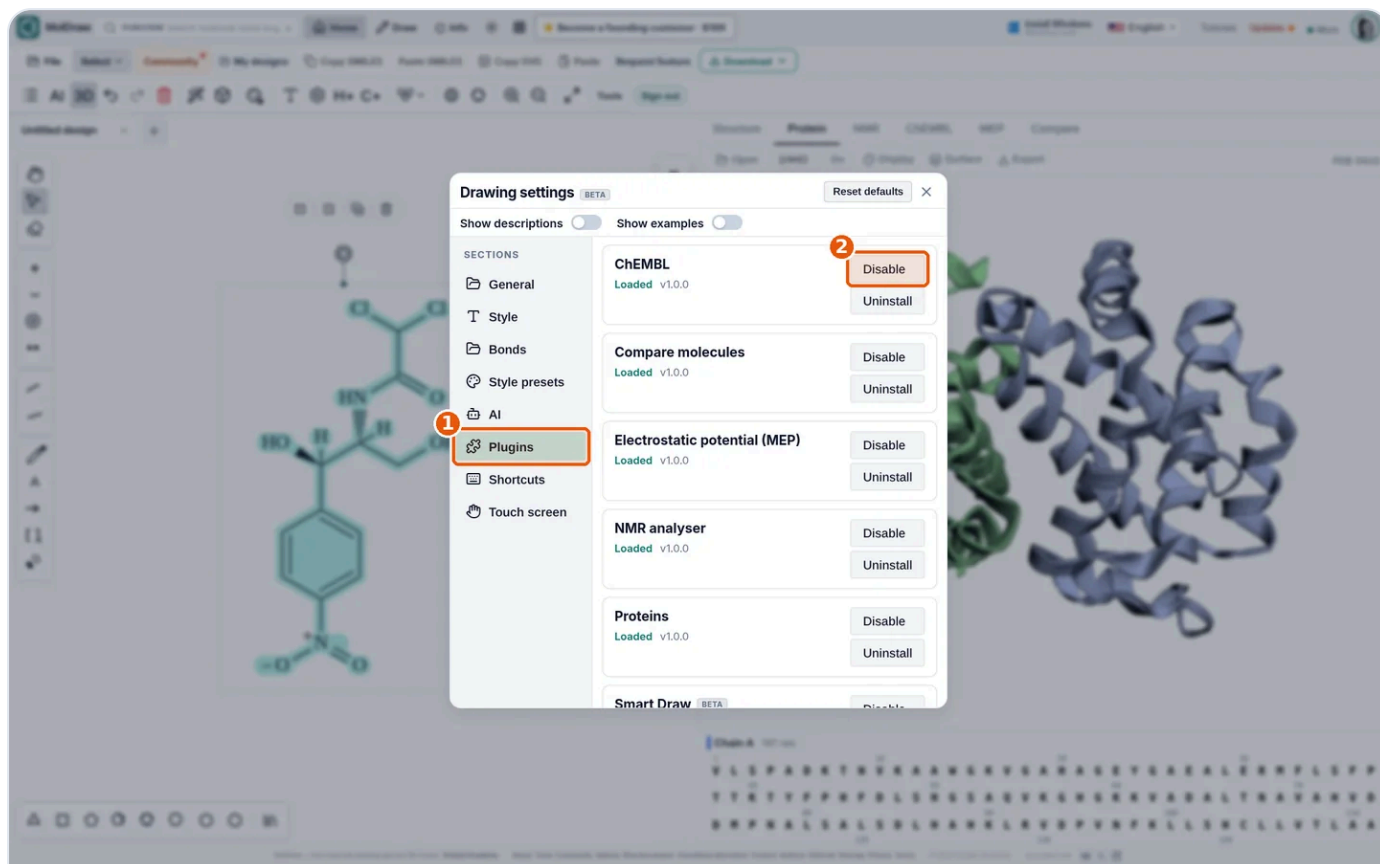


Plugins

MolDraw Docs · LabCanvas · 9 pages · moldraw.com/docs/

Plugins overview

Short answer: Plugins add extra features to MolDraw. Open Settings, then Plugins, and click Install. Most need a free account.



1 Plugins section. 2 Install, Disable or Uninstall.

- 1 Sign in to MolDraw.
- 2 Click **Settings** (gear icon).
- 3 Click **Plugins**.
- 4 Click **Install** next to the plugin you want.

All plugins

- NMR Analyser: Predict ^1H , ^{13}C , COSY, HSQC and HMBC spectra. You get peak tables and atom labels.
- ChEMBL: Look up bioactivity, targets and similar compounds in ChEMBL for any molecule.
- Electrostatic Potential (MEP): Color a 3D surface by electrostatic potential from Gasteiger charges.
- Compare Molecules: Compare structures side by side. See Tanimoto similarity, group changes and export CSV.
- Protein Viewer: Load a PDB entry by ID or file. Show cartoon or surface and export images.
- Smart Draw: Sketch with a pen, mouse or finger. Strokes turn into bonds, rings and labels.
- AI Spectroscopy: Ask the AI chat for NMR, mass and UV-Vis predictions of your molecule.
- Themes (Ball-and-Stick): Switch the 2D canvas to a colored ball and stick look for slides and posters.

NOTE

Protein viewer and Themes are on by default. They work without an account.

