

# 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><b>1. Structure Search Window</b></p> <p>A. Click <b>Structure Search</b>.</p> <p>B. Either <b>import, paste</b> or <b>draw structure</b>:</p> <ol style="list-style-type: none"><li>a. Use <b>Import</b> or <b>Paste</b> to retrieve a structure from a .mol file. You can save .mol files from structures drawn in ChemDraw.</li><li>b. OR Click <b>Edit</b> to draw the chemical structure.</li></ol> <p>C. If <b>drawing</b> a structure:</p> <ol style="list-style-type: none"><li>1) Draw the backbone of the structure using bonds and/or rings</li><li>2) To change an atom to something other than carbon, click the <b>C</b> 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.</li><li>3) When you are finished, click the escape icon on the drawing window to return your structure to the search screen.</li></ol>	

#### 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 this criteria. Please deselect one of the catalogues to make it available.

##### Basic-→Equal search

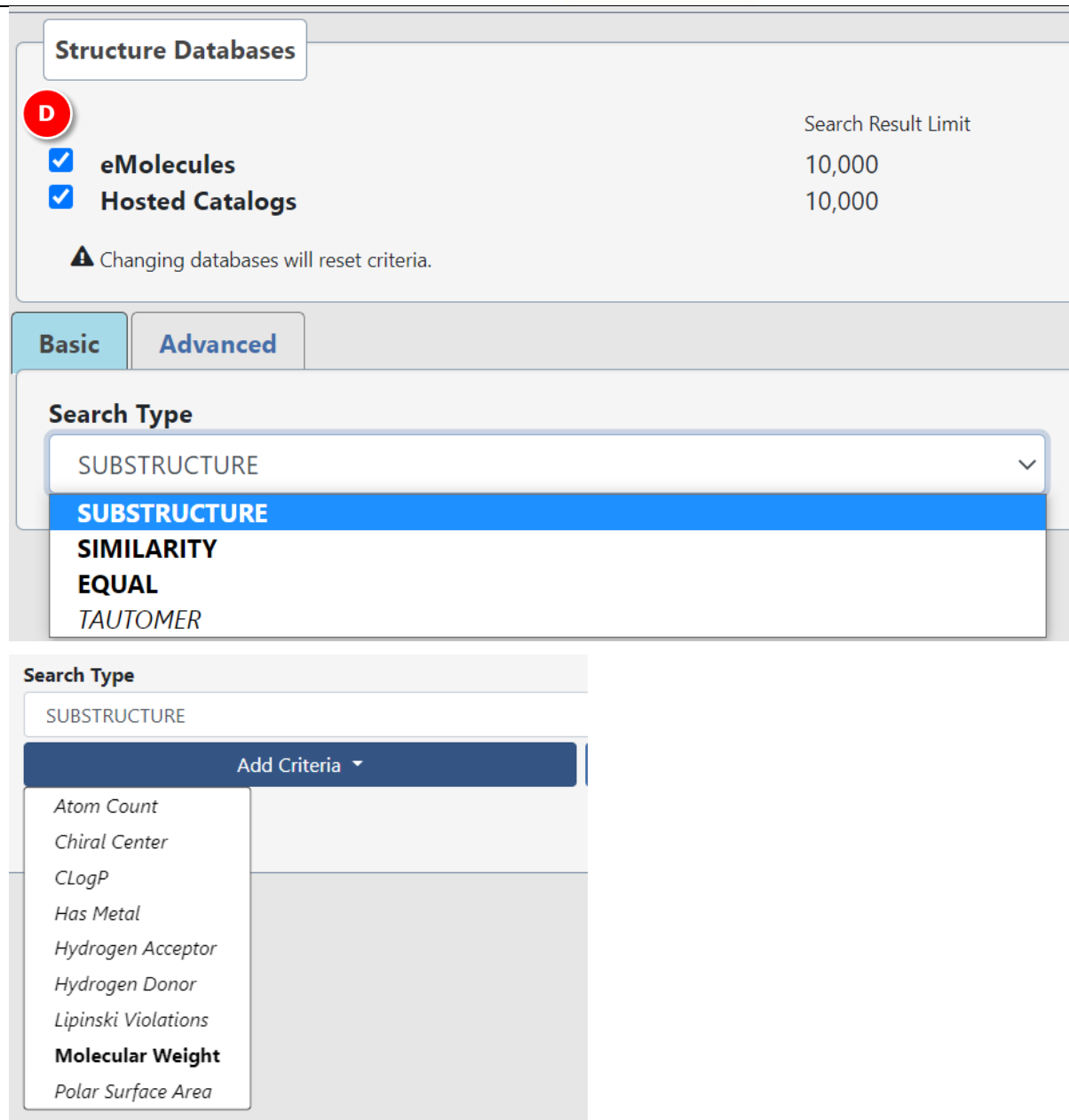
This can be used to find the exact structure in the hosted catalogues or internal inventory.

