Tutorial for browsing and searching the Chemical Functional Ontology (ChemFOnt)

August 15, 2022

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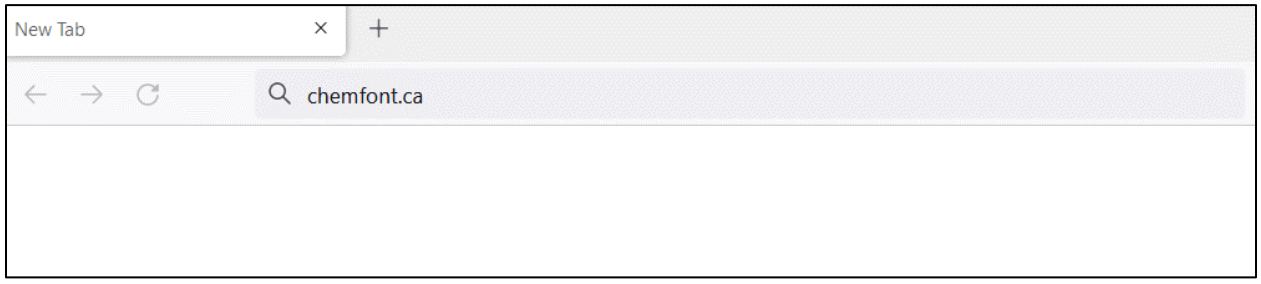
1. Structure and design of ChemFOnt.

- In simple terms, the **Chem**ical **F**unctional **O**ntology or ChemFOnt (https://chemfont.ca) is a hierarchical ontology describing the functions and actions of biologically important chemicals.
- ChemFOnt contains information on >319,000 chemicals, including primary metabolites, secondary metabolites, natural products, food chemicals, synthetic food additives, drugs, herbicides, pesticides, and environmental chemicals.
- Within the entry (Molecule Card) of each chemical, a functional ontology describes the roles, disposition, physiological effects, and processes associated with the chemical. Other sections include a chemical taxonomy and physical properties.

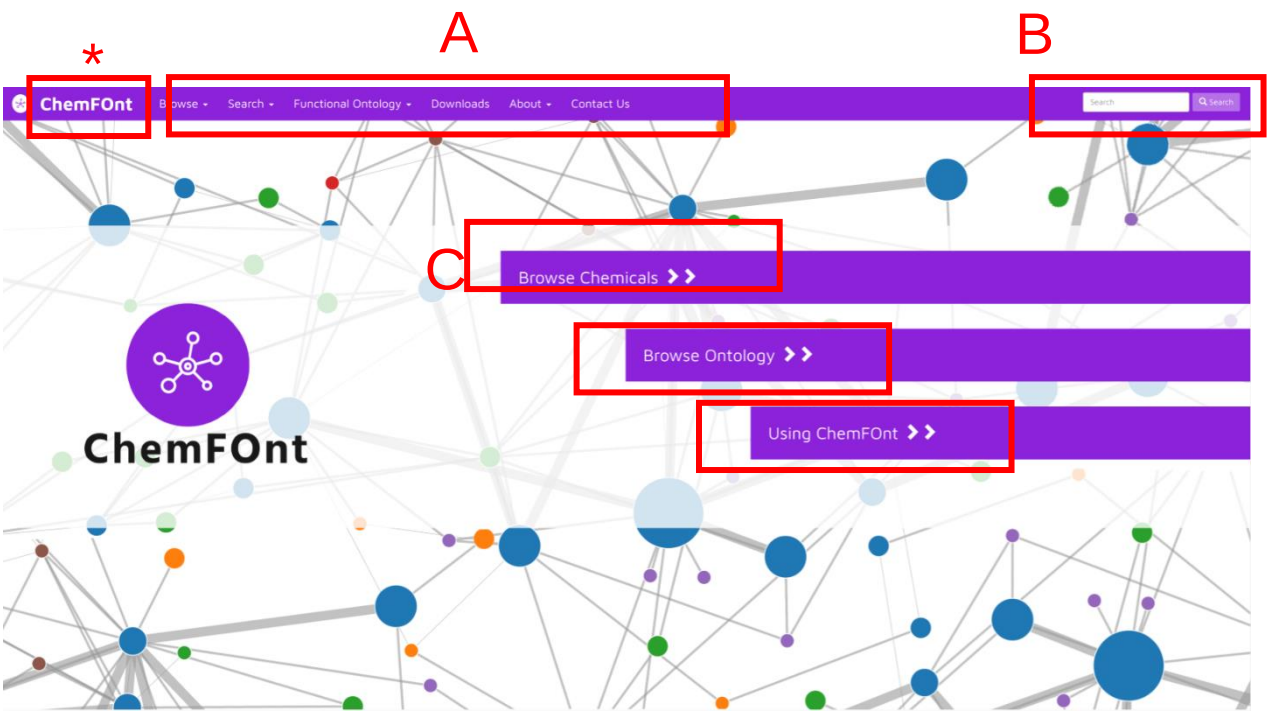
The next sections provide details about how to browse and search ChemFOnt.