Questions and answers

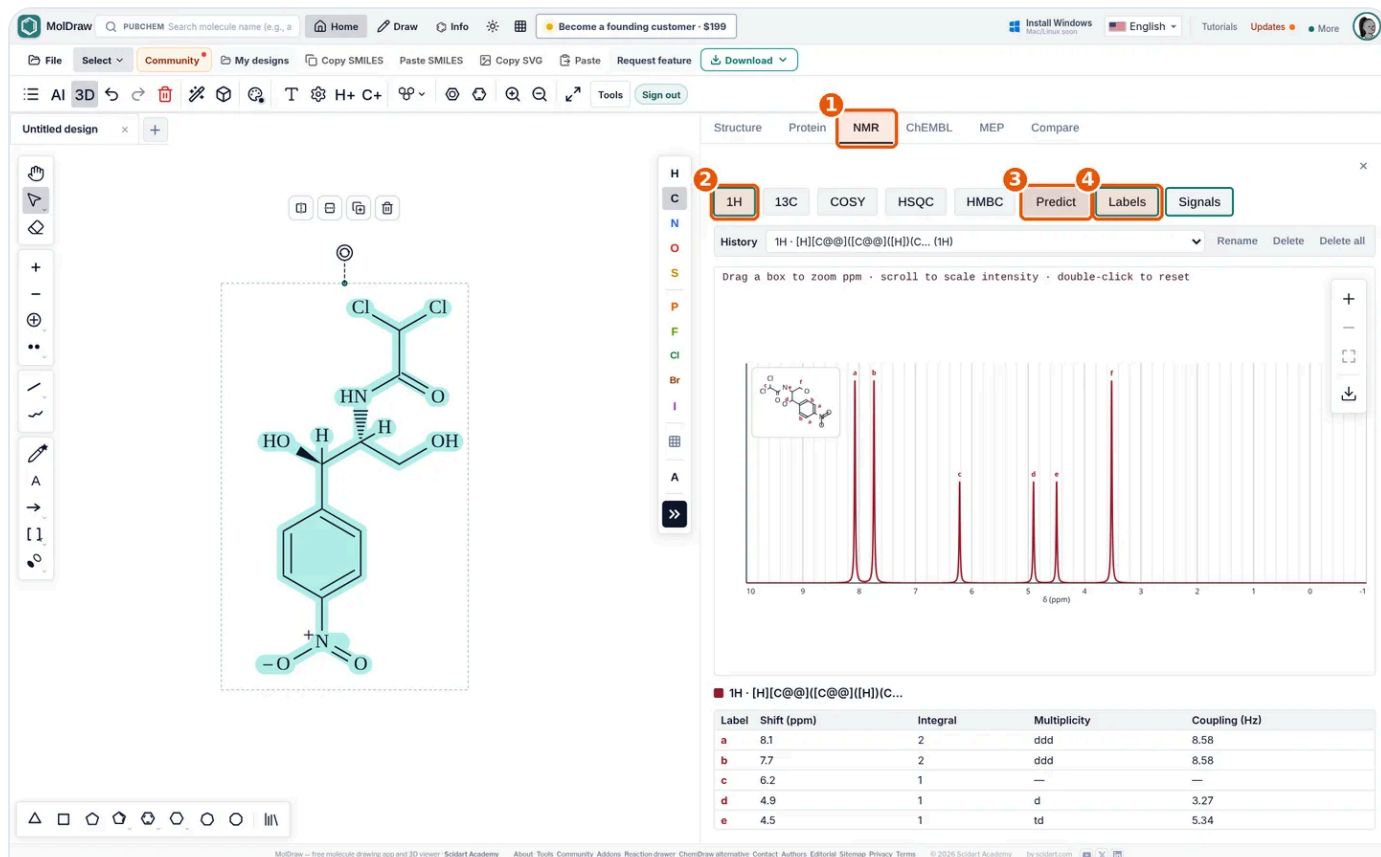
Are plugins free?

Where do plugin panels open?

Source: <https://www.moldraw.com/docs/plugins/moldraw-plugins-overview-and-how-to-install/>

NMR Analyser plugin

Short answer: Install NMR Analyser from Settings, Plugins, draw a molecule, open the NMR tab, pick an experiment and press Predict.



Predicted 1H spectrum of chloramphenicol. Each signal has a letter. The table lists shift, integral, splitting and J.

1. NMR tab in the right-hand analysis panel.
2. Experiment buttons: 1H, 13C, COSY, HSQC, HMBC.
3. Predict runs the prediction for the current canvas structure.
4. Labels / Signals toggle peak letters and the signal list.

What it does

The plugin predicts NMR spectra for the structure on your canvas.

- 1D 1H and 13C spectra show peaks with letters.
- The table gives shift, integral, splitting and coupling constant for each letter.
- 2D COSY, HSQC and HMBC show as contour plots. You can see which atoms are linked.
- Each run goes into **History**. Switch between molecules or experiments there.

To learn the basics, read [How to read an NMR spectrum](#).

Who it is for

Students who check a structure against a lab spectrum. Teachers who make worked examples. Chemists who want a quick sanity check.