##### Substructure search

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 Catalogues database to access most of the advanced search criteria.

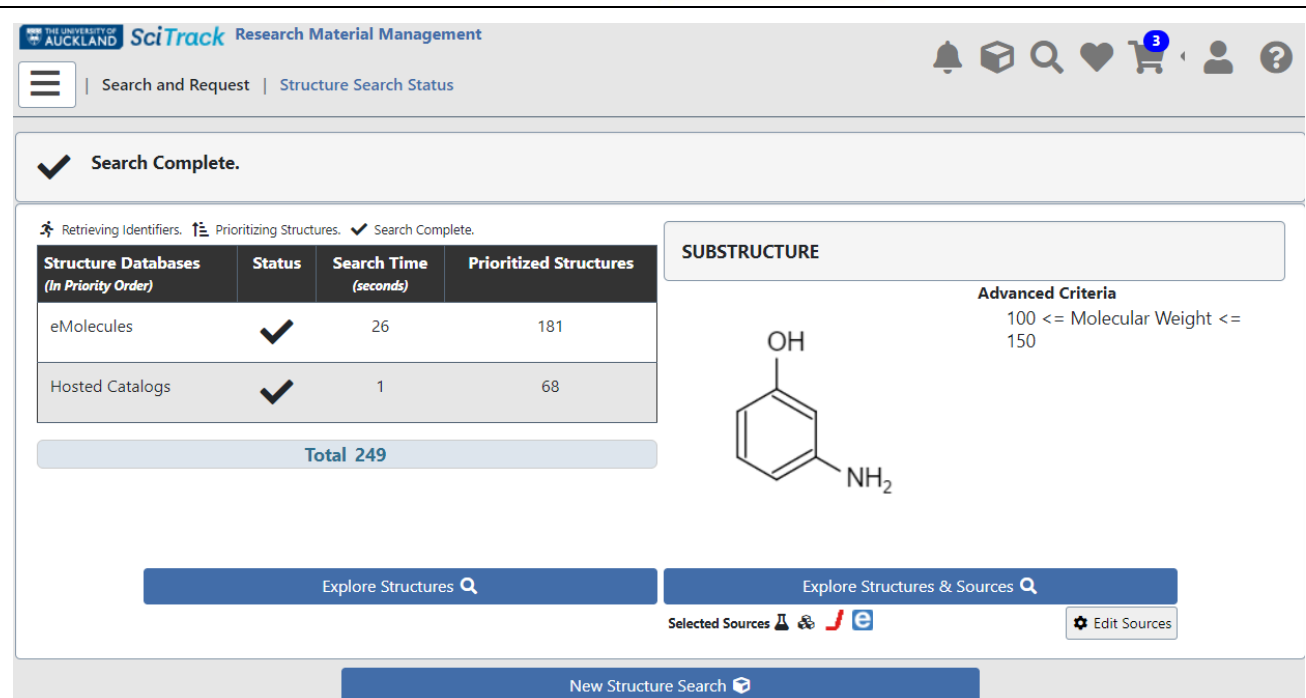


The screenshot shows the SciTrack search interface. At the top, there are two tabs: "Basic" and "Advanced". The "Advanced" tab is selected. Under "Structure Databases", there are two checked options: "eMolecules" and "Hosted Catalogs". A warning icon indicates that changing databases will reset criteria. To the right, the "Search Result Limit" is set to 10,000 for both. Below this, the "Search Type" dropdown menu is open, showing options: "SUBSTRUCTURE" (highlighted in blue), "SIMILARITY", "EQUAL", and "TAUTOMER". At the bottom, another "Search Type" dropdown is shown with "SUBSTRUCTURE" selected, and an "Add Criteria" button is visible, which has opened a list of search criteria including "Atom Count", "Chiral Center", "CLogP", "Has Metal", "Hydrogen Acceptor", "Hydrogen Donor", "Lipinski Violations", "Molecular Weight" (bolded), and "Polar Surface Area".

## 2. Retrieving identifiers

Allow some time for the search to complete.

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.

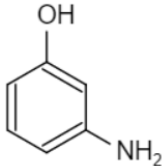
Retrieving Identifiers. Prioritizing Structures. Search Complete.



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



Explore Structures 
 Explore Structures & Sources 

Selected Sources    
 Edit Sources 

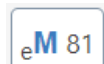
New Structure Search 

### 3. Explore Structures & Sources

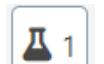
- A. Select the source you want to see results for.
- B. Find the structure you are interested in and click the relevant source icon to see the results in the source search page.



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

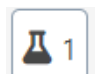
- To find a chemical in the internal inventory, click Yes in the "In Inventory" panel. To search for a chemical to purchase, leave this selection on All.
- Select individual structures using the check boxes or click Select Page from the drop-down to select all results on that page.
- View structures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

