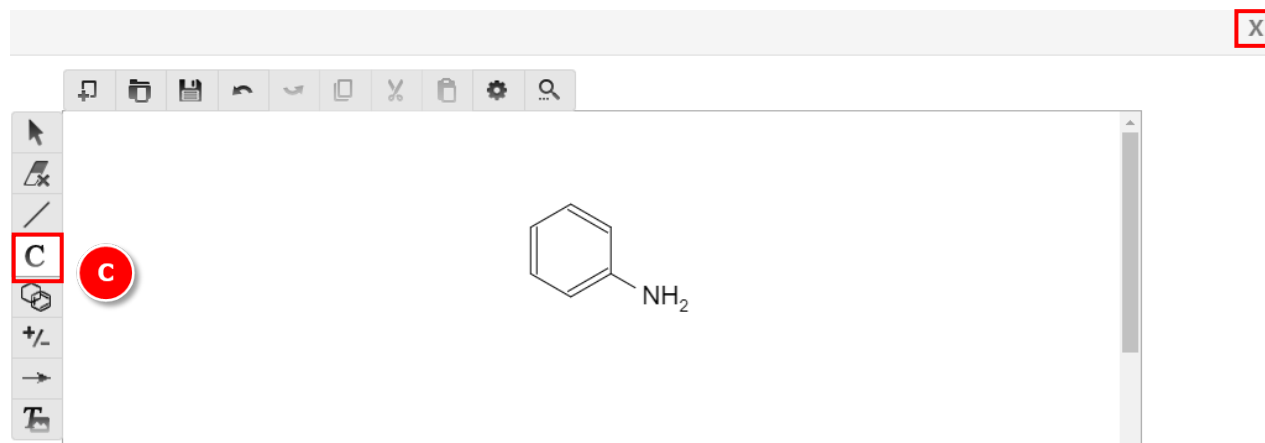
1. Structure Search Window
2. Retrieving Identifiers
3. Explore Structures & Sources OR
4. Explore Structures
5. Substructure Searches in the Inventory By Keyword

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 Research Material Management interface. At the top, there are three main navigation buttons: 'Source Search', 'Structure Search' (highlighted with a red box and labeled 'A'), and 'Shopping Cart'. Below these are several menu items: 'FulFill and Receive', 'Reports', 'Review and Approve', and 'Search and Request'. On the right side, there is a vertical list of options: 'Structure Search' (highlighted with a red box), 'Favorites', 'Add Type In Item', 'Shopping Cart', 'To Do List', and 'View My Requests'. At the bottom, there is a navigation bar with 'MOL File', 'Identifiers List', 'SD File', and 'SMILES' buttons (all highlighted with a red box), and a row of action buttons: 'Import', 'Paste', 'Edit' (labeled 'B'), and 'Clear'.</p>

SciTrack Quick Guide – Structure Search Procedure (Version 3.0)

C. If **drawing a structure:**

- 1) Draw the backbone of the structure using bonds and/or rings
- 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.