How to use it

- 1 Open the MolDraw editor and sign in. Click **Settings**, then **Plugins**, then **Install** next to NMR Analyser.
- 2 Draw or paste your structure (e.g. paste a SMILES with **Paste SMILES**).
- 3 Open the **NMR** tab in the right panel (callout 1).
- 4 Choose the experiment, **1H** or **13C** for 1D, or COSY/HSQC/HMBC for 2D (callout 2).
- 5 Press **Predict** (callout 3). The spectrum appears in a few seconds.
- 6 Drag a box to zoom into a ppm range, scroll to scale intensity, double-click to reset.
- 7 Turn on **Labels** (callout 4) to match peak letters with the table and hover a row to highlight the atoms.
- 8 Export the plot (PNG/SVG) or the peak list (CSV) with the download button.

Tips

- Draw explicit stereochemistry: diastereotopic protons can give different predicted shifts.
- Use HSQC to assign which H sits on which C, then HMBC to connect fragments across quaternary carbons.
- Predictions are for CDCl₃-like conditions; OH/NH shifts vary a lot with solvent and concentration.
- New to NMR. Read [how to read an NMR spectrum](#) first.

Questions and answers

How accurate is the predicted NMR?

Does the NMR Analyser need an account?

Can it predict 2D NMR?

Can I export the spectrum?

Source: <https://www.moldraw.com/docs/plugins/nmr-analyser-plugin-predict-1h-13c-and-2d-nmr-spectra/>

ChEMBL plugin

Short answer: Install ChEMBL from Settings, Plugins, open the ChEMBL tab, click Use canvas or type a name/ID, then press Lookup.

The screenshot illustrates the MolDraw interface with the ChEMBL plugin. The main canvas shows a chemical structure of aspirin. The right-hand panel is the ChEMBL analysis panel, with the 'ChEMBL' tab selected. The search bar contains the text 'aspirin', and the 'Lookup' button is highlighted. Below the search bar, the 'Overview' tab is active, displaying details for CHEMBL25 Aspirin, including its type (Small molecule), phase (Max phase Approved), and InChIKey. The bottom of the panel shows 21 protein targets and 4 other 158 measurements with pChEMBL.

Searching "aspirin" finds CHEMBL25. You can load it, add it to the canvas or send it to Compare.

1. ChEMBL tab in the analysis panel.
2. Query box: a name, ChEMBL ID (e.g. CHEMBL25) or the canvas structure.
3. Lookup runs the search.
4. Result tabs: Overview, Targets, Activity and Similar.

What it does

ChEMBL is a free database of drug-like molecules. EMBL-EBI runs it. It holds millions of activity data points.

- **Search** finds a compound by name, ChEMBL ID or your drawing.
- **Targets** lists proteins the compound was tested on.
- **Activity** lists values like IC50 and Ki.
- **Similar** finds look-alike compounds. Load any of them to the canvas.

Who it is for

Medicinal chemistry students. Researchers who check known activity. Teachers who show real drug data.

How to use it

- 1 Open the MolDraw editor and sign in. Click **Settings**, then **Plugins**, then **Install** next to ChEMBL.
- 2 Draw a molecule or leave the canvas empty if you will search by name.
- 3 Open the **ChEMBL** tab (callout 1).
- 4 Type a name or ChEMBL ID in the query box (callout 2) or press **Use canvas**.
- 5 Press **Lookup** (callout 3).
- 6 Browse the **Overview**, **Targets**, **Activity**, **Similar** tabs (callout 4).
- 7 Use **Load to canvas**, **Append** or **Send to Compare** to keep working with a hit.

Tips

- If a drawn structure is not found, check stereochemistry and charges; InChIKey matching is exact.
- Activity values from different assays are not directly comparable; open the assay link for conditions.
- Pair with Lipinski's rule of five and drug-likeness to screen hits.

Questions and answers

What is ChEMBL?

Is the ChEMBL plugin free?

Can I search by structure?

Source: <https://www.moldraw.com/docs/plugins/chembl-plugin-bioactivity-and-drug-target-lookup/>

Electrostatic Potential (MEP) plugin

Short answer: Install MEP from Settings, Plugins, draw a molecule, open the MEP tab and press Show in 3D.

The screenshot shows the MolDraw software interface. On the left is a 3D model of a chloramphenicol molecule. On the right is the 'Electrostatic potential (MEP)' panel. The panel includes a color scale from red (electron-rich) to blue (electron-poor), a 'Show in 3D' button, a 'Refresh charges' button, and an 'Opacity' slider set to 85%. Below these is a table of heavy-atom partial charges (most negative first).

Atom	Element	Charge
6	O	-0.445
5	O	-0.200
3	O	-0.169
4	O	-0.166
8	N	-0.151
1	Cl	-0.083
2	Cl	-0.083
12	C	-0.005
14	C	+0.002
15	C	+0.002
9	N	+0.012
17	C	+0.059
18	C	+0.059
7	O	+0.073
10	C	+0.079
11	C	+0.108

MEP for chloramphenicol. Oxygen atoms are most negative (red). Carbons with H are a bit positive (blue).

1. MEP tab in the analysis panel.
2. Colour scale from most electron-rich (red) to electron-poor (blue).
3. Show in 3D draws the coloured surface on the 3D model; Refresh charges recalculates after edits.
4. Opacity slider for the surface.
5. Charge table: Gasteiger partial charge for every heavy atom, sorted most negative first.