2. Open your Internet browser and type “https://chemfont.ca” or simply “chemfont.ca” into the search bar and press the “return” (“Enter”) key. Below is an example of having typed in the url (web address) of the ChemFOnt database into the search bar.



- After submitting the search (pressing the Enter key), you will be taken to the ChemFOnt homepage (shown below).

- Next: a few points about the choices available on the homepage.



3. **A.** Across the top of the homepage, there are six different menu headings, some with their own pulldown menu: **Browse**, **Search**, **Ontology**, **Downloads**, **About**, and **Contact Us**.

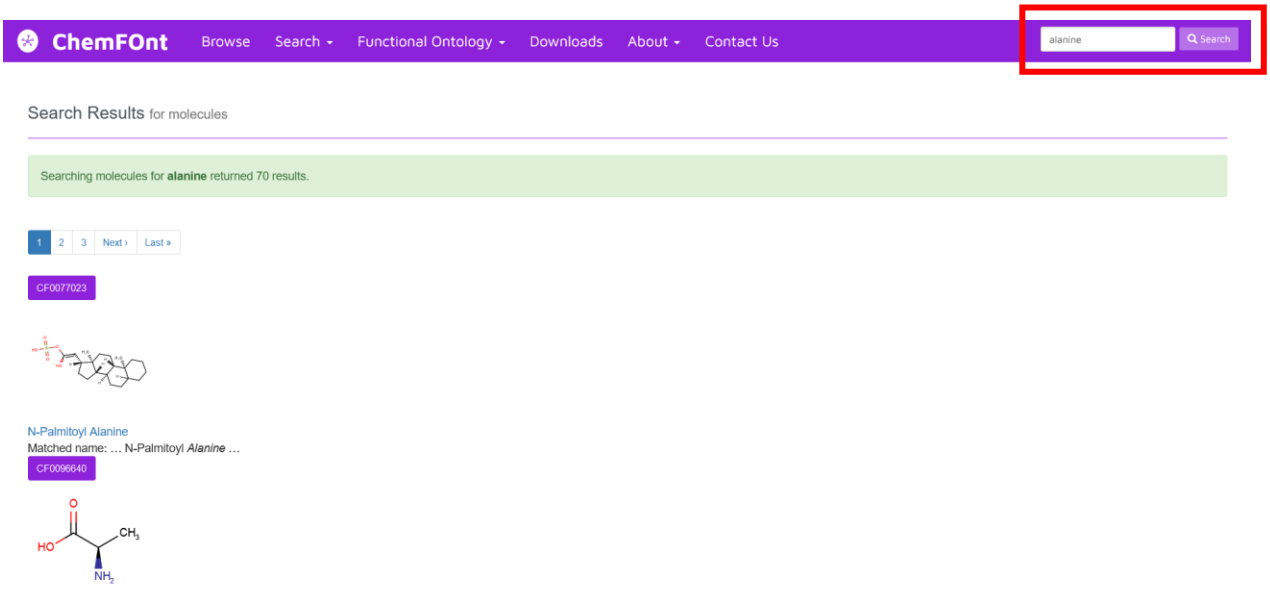
B. There is also a convenient general-text "**Search**" box in the top right corner which enables you to search the entire database. Clicking the purple "Search" button will return a list of results that match closely your query.

C. You can also "Browse Data", "Search Data", or learn more about "Using ChemFOnt" by clicking on these hyperlinked bars in the centre of the homepage.

*Clicking on "ChemFOnt" at the top left any time brings you back to this homepage.

