MolView manual

This is the manual for MolView version 2.2

MolView can be found at <u>molview.org</u>

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1. Drawing structural formulas

You can draw structural formulas using the Sketcher component.

Top toolbar

The top toolbar contains all general editing tools. The *2D to 3D* tool converts the structural formula into a 3D molecule which is displayed in the model window.

Top toolbar, from left to right: delete all, erase, undo, redo, move atoms/bonds, center view, rectangle select, lasso select, clear selection, clean structural formula, 2D to 3D conversion

Left toolbar

In the left toolbar, you can select a tool you want to use in order to modify or extend the structural formula. You can draw a carbon chain using the chain tool (11th button in image) Just click a start point or atom and drag a chain.

Left toolbar (rotated), from left to right: single bond, double bond, triple bond, up/down bond, benzene, cyclopropane/butane/pentane/hexane/heptane, chain, charge+, charge-

Right toolbar

The right toolbar contains some common elements and a periodic table tool in case you want to use another element. You can select an atom and click an existing atom in order to replace it with the selected atom. Note that you can only replace existing atoms. In order to add an atom, you will first have to add a new bond using the tools from the left toolbar.

Right toolbar (rotated), from left to right: hydrogen, carbon, nitrogen, oxygen, sulfur, phosphorus, fluorine, iodine, chlorine, bromine, table of elements, info (about dialog)

2. Finding structures

You can load structures from large databases like PubChem via the search bar located on the right side of the menubar. Just type what you are looking for and find it in the autocomplete dropdown or click one of the search categories listed below to perform a more extensive search.

- **Compounds:** small molecules from the PubChem database

- **Macromolecules:** biological macromolecules from the RCSB database

- **Crystals:** crystal structures from the Open Crystallography Database

You can also enter a PubChem CID via *Compounds*, a PDB ID via *Macromolecules* or a COD ID via *Crystals*. It is also possible to enter a SMILES, InChi or InChiKey string in the search field.

You can show or hide search results using the leftmost button (contains an eye) Note that *Macromolecules* search is absent on mobile devices which do not support WebGL since they can't display macromolecules anyway.

| Name, InChiKey, SMILES … | **Q** | Compounds | Macromolecules | Crystals | 👁 |
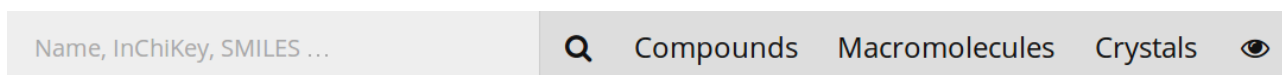
Search bar, from left to right: input field, fast search, compounds search (PubChem), macromolecules search (RCSB) and crystals search (COD)

3. Tools

The **Tools** menu contains several utility functions which are listed below.

Link

You can embed or share a specific compound, biomolecule or crystal using the provided URL or HTML code. Note that the linked structure is the one which is currently displayed in the model window. You can also copy the URL from the address bar in order to link to the current structure.

Export

Export options in the Export menu:

- **Structural formula image:** sketcher snapshot (PNG with alpha channel)

- **3D model image:** model snapshot (PNG, alpha channel in GLmol and ChemDoodle)

- **SDF file:** MDL Molfile from the 3D model **(common molecules)**

- **PDB file:** Protein Data Bank file from the 3D model **(macromolecules)**

- **CIF file:** Crystallographic Information File from the 3D model **(crystal structures)**

Information card

This function collects and displays information about the current structural formula (loaded from the Sketcher) You can also find a database reference for the current 3D model.

Spectroscopy

This function shows a new layer where you can view molecular spectra of the current structural formula (loaded from the Sketcher) More details are covered in the Spectroscopy chapter.

Advanced search

These functions allow you to perform some advanced searches through the PubChem database using the structural formula from the sketcher.

1. **Similarity search:** search for compounds with a similar structural formula

2. **Substructure search:** search for compounds with the current structure as subset

3. **Superstructure search:** search for compounds with the current structure as superset

4. Spectroscopy

You can open the Spectroscopy view via **Tools > Spectrocopy**. You can view three kinds of molecular spectra.

1. Mass spectrum

2. IR spectrum

3. H1-NMR prediction

Export data

You can also export different kinds of data from the currently selected spectrum.

1. **PNG image:** snapshot from interactive spectrum

2. **JCAMP file:** JCAMP-DX file of the current spectrum

5. 3D model

The **Model** menu contains some general functions for the 3D model.

Reset
This function sets the model position, zoom and rotation back to default.