What it does

The plugin works out Gasteiger partial charges for each atom. Then it colors a surface around the 3D model. Red is negative. Blue is positive.

It is fast, but it is not a quantum calculation. Use it to compare, not for exact energies. For example, see which end is more negative or where a nucleophile will attack.

Who it is for

Students who learn polarity. Teachers who make slides about charge. Anyone who wants a quick picture of charge in a molecule.

How to use it

- 1 Open the MolDraw editor and sign in. Click **Settings**, then **Plugins**, then **Install** next to Electrostatic Potential (MEP).
- 2 Draw a molecule (or load one by name using the PubChem search box).
- 3 Open the **MEP** tab (callout 1); charges are calculated immediately.
- 4 Read the colour scale (callout 2) and the charge table (callout 5).
- 5 Press **Show in 3D** (callout 3) to paint the surface on the 3D model.
- 6 Adjust **Opacity** (callout 4) to see the ball-and-stick model through the surface.
- 7 Use **Turn surface off** to return to the plain 3D view.

Tips

- Compare related molecules, e.g. phenol vs. aniline, to see how substituents change charge.
- After editing the 2D drawing, press Refresh charges.
- For bond polarity, see the Lewis structure generator and VSEPR calculator.

Questions and answers

What does an electrostatic potential map show?

How is the MEP calculated in MolDraw?

Is it free?

Source: <https://www.moldraw.com/docs/plugins/mep-plugin-molecular-electrostatic-potential-surface/>

Compare Molecules plugin

Short answer: Install Compare molecules, open the Compare tab, press Add canvas for the reference, paste other SMILES and press Add SMILES.

The screenshot shows the MolDraw software interface. The 'Compare' tab is selected in the top right. The 'Compare molecules' panel is open, showing a comparison between a reference molecule (Chloramphenicol) and a selected molecule (Salicylic acid). The panel includes a text input for pasting SMILES, buttons for 'Add canvas', 'Add SMILES', 'Clear', and 'CSV', and a table of comparison results.

#	Drawing	Structure similarity	Functional similarity	Changes
1		ref	ref	
2		11%	37%	NO ₂ → O ₂ ; - acetamido acid; + O
3		17%	36%	modified O ₂ ; - acetamido acid; O → carboxylic acid

Chloramphenicol as the reference, next to salicylic acid and paracetamol. You see two similarity scores and a list of changes.

1. Compare tab.
2. Add canvas adds the current drawing (the first molecule is the reference).
3. SMILES box: one SMILES per line, optional name after a space.
4. Add SMILES adds them all to the table.
5. CSV exports the comparison table.

What it does

Pick one molecule as the reference. Add others to compare.

- **Structure similarity** is a Tanimoto score from fingerprints.
- **Functional similarity** compares the groups each molecule has.
- **Changes** lists groups gained, lost or changed.

- Export the table as CSV.

Who it is for

Medicinal chemists who look at analogues. Students who compare isomers or drug series.

How to use it

- 1 Open the MolDraw editor and sign in. Click **Settings**, then **Plugins**, then **Install** next to Compare Molecules.
- 2 Draw the reference molecule.
- 3 Open the **Compare** tab (callout 1) and press **Add canvas** (callout 2).
- 4 Paste more structures as SMILES, one per line (callout 3), then press **Add SMILES** (callout 4).
- 5 Click a row to see reference and selected structures side by side with the shared core highlighted.
- 6 Sort by similarity, and press **CSV** (callout 5) to export.

Tips

- Tanimoto 1.00 can still hide stereo differences; check the stereo flag column.
- Use the ChEMBL plugin's Send to Compare to add database hits directly.
- To get SMILES, convert names with name to SMILES.

Questions and answers

What is Tanimoto similarity?