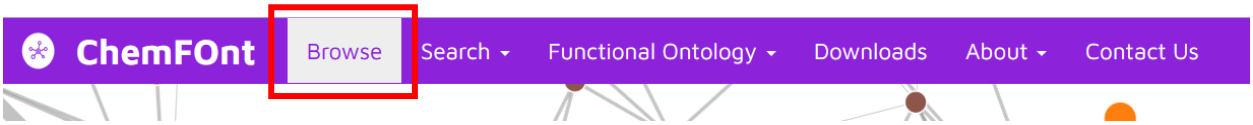
➡ Next, we provide examples of general text searches using the "Search" box.

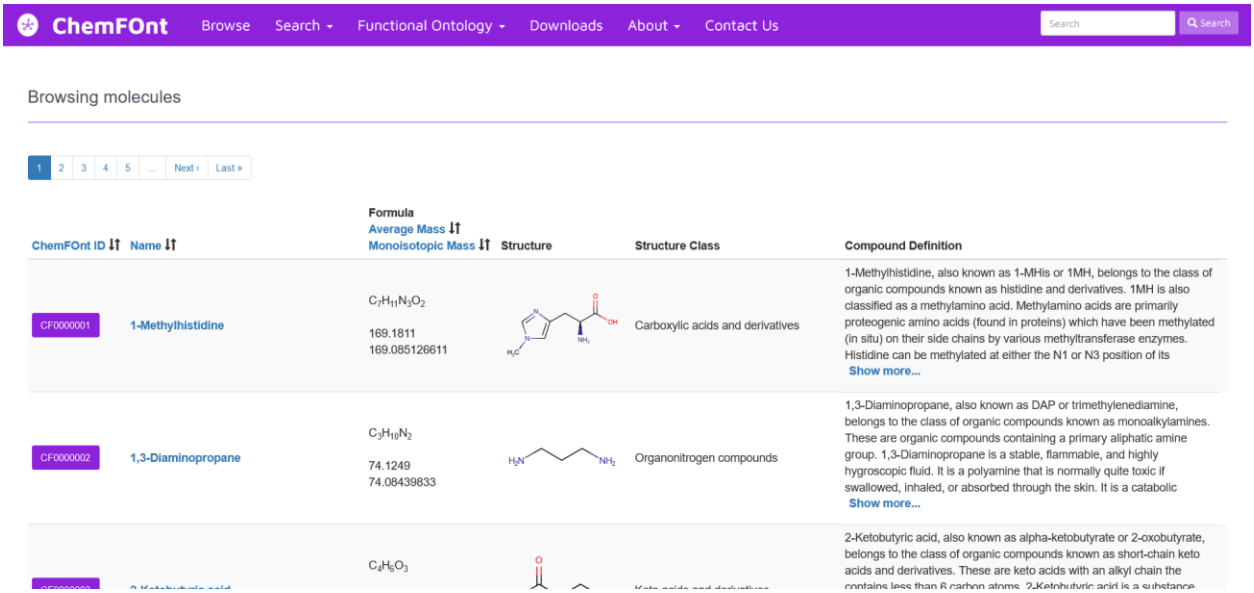
- If you entered "alanine" in the "Search" box, 70 results are returned in which "alanine" is found in the name or definition.



4. “Browse” option. Clicking on the “Browse” option at the top left of the homepage will allow you to browse either the chemicals or the ontology.

a. Clicking “Browse Chemicals will bring you to the Molecule Table, showing chemicals in order of their ChemFOnt ID number. Clicking the “Browse Data” hyperlink bar in the centre of the homepage will bring you to the same Molecule Table.