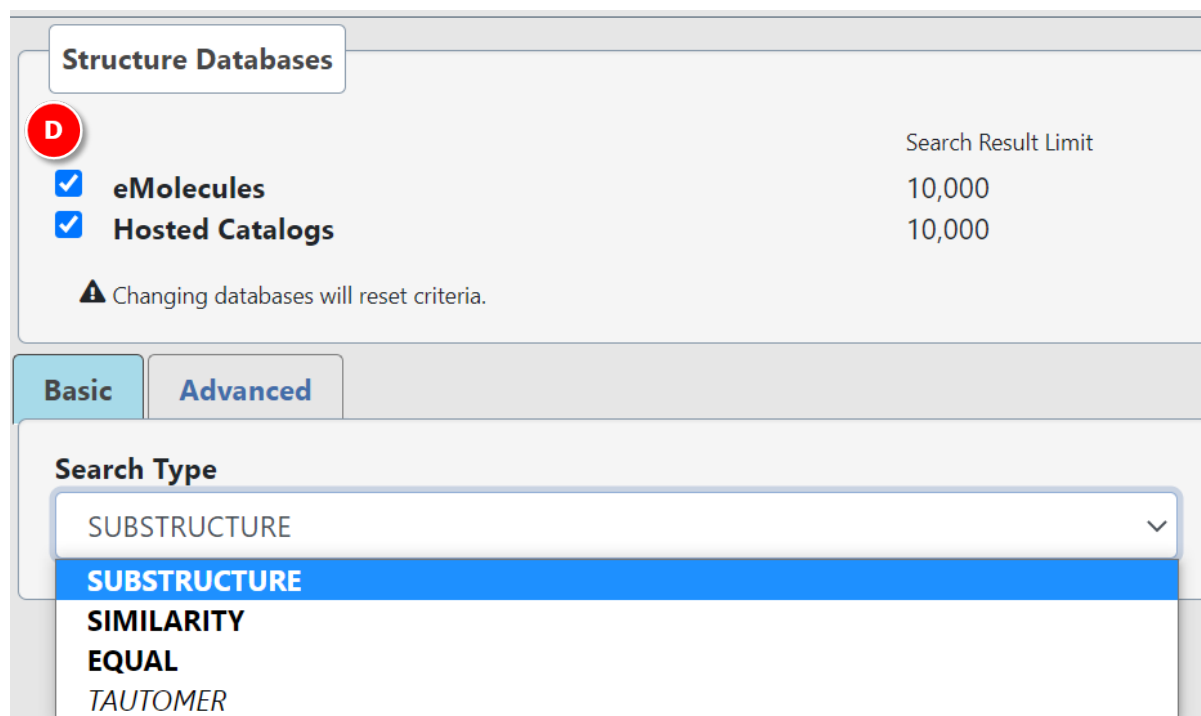

D. Select search criteria:
Structure Databases

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.



Structure Databases

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

⚠ Changing databases will reset criteria.

Basic | Advanced

Search Type

- SUBSTRUCTURE
- SUBSTRUCTURE**
- SIMILARITY
- EQUAL
- TAUTOMER

SciTrack Quick Guide – Structure Search Procedure (Version 3.0)

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.