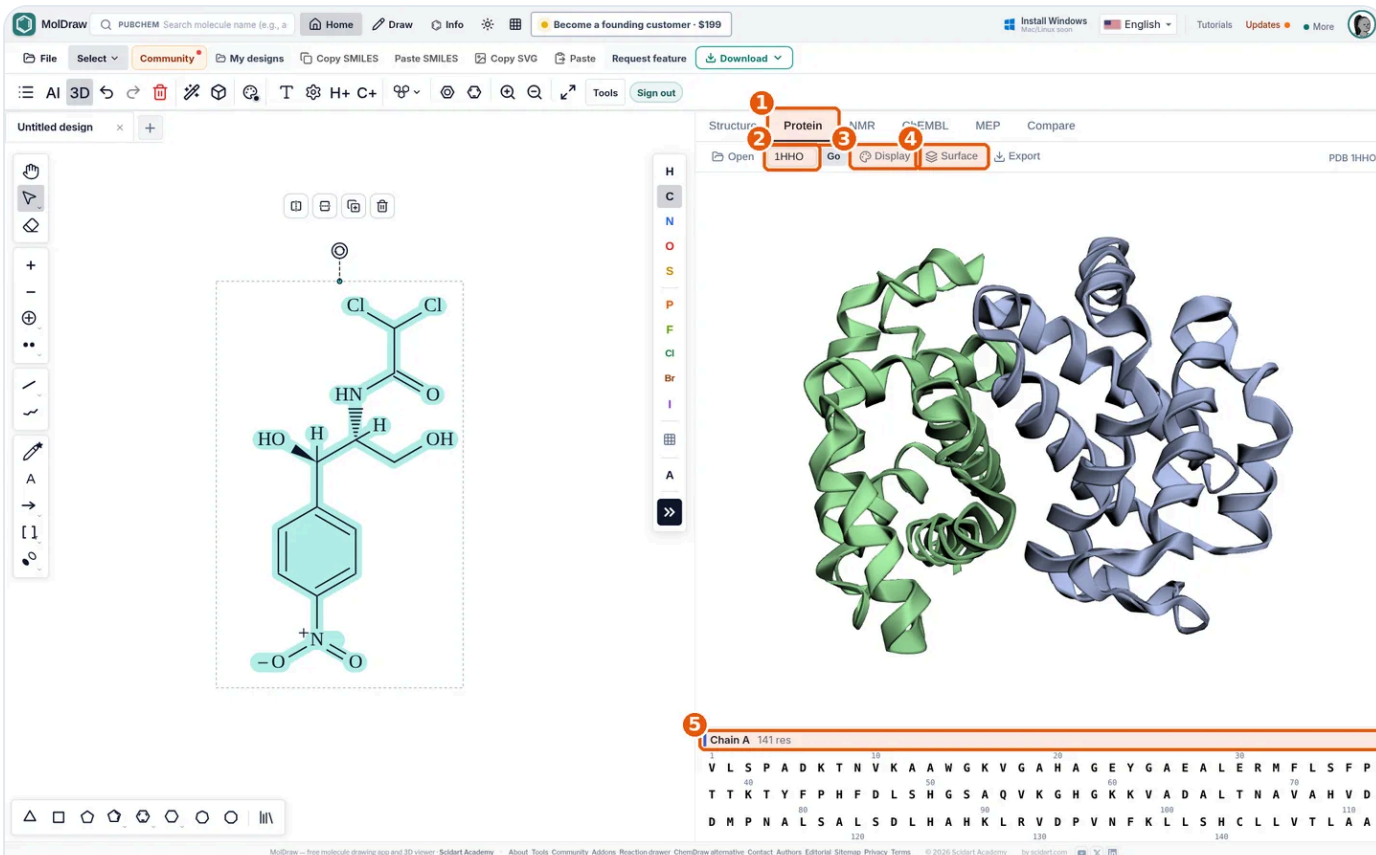
How many molecules can I compare?

Does it detect stereoisomers?

Source: <https://www.moldraw.com/docs/plugins/compare-molecules-plugin-tanimoto-similarity/>

Protein Viewer plugin

Short answer: Open the Protein tab, type a PDB ID such as 1HHO and press Go. It is installed by default and works without signing in.



Haemoglobin (PDB 1HHO) as a cartoon. Each chain has its own color. The sequence of chain A is below.

1. Protein tab.
2. PDB ID box: type an ID and press Go (or use Open for a file).
3. Display menu: cartoon, sticks, lines, spheres and colouring.
4. Surface: molecular surface with opacity and colour.
5. Sequence strip: click residues to select and style them.

What it does

Open the **Protein** tab next to Structure. Type a PDB ID like 1HHO, or load a file.

- **Display** sets the style: cartoon, stick or surface.
- Color by chain, secondary structure or element.
- Click the sequence strip to select residues.
- Export a PNG of the view.

Who it is for

Biochemistry students. Teachers who need protein figures. Researchers who want a quick look at a structure.

How to use it

- 1 Open the editor (no sign-in needed) and click the **Protein** tab (callout 1).
- 2 Type a PDB ID, e.g. `1HHO` , and press **Go** (callout 2), or press Open to load a local file.
- 3 Use **Display** (callout 3) to switch cartoon/sticks and colour by chain.
- 4 Add a **Surface** (callout 4) and lower its opacity to see the backbone.
- 5 Click residues in the **sequence strip** (callout 5) to highlight them.
- 6 Press **Export** to download an image.

Tips

- Try 1HHO (haemoglobin), 1BNA (B-DNA), 6LU7 (SARS-CoV-2 main protease) or 1GFL (GFP).
- Calculate a protein's mass from its sequence with the protein molecular weight calculator.
- For docking prep, use PDB to PDBQT.

Questions and answers

Do I need an account to view proteins?