Representation
You can choose from a list of different molecule representations including; ball and stick, stick, van der Waals spheres, wireframe and lines. Macromolecules are automatically drawn using ribbons.

Background
You can switch between a black, gray or white background. The default background is black (exported images from GLmol or ChemDoodle have a transparent background)

Engines
You can choose from three different render engines: **GLmol**, **Jmol** and **ChemDoodle**. GLmol is used as default render engine. GLmol and ChemDoodle are based on WebGL, a browser technology to support 3D graphics. If WebGL is not available in your browser, Jmol wil be used for all rendering.

MolView automatically switches to:

1. **Jmol** if you execute functions from the Jmol menu

2. **GLmol** if you load macromolecules and WebGL is available (due to significant higher performance)

3. **ChemDoodle** if you load a cr*ystal structure and WebGL is available (GLmol cannot render crystal structures)*

You might want to switch back to GLmol when you do no longer need Jmol or ChemDoodle since GLmol has a better performance.

Note that macromolecules are drawn slightly different in each engine. ChemDoodle provides the finest display. You should, however, avoid using ChemDoodle for very large macromolecules.

Model transformation

You can rotate, pan and zoom the 3D model. Use the right button for rotation, the middle button for translation (except for ChemDoodle) and the scrollwheel for zooming. On touch devices, you can rotate the model with one finger and scale the model using two fingers.

Crystallography

You can load an array of crystal cells (2x2x2 or 1x3x3) or a single unit cell when viewing crystal structures.

Fog and clipping

When you are viewing large structures, like proteins, it can be useful to hide a certain part using fog or a clipping plane. GLmol offers a few options to do this.

1. **Fog:** you can move the fog forward by dragging the mouse **up** while holding **CTRL + SHIFT** (drag in the opposite direction to move the fog backward)

2. **Clipping plane:** you can move a frontal clipping plane into the structure by dragging the mouse to the **left** while holding **CTRL + SHIFT** (drag in the opposite direction to move the clipping plane back)

6. Protein display

Proteins can be displayed in a number of different ways including different color types and different chain representations. These settings are located under the **Protein** menu in the menubar.

Biological assembly

Some macromolecules are only a small unit (asymmetric unit) from a much larger structure (biological unit) This function allows you to view the full biological unit.

Chain representation

You can choose from four different chain representations. You can also view the full chain structure by enabling the **Bonds** option.

1. **Ribbon:** draws ribbon diagram *(default representation)*

2. **Cylinder and plate:** solid cylinders for α-helices and solid plates for β-sheets

3. **B-factor tube:** tube were thickness is calculated from the B-factor *(thermal motion)*

4. **C-alpha trace:** lines between central carbon atom in amino-acids *(very fast rendering)*

Chain coloring

You can choose from six chain color schemes.

1. **Secondary structure:** different colors for α-helices, β-sheets, etc.

2. **Spectrum:** color spectrum *(rainbow)*

3. **Chain:** each chains gets a different color

4. **Residue:** all amino-acid residues are colored differently

5. **Polarity:** colors polar amino-acids red and non polar amino-acids white

6. **B-factor:** blue for low B-factor and red for high B-factor *(if provided)*

7. Advanced Jmol functions

Jmol offers some advanced functions. You can find them in the **Jmol** menu in the menubar. Note that all functions (except for render modes) are disabled when viewing proteins.

Clear
Clears all executed calculations and measurements.

High Quality
Enables High Quality rendering in Jmol (enabled by default on fast devices) When turned off, anti-aliasing is disabled and the model is drawn using lines while transforming it.

Calculations
You can perform the following Jmol calculations in Jmol:

- **MEP surface lucent/opaque:** calculates and projects molecular electrostatic potential on a translucent or opaque on van der Waals surface

- **Charge:** calculates and draws the atomic charge as labels

- **Bond dipoles:** calculates and draws the individual bond dipoles

- **Overall dipole:** calculates and draws the netto bond dipole

- **Energy minimization:** executes an interactive MMFF94 energy minimization

(note that this function only executes a maximum of 100 minimization steps at a time)

Measurement
You can measure distance, angle and torsion using Jmol. You can activate and deactivate one of these measurement types via the Jmol menu.

- **Distance:** distance between two atoms in **nm** *(select two atoms)*

- **Angle:** angle between two bonds in **deg** *(select three atoms)*

- **Torsion:** torsion between four atoms in **deg** *(select four atoms)*

Note that the resolved 3D model is only an approach of the real molecule, this means you have to execute an **Energy minimization** in order to do reliable measurements.