Search Type

SUBSTRUCTURE

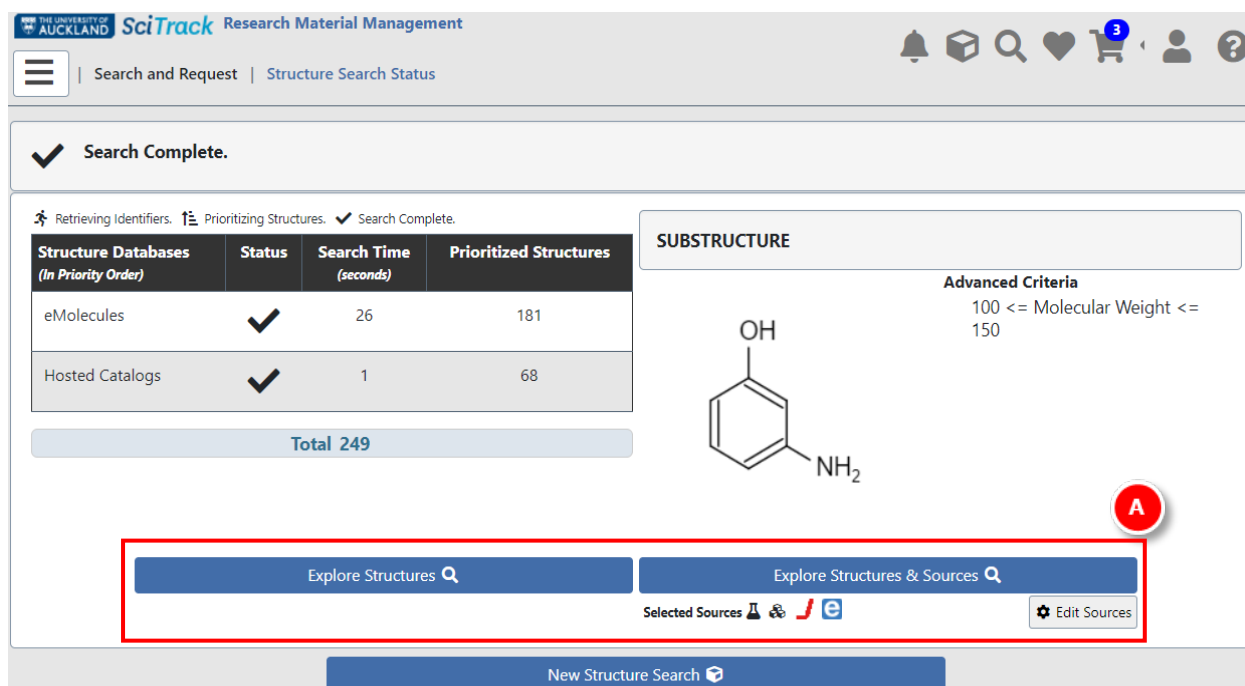
Add Criteria ▾

Atom Count
 Chiral Center
 CLogP
 Has Metal
 Hydrogen Acceptor
 Hydrogen Donor
 Lipinski Violations
Molecular Weight
 Polar Surface Area

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.



THE UNIVERSITY OF AUCKLAND **SciTrack** Research Material Management

Search and Request | Structure Search Status

Search Complete.

Retrieving Identifiers. Prioritizing Structures. Search Complete.


Structure Databases (In Priority Order)	Status	Search Time (seconds)	Prioritized Structures
eMolecules	✓	26	181
Hosted Catalogs	✓	1	68
Total 249			


SUBSTRUCTURE

Advanced Criteria
 100 <= Molecular Weight <= 150

Nc1cccc(O)c1

Explore Structures 🔍 | Explore Structures & Sources 🔍

Selected Sources  Edit Sources

New Structure Search 

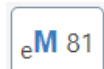
SciTrack Quick Guide – Structure Search Procedure (Version 3.0)

3. Explore Structures & Sources

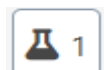
- A. Toggle the sources you want to see results for.
- B. Find the structure you are interested in and click the relevant source icon to see the results in the source search page.



shows Hosted Catalogue search results.