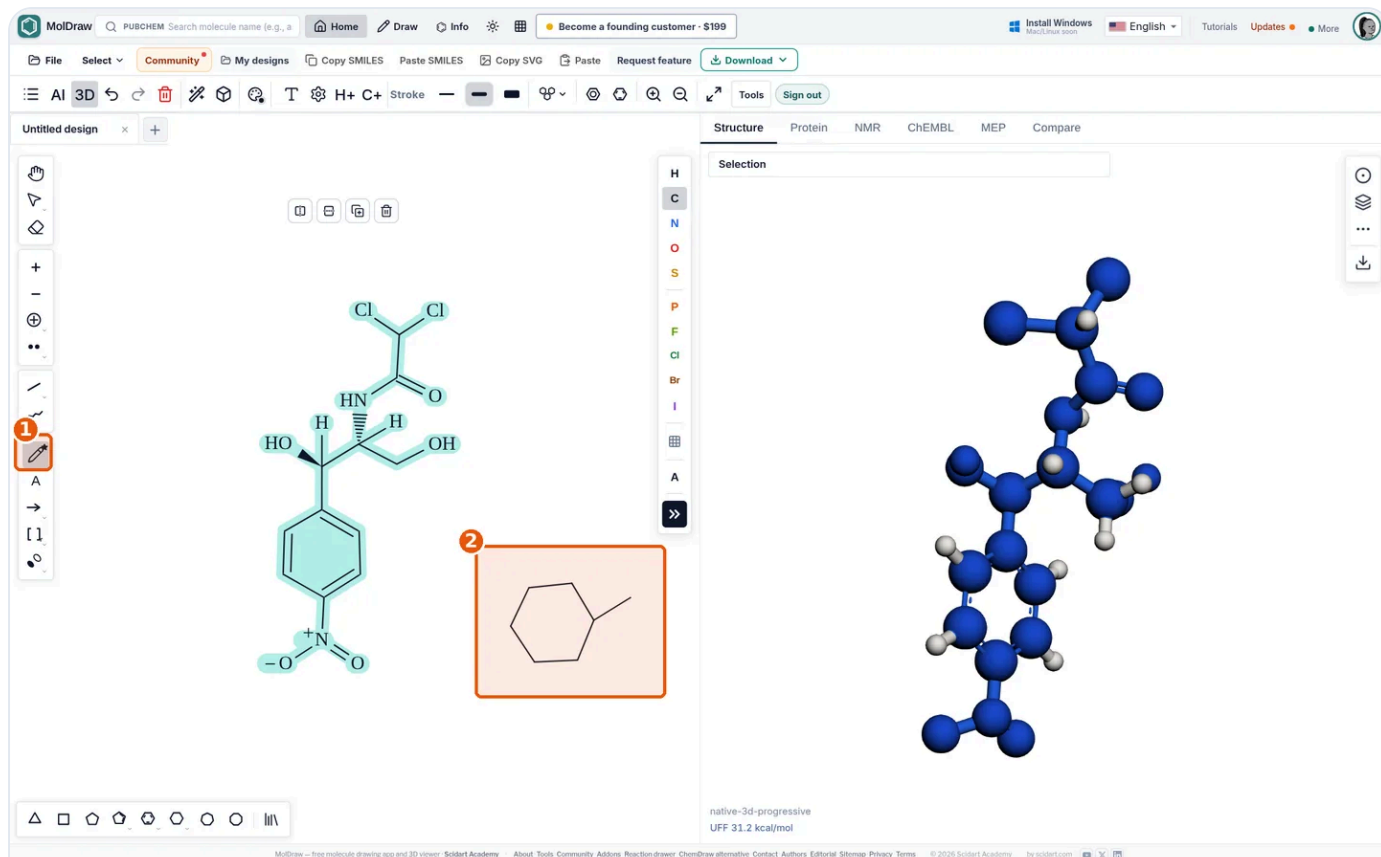
Which file formats can I open?

Can I show a ligand as sticks?

Source: <https://www.moldraw.com/docs/plugins/protein-viewer-plugin-view-pdb-structures-in-3d/>

Smart Draw plugin

Short answer: Install Smart Draw, pick the Smart Draw pencil in the left toolbar, sketch, then pause or press Enter to convert.



A hand-drawn hexagon with one extra stroke. Smart Draw turns it into methylcyclohexane.

1. Smart Draw tool in the left toolbar.
2. Sketch area: freehand strokes are recognised as a ring plus a substituent bond.

What it does

Draw with the Smart Draw pencil. MolDraw reads your strokes.

- Straight strokes become bonds.
- Closed shapes become rings of the same size.
- Written letters become atom labels.

The result is a normal MolDraw structure. You can edit it, clean it up or export it.

Who it is for

Tablet and stylus users. Teachers who draw on a whiteboard. Students who find clicking slow.

How to use it

- 1 Open the MolDraw editor and sign in. Click **Settings**, then **Plugins**, then **Install** next to Smart Draw.
- 2 Install Smart Draw from Settings , Plugins.
- 3 Select the **Smart Draw** tool in the left toolbar (callout 1).
- 4 Sketch bonds or a ring on the canvas (callout 2). Keep strokes reasonably straight.
- 5 Pause for about 1.2 s, or press **Enter**, to convert the strokes.
- 6 Write a letter at a bond end to place a heteroatom, or switch to the normal tools to refine.
- 7 Use **Cleanup** to tidy bond lengths and angles.

Tips

- Draw rings in one continuous stroke for the best recognition.
- On iPad, use Apple Pencil and enable the touch-screen settings in Settings , Touch screen.
- After converting, copy the SMILES with Copy SMILES or check the formula with the SMILES to formula tool.

Questions and answers

Does Smart Draw work offline?

