Searching with PubChem Sketcher

- PubChem Sketcher is a web-based chemical structure sketching tool
- Allows users to search a manually drawn or modified structure
- Supports CID, SMILES, SMARTS, InChI, Molecular Formula, and select uploaded file formats
- More information at PubChem Sketcher Help

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Beginning of Exercise 2

Searching with PubChem Sketcher (1/10)

Go to the PubChem homepage . You can search by structure from the start by clicking on Draw Structure:

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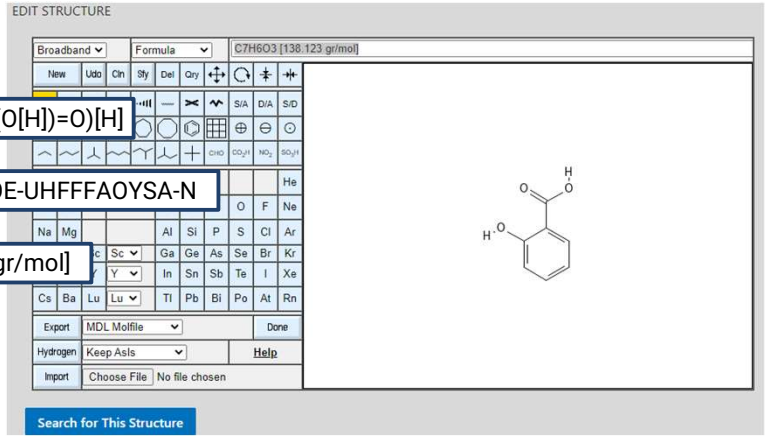
Searching with PubChem Sketcher (2/10)

And manually drawing a structure of interest or inputting SMILES, SMARTS, InChI, and InChiKey information:

SMILES O(C1=CC=CC=C1C(O[H])=O)[H]

InChIKey=YGSDEFSMJLZEOE-UHFFFAOYSA-N

Formula C7H6O3 [138.123 gr/mol]



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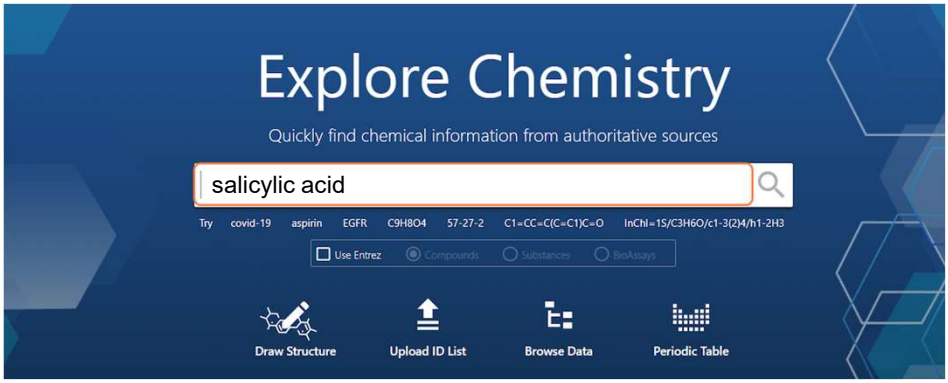
Searching with PubChem Sketcher (3/10)

Or you can find a similar structure during a text query. Here we will type "salicylic acid" into input:



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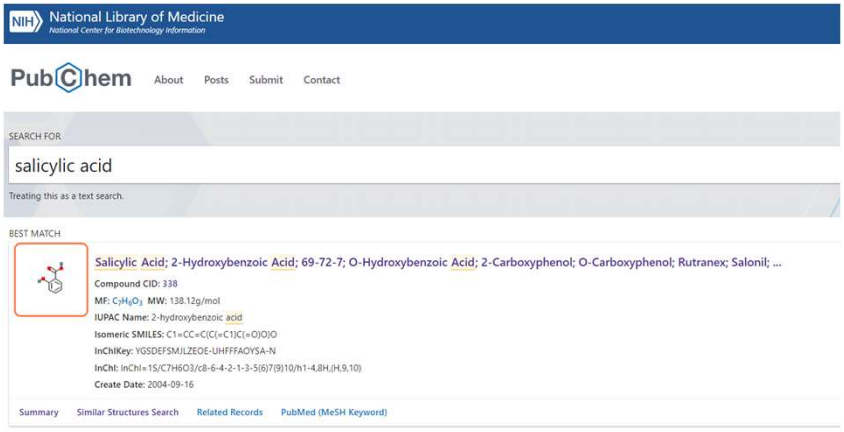
Searching with PubChem Sketcher (4/10)

And click on the Structure image:

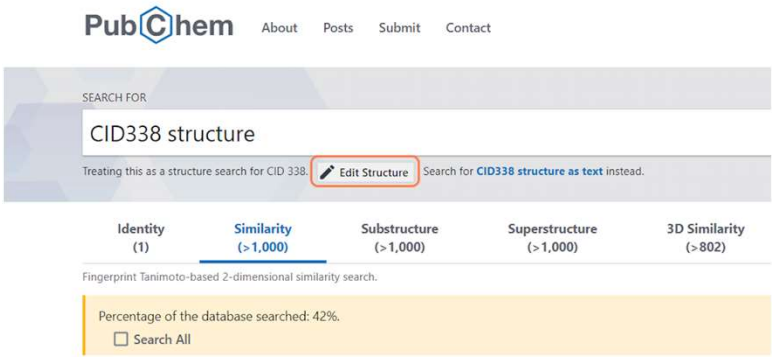


Searching with PubChem Sketcher (5/10)

Select Find Similar Structures:

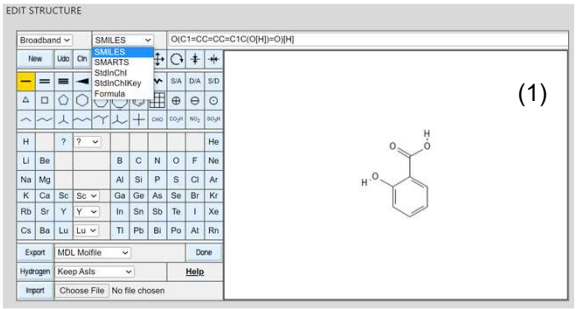
Searching with PubChem Sketcher (6/10)

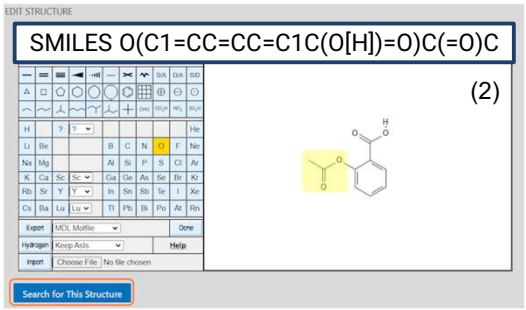
And select Edit Structure to make any changes:



Searching with PubChem Sketcher (7/10)

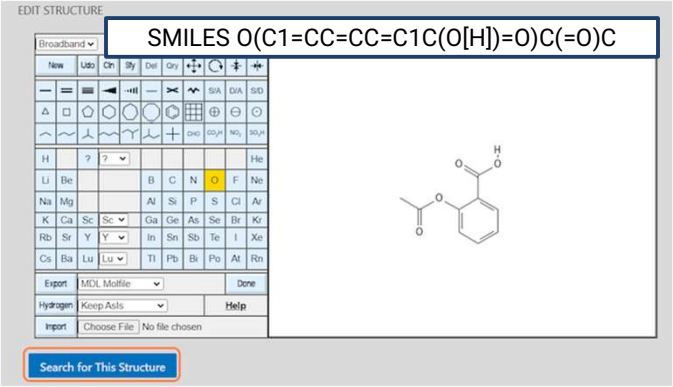
Here, you can replace the phenol (1) with a carboxyl manually (2) or change the SMILES String to O(C1=CC=CC=C1C(O[H])=O)C(=O)C:





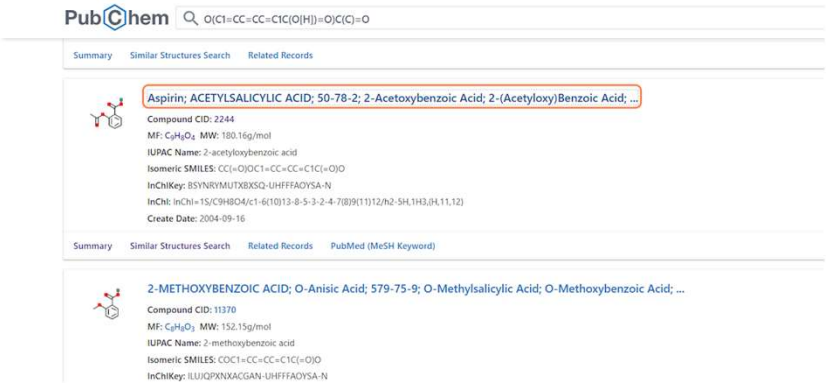
Searching with PubChem Sketcher (8/10)

And click on Search for This Structure to see how this effects the PubChem results:



Searching with PubChem Sketcher (9/10)

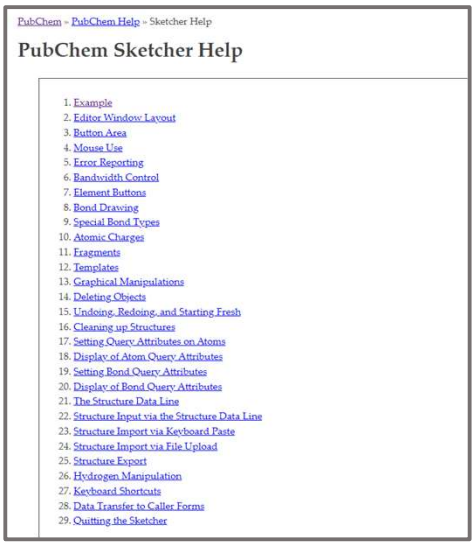
You will find a handful of results, one that may be of interest is Aspirin; ACETYLSALICYLIC ACID. You can open this entry to learn more:



Searching with PubChem Sketcher (10/10)

More information about the PubChem Sketcher can be found here:

5-minute break!


PubChem » PubChem Help » Sketcher Help

PubChem Sketcher Help

1. Example
2. Editor Window Layout
3. Button Area
4. Mouse Use
5. Error Reporting
6. Bandwidth Control
7. Element Buttons
8. Bond Drawing
9. Special Bond Types
10. Atomic Charges
11. Fragments
12. Templates
13. Graphical Manipulations
14. Deleting Objects
15. Undoing, Redoing, and Starting Fresh
16. Cleaning up Structures
17. Setting Query Attributes on Atoms
18. Display of Atom Query Attributes
19. Setting Bond Query Attributes
20. Display of Bond Query Attributes
21. The Structure Data Line
22. Structure Input via the Structure Data Line
23. Structure Import via Keyboard Paste
24. Structure Import via File Upload
25. Structure Export
26. Hydrogen Manipulation
27. Keyboard Shortcuts
28. Data Transfer to Caller Forms
29. Quitting the Sketcher

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