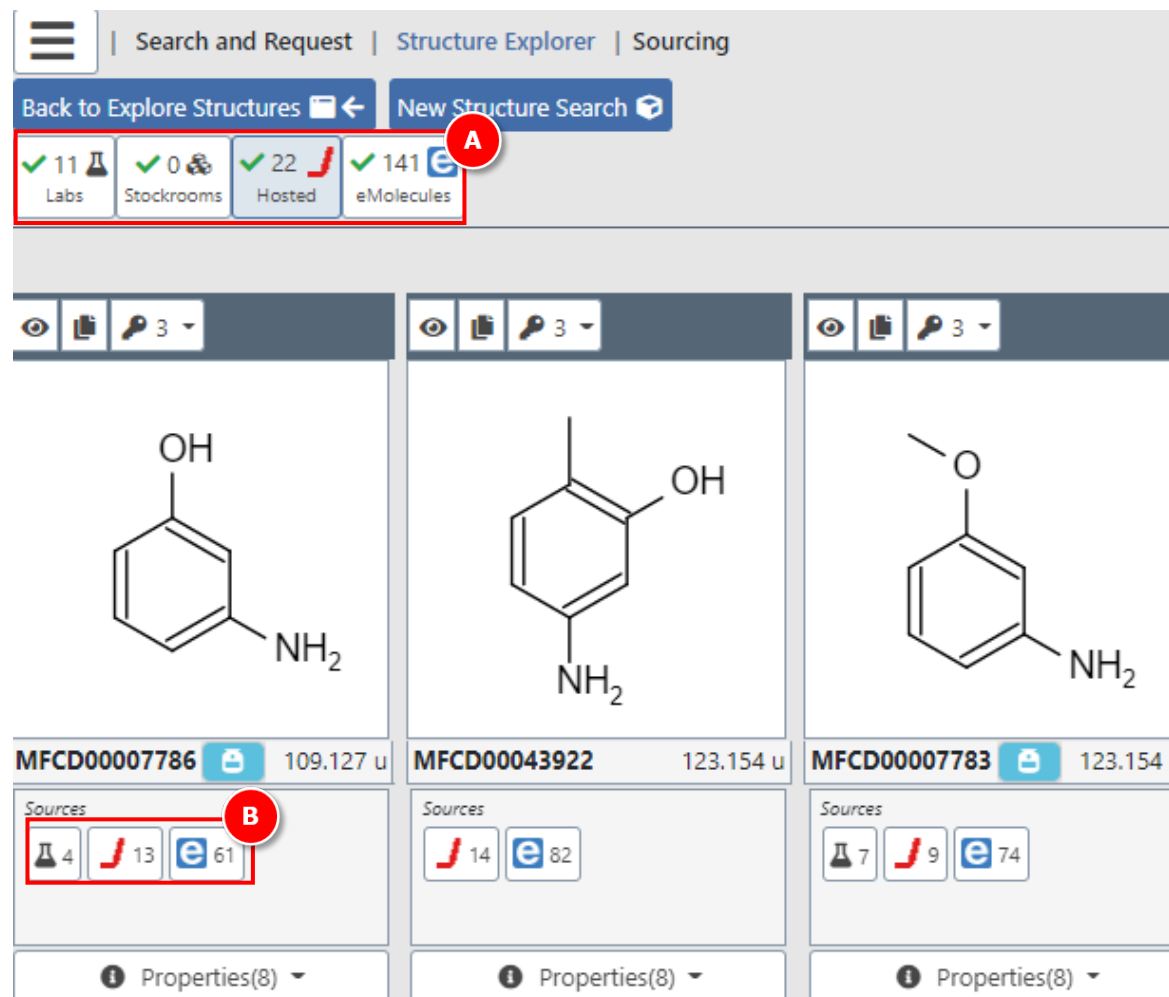
shows eMolecules results



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".



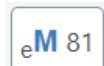
SciTrack Quick Guide – Structure Search Procedure (Version 3.0)

4. Explore Structures

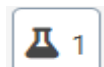
- To find a chemical in the internal inventory, click Yes in the “In Inventory” panel. To search for a chemical to purchase, leave this selection on All.
- Select individual structures using the check boxes or click Select Page from the drop-down to select all results on that page.
- View structures 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.