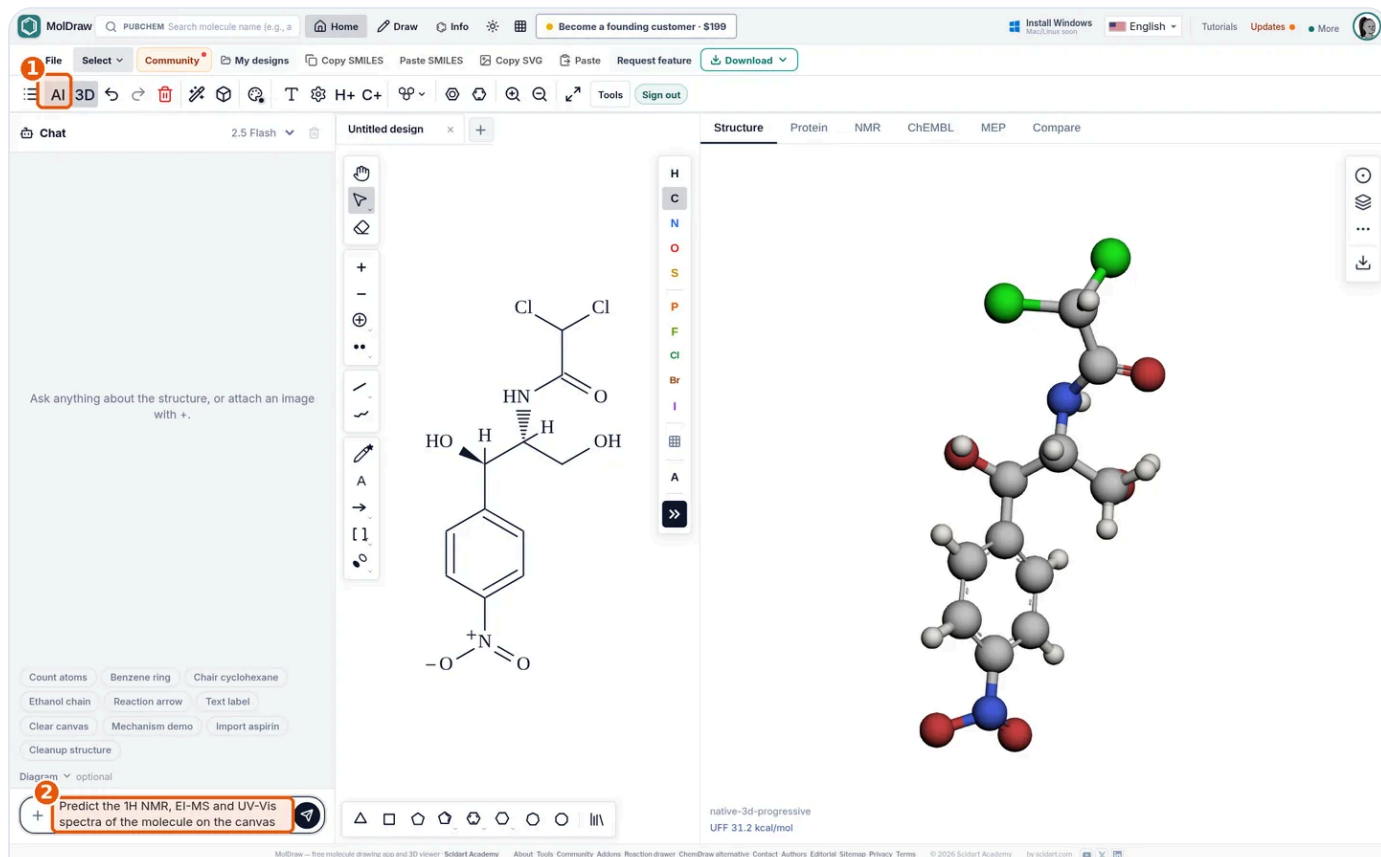
Can I draw on a phone or tablet?

What can it recognise?

Source: <https://www.moldraw.com/docs/plugins/smart-draw-plugin-hand-drawn-sketch-to-structure/>

AI Spectroscopy plugin

Short answer: Add a Gemini API key in Settings, AI, install Spectroscopy, open AI chat and ask e.g. "Predict the EI mass spectrum of this molecule".



The AI chat predicts NMR, EI mass and UV-Vis data for the structure on the canvas.

1. AI chat button in the toolbar.
2. Prompt box: describe which spectrum you want.

What it does

The plugin sends your structure to the AI model. The model returns peaks in a fixed format. MolDraw shows them as tables and charts.

The values come from a language model. Use them to learn and explain. Do not use them as reference data. Check real spectra in SDBS or NIST.

Who it is for

Students who want a quick guess at a spectrum. Teachers who make practice problems.

How to use it

- 1 Open the MolDraw editor and sign in. Click **Settings**, then **Plugins**, then **Install** next to AI Spectroscopy.
- 2 Open Settings , AI and paste your Gemini API key (stored only in your browser).
- 3 Install **Spectroscopy** from Settings , Plugins.
- 4 Draw the molecule.
- 5 Click **AI chat** (callout 1).
- 6 Type a request in the prompt box (callout 2), e.g. "Predict the ^1H NMR spectrum".
- 7 Open the result window to see the spectrum, peak table and notes.

Tips

- Ask follow-up questions such as "Why is the base peak at m/z 43?"
- Check the molecular ion with the exact mass calculator.
- Learn to read the plots with the mass spectrum, IR and NMR guides.

Questions and answers

Does the AI Spectroscopy plugin cost money?

