

Lab: Visualizing Chemical Structures with MolView

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Visualizing Chemical Structures

Chemists and students studying Chemistry typically need to draw visual representations of chemical structures. Before computers were common, chemists had plastic templates to trace different features to build up structures.

There are now several expensive software packages to do this. Examples are ACD/ChemSketch which has a free version for personal/academic use. It runs on Windows 64 bit computers. ACD/Labs notes that it will run on MacOS in a Windows Virtual Machine.

There is also a package called Chem Doodle that runs on Windows, MacOS, and Linux. It sounds great, right? There is a problem: The license costs \$15/month or \$150/year or \$750/life. Ouch!

Here is the good news: There is a website online that serves an Open Source package called MolView. This is great: No software to download. It runs in your Web Browser!

There is a manual available in PDF format [here](#). There is a helpful video by Roger Nixon on YouTube that demonstrates how to use MolView.

One advantage of Molview is that one can find input data for many organic molecules on the Pubchem website. This makes it easy to find molecular structures.

One can query for a molecule like toluene. Note that Pubchem lists an **InChIKey** for toluene: **YXFVABEGXRONW-UHFFFAOYSA-N**. If one types that key into the Molview **search** box at the top, Molview will draw the structure. That is really helpful!

We can also toggle certain features (like bonds and H) in the display

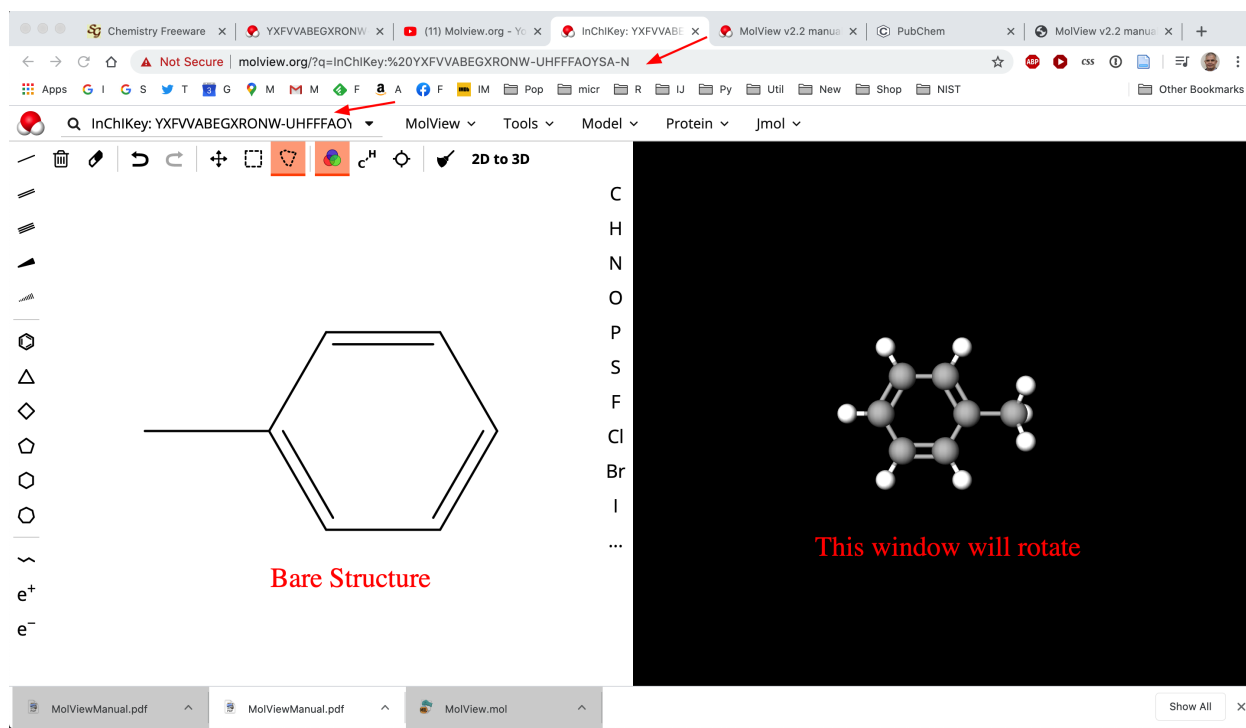
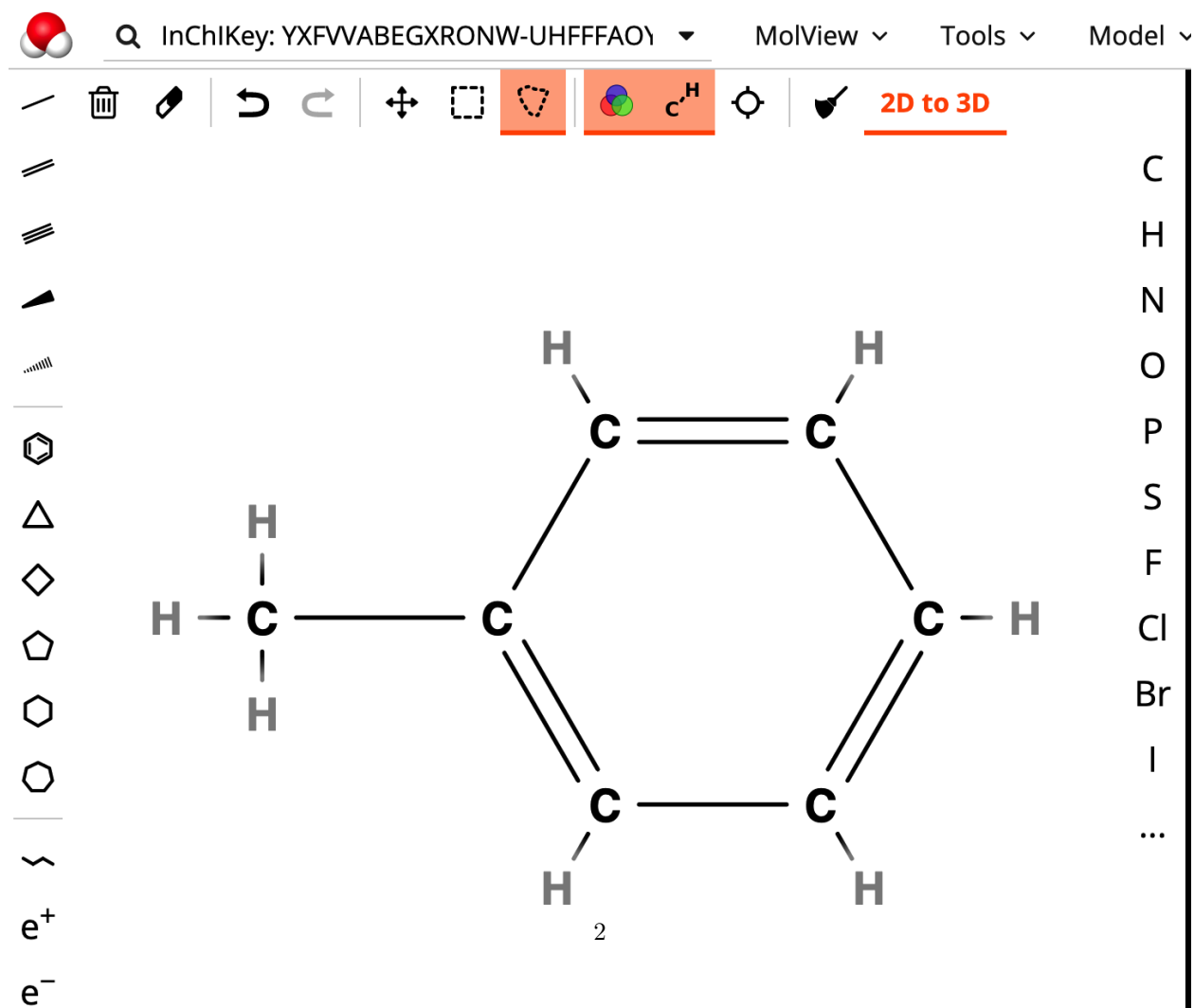


Figure 1: Toluene Example



We can search for benzoic acid on PubChem. The search returns

The screenshot shows the PubChem website interface. At the top, the browser address bar displays the URL `pubchem.ncbi.nlm.nih.gov/#query=benzoic%20acid`. Below the address bar is a navigation bar with the PubChem logo and links for About, Blog, Submit, and Contact. A search bar is prominently displayed with the text "benzoic acid" entered. Below the search bar, a message states "Treating this as a text search." The main content area is titled "COMPOUND BEST MATCH" and features a chemical structure of benzoic acid (a benzene ring with a carboxylic acid group). To the right of the structure, the following text is displayed: "Benzoic Acid; 65-85-0; Dracrylic Acid; Benzenecarboxylic Acid; Carboxybenzene; Benzeneformic Acid; Phenylformic Acid; Phenylcarboxylic Acid; ...". Below this, the following information is provided: "Compound CID: 243", "MF: C₇H₆O₂ MW: 122.12g/mol", "InChIKey: WPYMKLBDIGXBTP-UHFFFAOYSA-N", "IUPAC Name: benzoic acid", and "Create Date: 2004-09-16". At the bottom of the main content area, there are four tabs: "Summary", "Similar Structures Search", "Related Records", and "PubMed (MeSH Keyword)".

