

## 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](#)

## Searching with [PubChem Sketcher](#) (1/10)

Go to the [PubChem homepage](#). You can search by structure from the start by clicking on Draw Structure:



## 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=YGSDEFSMJLZE0E-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:

Explore Chemistry

Quickly find chemical information from authoritative sources

salicylic acid

Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)/h1-2H3

Use Entrez  Compounds  Substances  BioAssays

Draw Structure Upload ID List Browse Data Periodic Table

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## Searching with [PubChem Sketcher](#) (4/10)

And click on the Structure image:


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SEARCH FOR  
salicylic acid

Treating this as a text search.

BEST MATCH

 Salicylic Acid; 2-Hydroxybenzoic Acid; 69-72-7; O-Hydroxybenzoic Acid; 2-Carboxyphenol; O-Carboxyphenol; Rutranex; SaloniL; ...  
Compound CID: 338  
MF: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub> MW: 138.12g/mol  
IUPAC Name: 2-hydroxybenzoic acid  
Isomeric SMILES: C1=CC=C(C(=O)O)C(=O)O  
InChIKey: YGSEFSMLZEO-UHFFFAOYSA-N  
InChI: InChI=1S/C7H6O3/c8-6-4-2-1-3-5(6)/7(10)/h1-4,8H,(H,9,10)  
Create Date: 2004-09-16

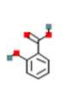
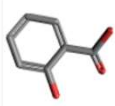
Summary Similar Structures Search Related Records PubMed (MeSH Keyword)

## Searching with [PubChem Sketcher](#) (5/10)

Select Find Similar Structures:

PubChem CID 338




Structure

2D 3D Crystal

[Find Similar Structures](#)

Chemical Safety

## Searching with [PubChem Sketcher](#) (6/10)

And select Edit Structure to make any changes:

PubChem About Posts Submit Contact

SEARCH FOR  
CID338 structure

Treating this as a structure search for CID 338. [Edit Structure](#) Search for **CID338 structure as text** instead.

Identity (1) **Similarity (>1,000)** Substructure (>1,000) Superstructure (>1,000) 3D Similarity (>802)

Fingerprint Tanimoto-based 2-dimensional similarity search.

Percentage of the database searched: 42%  
 Search All

## 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:

EDIT STRUCTURE

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

New Lib On SMARTS SDF InChI InChIKey Formula B/A D/A S/D

H ? ? ? ? ? ? ? ? ? ? He

Li Be B C N O F Ne

Na Mg Al Si P S Cl Ar

K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr

Rb Sr Y Zr Nb Mo Ru Rh Pd Ag Cd In Sn Sb Te I Xe

Cs Ba La Lu Hf Ta Pt Au Hg

Export MDL Molfile Done

Hydrogen Keep AsIs Help

Import Choose File No file chosen

(1)

EDIT STRUCTURE

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

Li Be B C N O F Ne

Na Mg Al Si P S Cl Ar

K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr

Rb Sr Y Zr Nb Mo Ru Rh Pd Ag Cd In Sn Sb Te I Xe

Cs Ba La Lu Hf Ta Pt Au Hg

Export MDL Molfile Done

Hydrogen Keep AsIs Help

Import Choose File No file chosen

Search for This Structure

(2)

## Searching with [PubChem Sketcher](#) (8/10)

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

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## 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:

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National Center for Biotechnology Information

## 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
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11. Fragments
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15. Undoing, Redoing, and Starting Fresh
16. Cleaning up Structures
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20. Display of Bond Query Attributes
21. The Structure Data Line
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26. Hydrogen Manipulation
27. Keyboard Shortcuts
28. Data Transfer to Caller Forms
29. Quitting the Sketcher