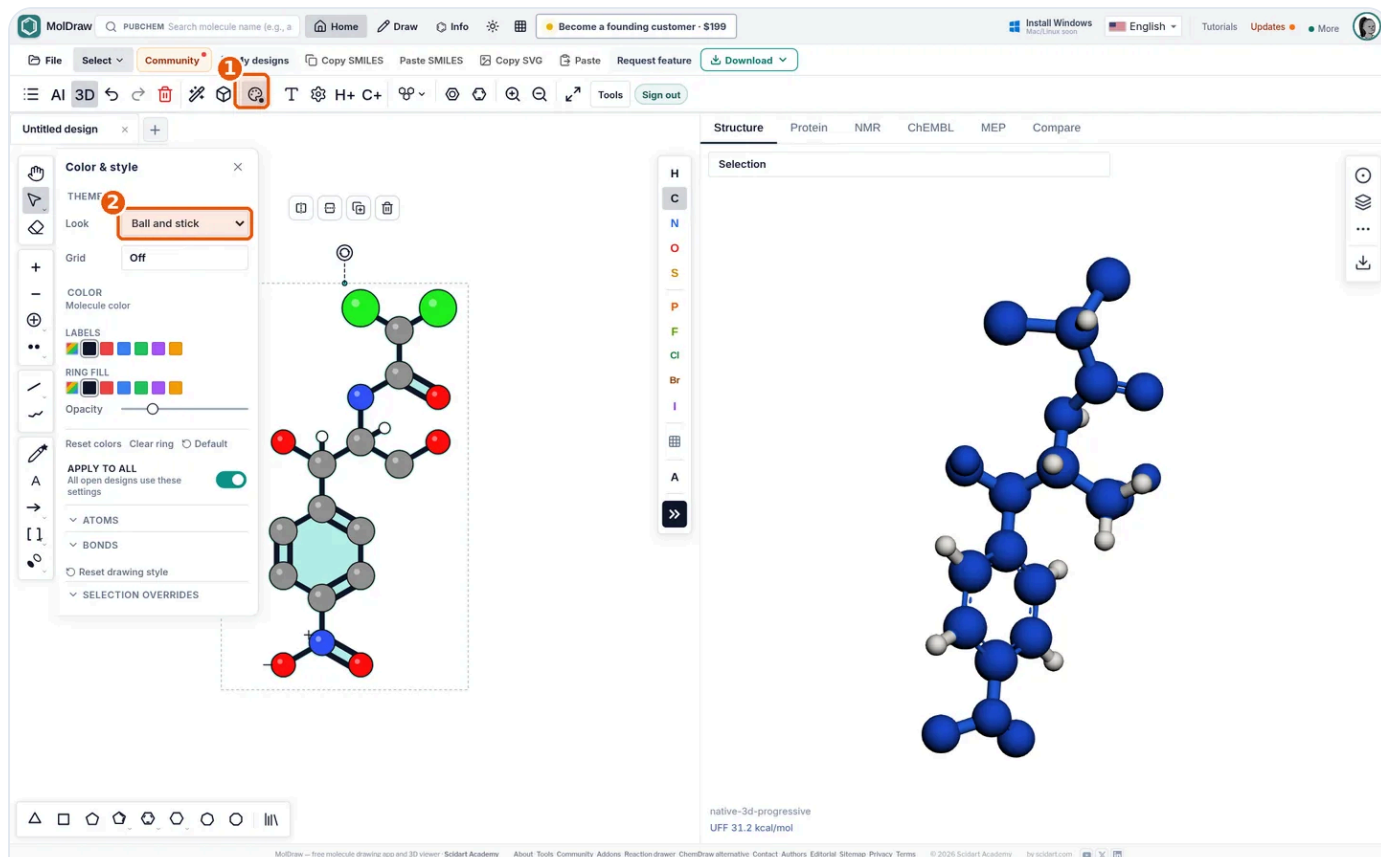
Are AI-predicted spectra accurate?

Which spectra can it predict?

Source: <https://www.moldraw.com/docs/plugins/ai-spectroscopy-plugin-predict-nmr-ms-and-uv-vis/>

Themes (Ball-and-Stick) plugin

Short answer: Click Color & style in the toolbar and set Look to Ball and stick. Themes is installed by default.



Chloramphenicol in the Ball and stick theme. Cl is green, O red, N blue and C grey.

1. Color & style button in the toolbar.
2. Look menu: choose Default or Ball and stick.

What it does

Themes change only how structures are drawn, not the chemistry. You can apply the look to the selection or, with *Apply to all*, to every design. Label and ring-fill colours, opacity and atom/bond overrides in the same panel still work, and exports (PNG/SVG) keep the theme.

Who it is for

Teachers and students making visually clear figures, and anyone who wants a 3D-style image without opening the 3D viewer.

How to use it

- 1 Draw or load a structure.
- 2 Click **Color & style** (callout 1).
- 3 Set **Look** to **Ball and stick** (callout 2).
- 4 Toggle *Apply to all* to restyle all open designs.
- 5 Export with Download , PNG or SVG.

Tips

- For a true rotatable 3D model use the 3D molecular model viewer.
- Explore ready-made 3D pages in the molecule library.
- Switch back to Default for journal-style skeletal structures.

Questions and answers

Is the ball-and-stick theme 3D?

Does it need an account?

Which colours are used?

Source: <https://www.moldraw.com/docs/plugins/themes-plugin-ball-and-stick-2d-style/>