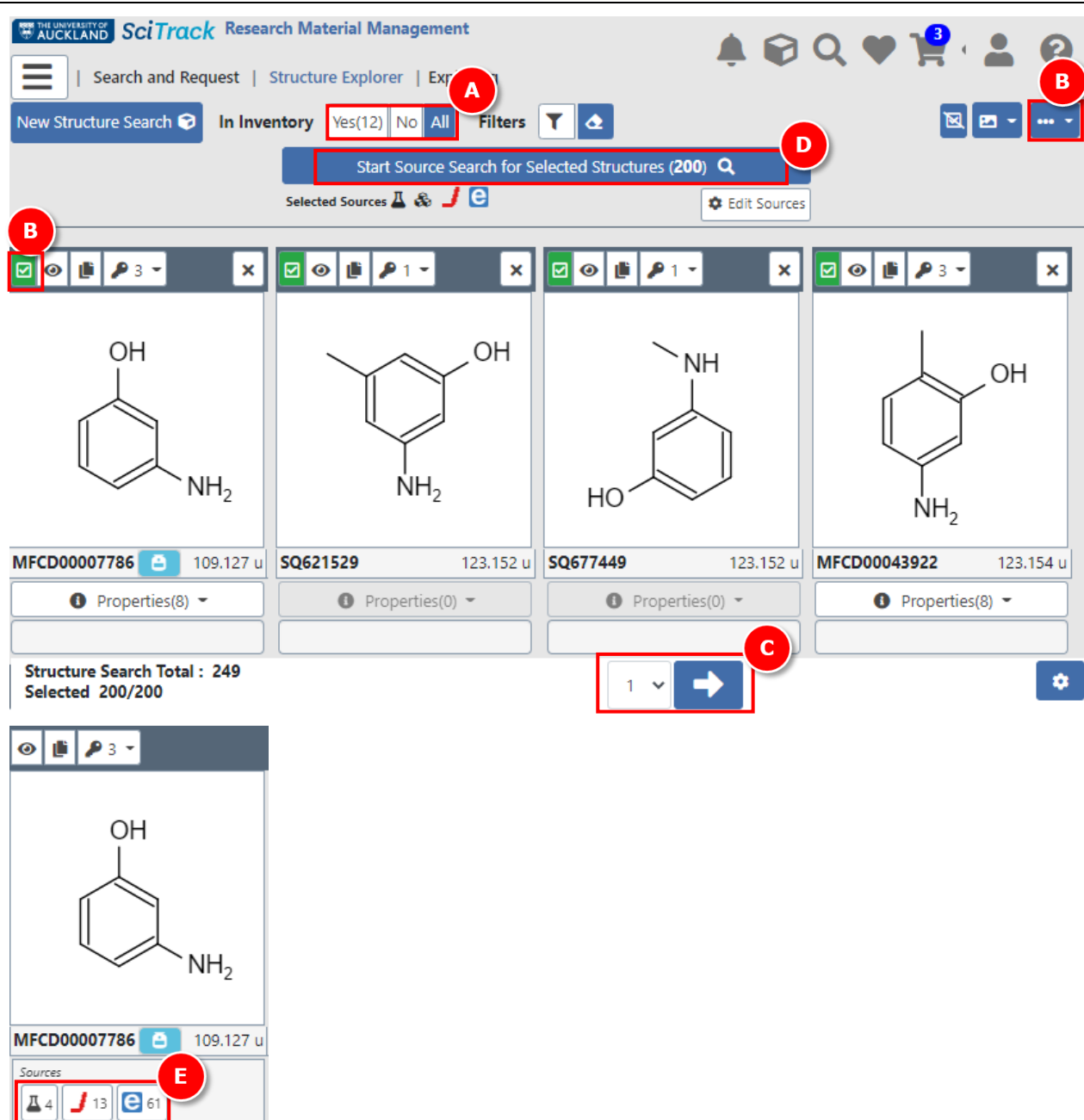


shows eMolecules results



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 Research Material Management interface. At the top, there are navigation tabs: "Search and Request", "Structure Explorer", and "Exp". Below this is a search bar with "Start Source Search for Selected Structures (200)" and a search icon. To the left of the search bar are filters for "In Inventory" (Yes(12), No, All) and "Filters".

The main area shows a grid of chemical structures. Each structure is displayed in a card format with a chemical structure, a source ID, and a price. The first card shows a structure with an OH group and an NH<sub>2</sub> group, with source ID MFC00007786 and price 109.127 u. The second card shows a structure with an OH group and an NH<sub>2</sub> group, with source ID SQ621529 and price 123.152 u. The third card shows a structure with an NH group and an OH group, with source ID SQ677449 and price 123.152 u. The fourth card shows a structure with an OH group and an NH<sub>2</sub> group, with source ID MFC00043922 and price 123.154 u.

At the bottom of the grid, there is a "Structure Search Total : 249 Selected 200/200" summary. Below this is a navigation bar with a dropdown menu showing "1" and a right arrow button. At the bottom left, there is a "Sources" section with icons for different sources: a flask (4), a J (13), and an eM (61).