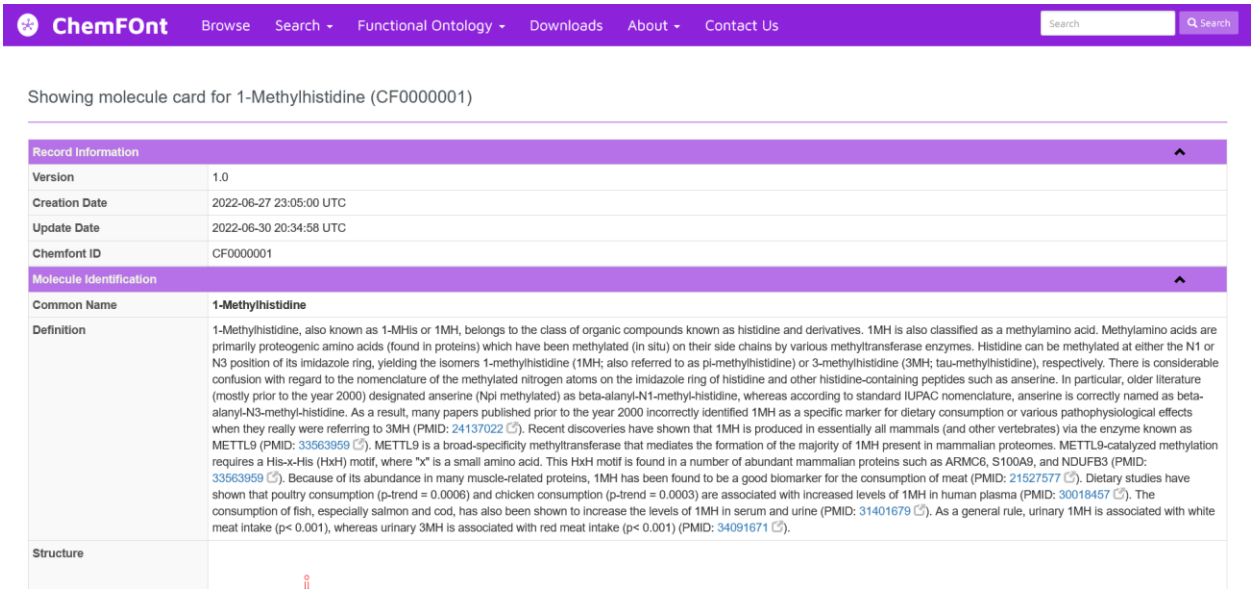
- The Molecule Table is sortable by selecting a column header in blue text, namely one of the ChemFOnt ID, Name, Average Mass, or Monoisotopic Mass. Other fields shown are the Formula, Structure, Structure Class, and Compound Definition.

➡ Next is an example result from the Molecule Table.

- Clicking on the ChemFOnt ID button or the compound name will take you to the ChemFOnt Molecule Card for that compound. The top portion of the ChemFOnt Molecule Card for 1-methylhistidine (CF0000001) is shown below.

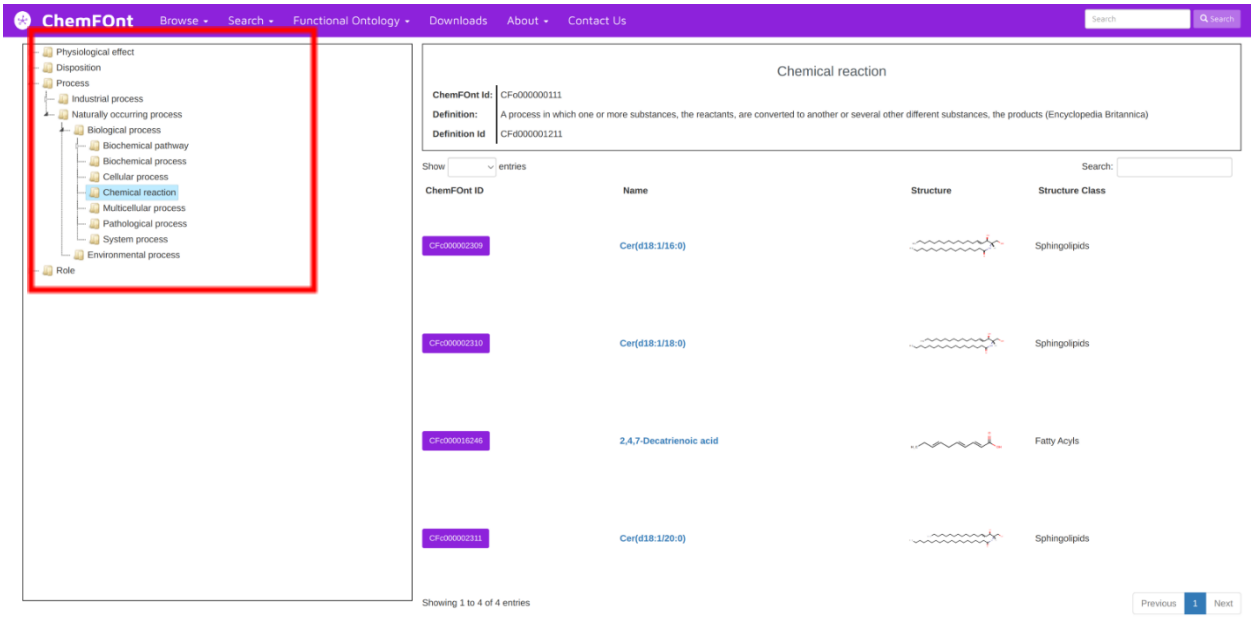
- Each ChemFOnt Molecule Card contains seven major data sections, each with various fields: 1) ChemFOnt Record Information; 2) Molecule Identification; 3) Chemical Taxonomy; 4) Functional Ontology; 5) Physical Properties; 6) External Links; and 7) References. The first four sections are open (expanded) by default.