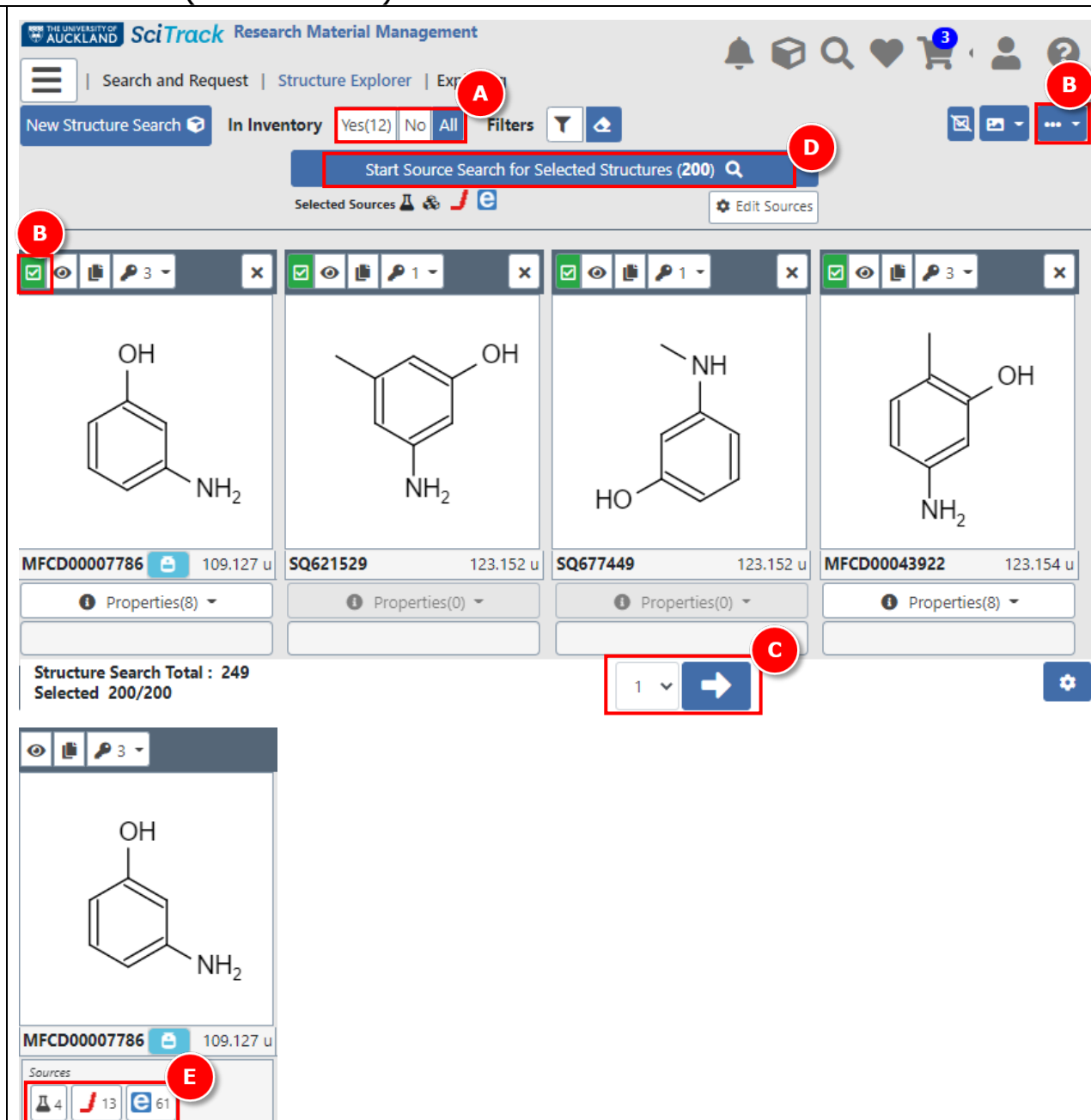


shows eMolecules results



shows results in the internal lab inventory

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



The screenshot displays the SciTrack interface for Research Material Management. At the top, there are navigation tabs for 'Search and Request', 'Structure Explorer', and 'Exp'. Below this, a search bar contains 'Start Source Search for Selected Structures (200)'. A filter panel shows 'In Inventory' with 'Yes(12)', 'No', and 'All' options. A 'Start Source Search' button is highlighted with a red box and callout D. Below the search bar, there are four structure cards. Each card shows a chemical structure, an ID (e.g., MFCD00007786), and a quantity (e.g., 109.127 u). A 'Properties' dropdown is visible below each card. At the bottom, a 'Structure Search Total : 249 Selected 200/200' summary is shown. A navigation bar at the bottom right has a dropdown set to '1' and a right-pointing arrow, highlighted with a red box and callout C. A 'Sources' panel at the bottom left shows icons for different sources with counts: a flask (4), a red 'J' (13), and 'eM' (61), highlighted with a red box and callout E. Other callouts include A (filter selection), B (checkbox selection), and C (navigation arrows).

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 interface for a source search. At the top, there are three navigation buttons: 'Source Search' (A), 'Structure Search', and 'Shopping Cart'. Below this is the 'Source Search' section with 'Search' and 'Advanced Search' tabs. A search bar (C) contains the text '*aniline*'. Below the search bar are 'Reset', 'Internal', 'External', and 'All' buttons. A 'Labs' checkbox is checked, and a 'Preferred (1)' button (B) is highlighted. The search results show '2,3-Dimethylaniline (2)' with a chemical structure, CAS # 87-59-2, MDL # MFCD00007732, and a quantity of 121.18 u. At the bottom, there is a 'Pre-SciQuest' section with a 'Sigma' logo and a '2,3-Dimethylaniline' entry. An info icon (E) is highlighted next to the entry. A pagination bar shows page 1 of 6.