## 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,

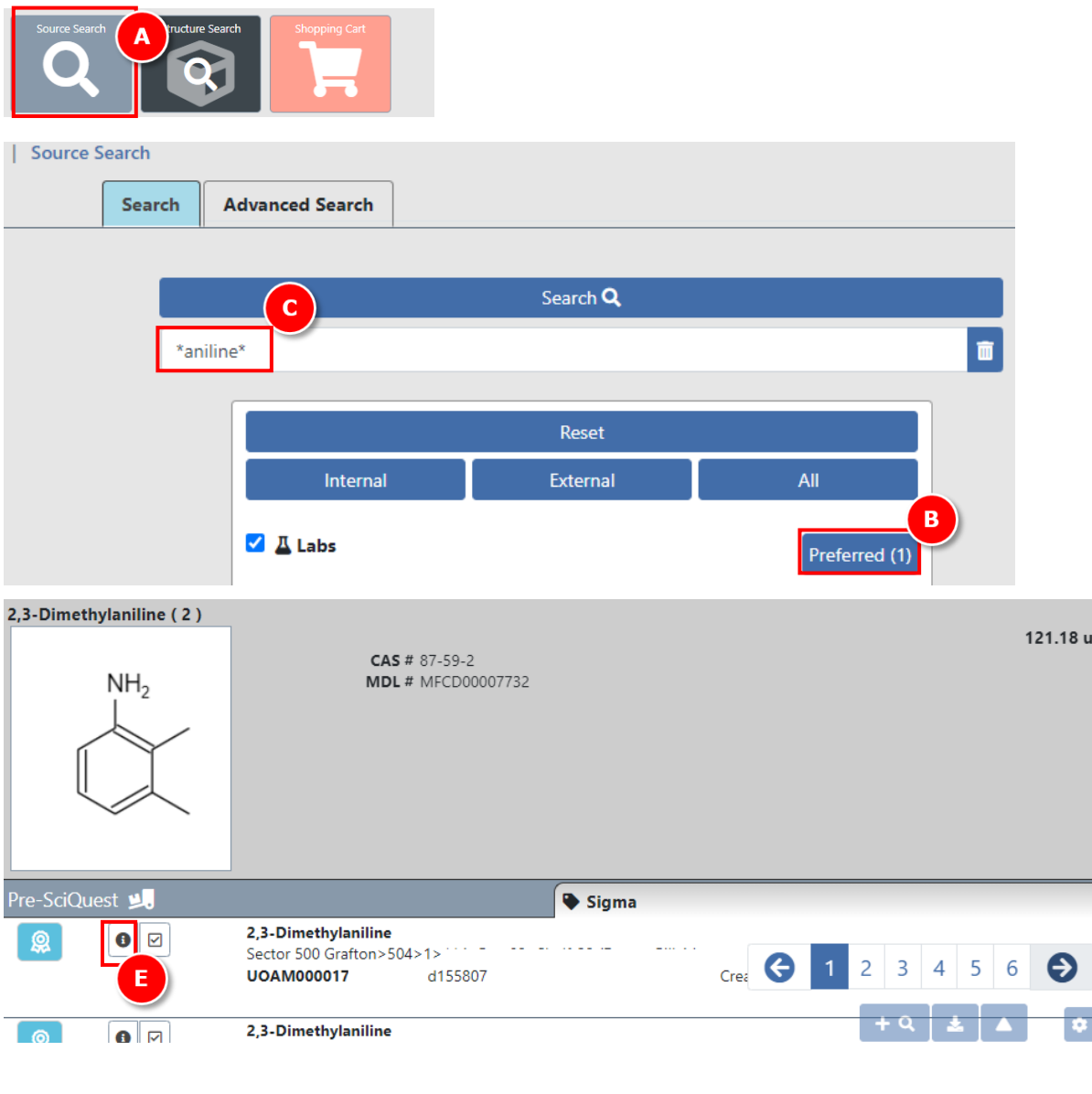
- A. Go to Source Search
- B. Optionally, click Preferred next to Labs to only search preferred search locations. See Quick Guide 2. Configure Preferences for more information.
- C. In the search criteria, enter key words with a wildcard (\*) on either side and in-between words as required, and click 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, 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' buttons. A search bar (C) contains the text '\*aniline\*'. Below the search bar are buttons for 'Reset', 'Internal', 'External', and 'All'. A 'Labs' checkbox is checked, and a 'Preferred (1)' button (B) is visible. 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 pagination bar with page numbers 1 through 6, and an info icon (E) for more details.