- For any collapsed section, clicking on the down arrow on the righthand side expands it and reveals further information about that molecule. Clicking on the up arrow for any expanded section collapses that section.

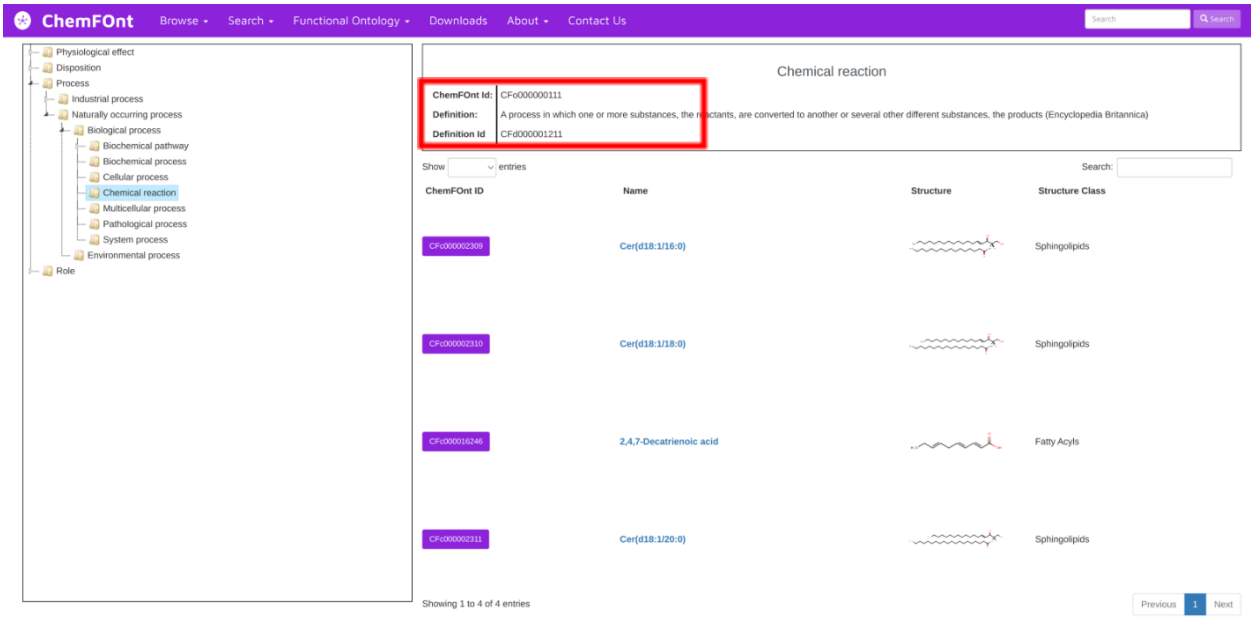


4.