Figure 2: Benzoic Acid on PubChem

Note the key information:

MF: C₇H₆O₂ MW: 122.12g/mol

InChIKey: WPYMKLBDIGXBTP-UHFFFAOYSA-N

IUPAC Name: benzoic acid

Let's use the InChIKey to get the structure in MolView

Export Data

Note what you can export from the `tools` menu:

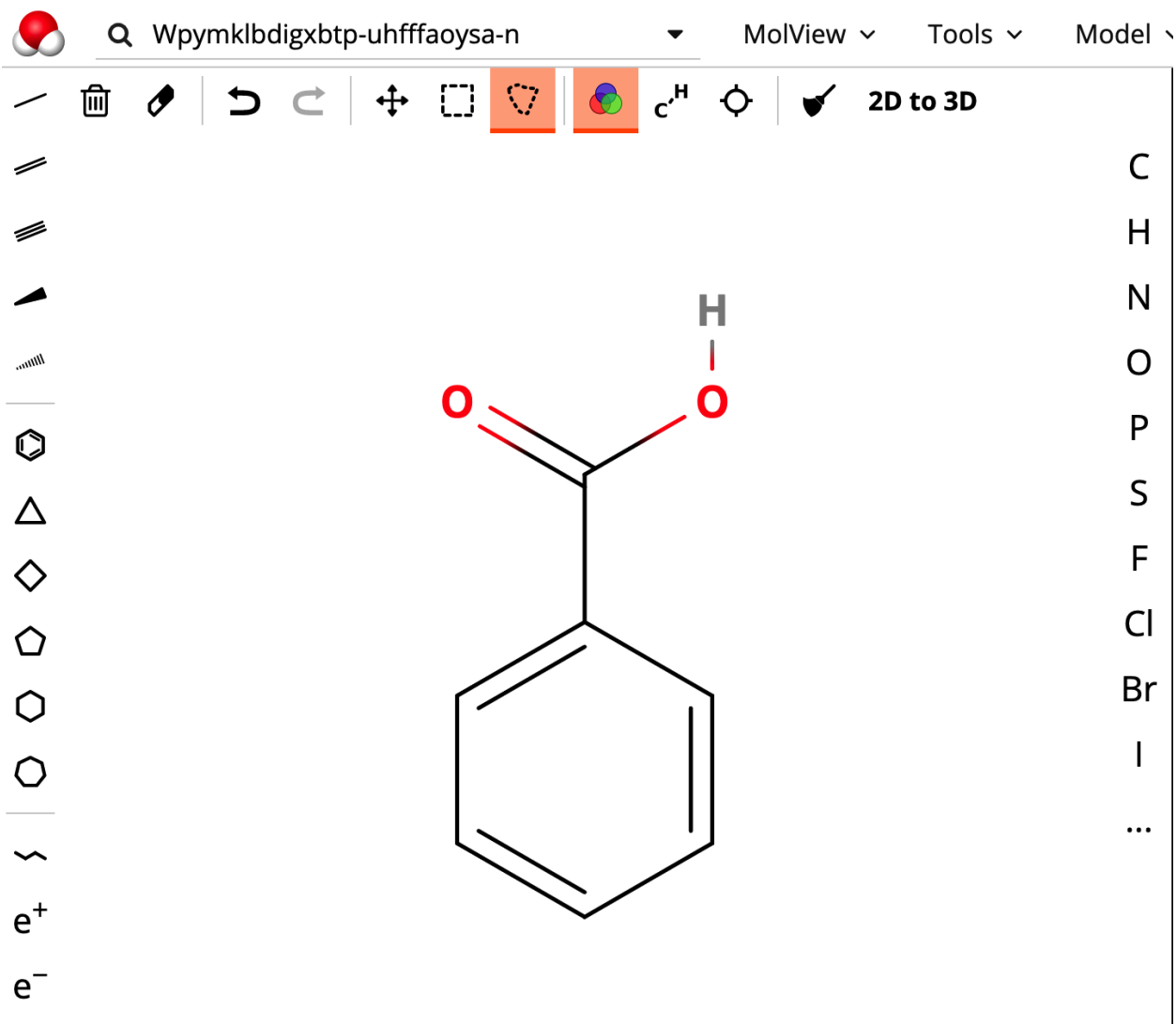


Figure 3: benzoic acid

Tools ▾

Model ▾

Protein

LINK

</> Embed

EXPORT

⬇️ Structural formula image

⬇️ 3D model image

⬇️ MOL file

CHEMICAL DATA

📊 Information card

📈 Spectroscopy

3D model source

ADVANCED SEARCH

≈ Similarity

⊂ Substructure

⊃ Superstructure