

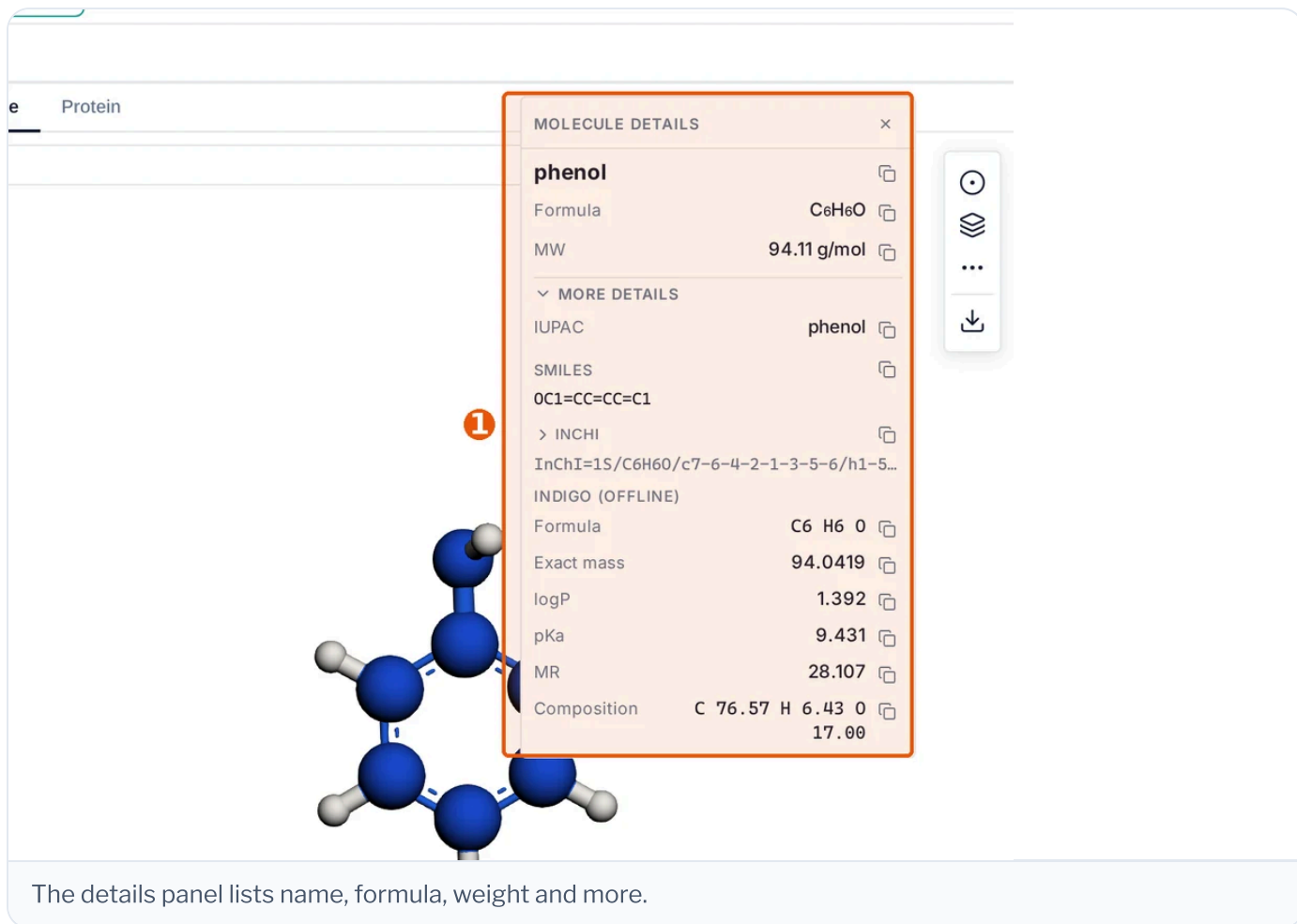
Analyze and 3D

MolDraw Docs · LabCanvas · 2 pages · mol draw.com/docs/

Names, formula and properties

Short answer: Select a molecule and click Info. You see the name, formula, weight, SMILES, InChI, exact mass, logP and more.

- 1 Select the molecule. Press **Ctrl** + **A** for everything.
- 2 Click **Info** at the top.
- 3 Click the copy icon next to any value.



The screenshot shows the MolDraw software interface. A 3D ball-and-stick model of a phenol molecule is displayed in the center. Overlaid on the right side is a 'MOLECULE DETAILS' panel. A red circle with the number '1' points to the 'Info' button at the top of this panel. The panel contains the following information:

MOLECULE DETAILS	
phenol	
Formula	C ₆ H ₆ O
MW	94.11 g/mol
▼ MORE DETAILS	
IUPAC	phenol
SMILES	<chem>Oc1ccccc1</chem>
> INCHI	InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5...
INDIGO (OFFLINE)	
Formula	C6 H6 O
Exact mass	94.0419
logP	1.392
pKa	9.431
MR	28.107
Composition	C 76.57 H 6.43 O 17.00

The details panel lists name, formula, weight and more.

For spectra, see NMR Analyser and the mass spectrum predictor.

Questions and answers

How do I get the IUPAC name?

Source: <https://www.moldraw.com/docs/analyze/how-to-find-iupac-name-molecular-formula-and-weight/>

3D viewer

Short answer: The 3D panel builds a 3D model from your drawing. Drag to rotate it. Use 3D Clean Up to show your 2D drawing in perspective.

- 1 Make sure the 3D panel is open. Click **3D** in the tools row if not.
- 2 Drag in the panel to rotate. Scroll to zoom.
- 3 Press **Ctrl** + **Shift** + **D** for 3D Clean Up on the canvas.

Use the **Protein** tab to load a PDB entry. See Protein viewer.

Questions and answers

How do I rotate my molecule in 3D?

Source: <https://www.moldraw.com/docs/analyze/how-to-view-molecules-in-3d/>