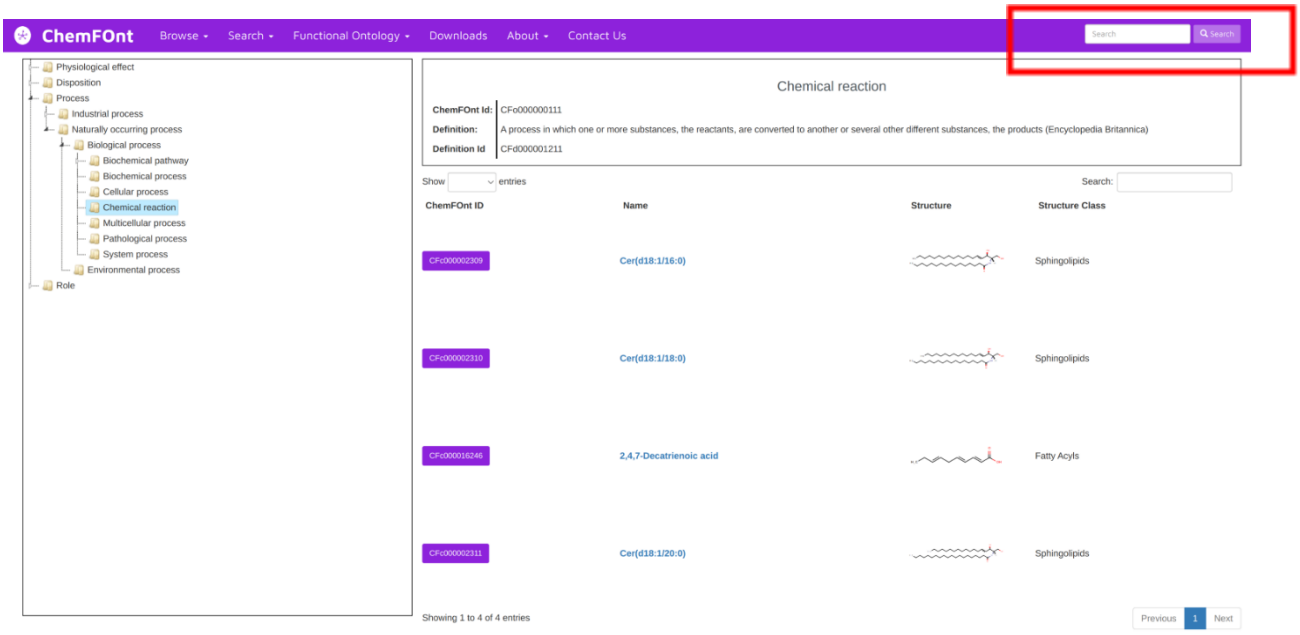
b. Clicking “Browse Ontology” will bring you to the Ontology Viewer, showing the ontology in a hierarchical format. Clicking the “Browse Ontology” hyperlink bar in the centre of the homepage will bring you to the same Ontology Viewer.



- The ontology can be browsed by clicking on any of the terms in the top left of the page. Clicking on one of these terms will show the child terms, as well as any chemicals belonging to the term.
- Clicking on a leaf node of the ontology browse will allow you to see any chemicals that belong to this term.



- Term information, including ChemFOnt ID, Definition and Definition ID can be found at the top of the page for any ChemFOnt term. Additionally, by clicking on either the ChemFOnt ID box or the Name, you can view the ChemFOnt Molecule Card.



- As with Compounds, ChemFOnt terms can be searched for via the top right search box.

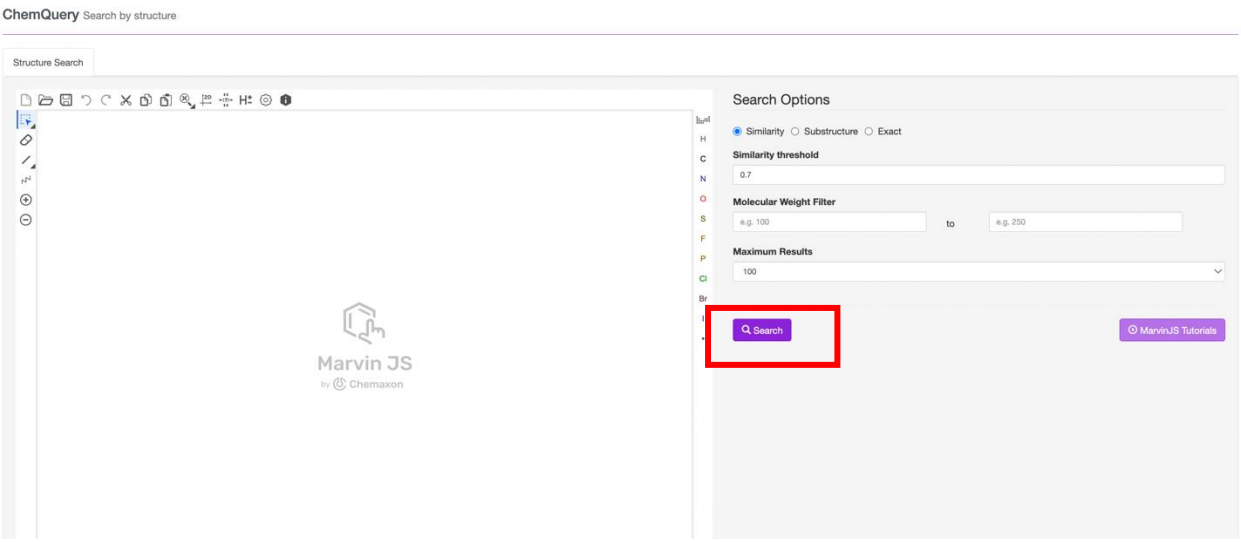
5. “Search” options. Clicking on the “Search” option at the top left of the homepage reveals a pulldown menu with three options including:

- Advanced Search (advanced search based on the textual fields of a Molecule Card);
- ChemQuery Structure Search (to search for a molecule by its chemical structure, whether by using its actual drawn structure or inserting its SMILES or InChI); and
- Text Query (the same search performed as using the search box in the top right of the homepage or the “Search Data” hyperlink bar in the centre of the homepage).

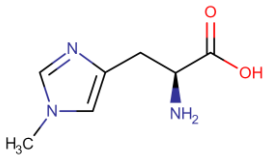
The website has provided online instructions for the Advanced Search and Text Query that are easy to follow.

➡ As the “ChemQuery Structure Search” is not straightforward, the following is an example to demonstrate how it is used.

For ChemQuery searches: The MarvinView applet from ChemAxon allows users to interactively draw structures or paste InChI or SMILES strings onto a palette. Click on the purple “Search” button and the MarvinView applet will be displayed.

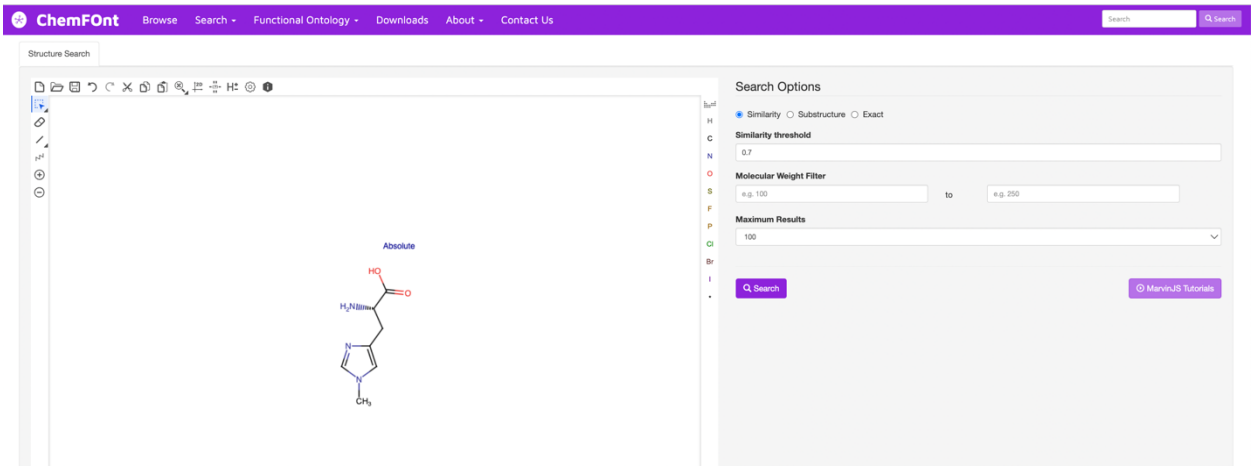


- If you were searching for the compound 1-methylhistidine, using the interactive palette,
  - you could draw its chemical structure as below;



  - insert its InChI (InChI=1S/C7H11N3O2/c1-10-3-5(9-4-10)2-6(8)7(11)12/h3-4,6H,2,8H2,1H3,(H,11,12)/t6-/m0/s1); or
  - insert one of its SMILES strings (e.g., CN1C=NC(C[C@H](N)C(O)=O)=C1).

- Inserting the SMILES string “CN1C=NC(C[C@H](N)C(O)=O)=C1” (without the quotation marks) generates the below chemical structure as shown within the applet.



- Selections for a narrowed search are also provided. Selecting the “Similarity” match option, then clicking the “Search” button returns these results.