

MolDraw editor documentation

How to use the editor: drawing, rings, stereochemistry, reactions, import and export, 3D, the AI assistant and plugins.

MolDraw (<https://www.moldraw.com>) · Help centre: <https://www.moldraw.com/support/> · Updated 2026-10-17

Introduction to MolDraw

<https://www.moldraw.com/docs/get-started/what-is-moldraw-free-online-chemical-structure-editor/>

MolDraw is a free chemical structure editor that runs in your browser. You can draw molecules and reactions, view them in 3D, and export figures for papers and slides.

What you can do with MolDraw

- Draw molecules, rings and reactions on an open canvas.
- Turn a name, SMILES or CAS number into a structure.
- See the formula, weight and name of what you draw.
- Rotate your molecule in 3D.
- Export PNG, SVG, PDF, MOL, CDXML and more.
- Add plugins for NMR, ChEMBL data and more.

Do you need an account

You do not need an account to draw. Your work saves in your browser. Sign in when you want plugins, Community posts or cloud features.

Where to start

1. Open the [MolDraw editor](#).
2. Follow [Draw your first structure](#).
3. Learn the [keyboard shortcuts](#) to work faster.

Tip: Every page has a short answer at the top. Read that first if you are in a hurry.

Questions and answers

Is MolDraw free? Yes. Drawing, 3D viewing and exports are free. You only need a free account for plugins and Community.

Does MolDraw work offline? The editor runs in your browser. Drawing and saving work without a server. Name lookup, PubChem and AI need the internet.

Which browsers work? Use a recent Chrome, Edge, Firefox or Safari. Phones and tablets work too.

Draw your first structure

<https://www.moldraw.com/docs/get-started/how-to-draw-your-first-chemical-structure-in-moldraw/>

Click the benzene ring, click the canvas, add a bond, then place an oxygen. Click Clean up and open Info to see the name, formula and weight. This guide draws phenol in six steps.

Before you start

Open the [MolDraw editor](#). You do not need to sign in. If the canvas has a drawing, click **Clear canvas** (the red bin) first.

Watch the whole thing

Animation: [The full walkthrough in 19 seconds](#). [Orange rings show each click](#). (Screen recording of drawing phenol in MolDraw: pick benzene, place it, add a bond, change the end to oxygen, clean up, then open Info)

The parts of the screen

The main parts of the screen. 1 Ring bar. 2 Left tool rail. 3 Atom palette. 4 Canvas.

Step by step

1. **Pick the benzene ring.** In the ring bar at the bottom left, click the benzene button. **Animation:** [Click the benzene button](#). (Animation: the pointer clicks the benzene button in the ring bar) *The benzene button in the ring bar.*
2. **Place the ring.** Click once on an empty part of the canvas. A benzene ring appears where you click. **Animation:** [One click places the ring](#). (Animation: one click on the canvas places a benzene ring) *Your ring on the canvas.*
3. **Add a bond.** Click the single bond tool in the left rail. Then click the top atom of the ring. A new bond grows from that atom. **Animation:** [Pick the bond tool, then click the top atom](#). (Animation: pick the single bond tool, then click the top ring atom to add a bond) *The single bond tool. The new bond, marked 2.*
4. **Make it an oxygen.** Click **O** in the atom palette. Then click the free end of the new bond. The end turns into OH. **Animation:** [Pick O, then click the end of the bond](#). (Animation: pick O in the atom palette, then click the end of the new bond) *The O button in the atom palette. The OH group is now on the ring.*
5. **Tidy the drawing.** Click **Clean up** in the tools row. MolDraw fixes bond lengths and angles. **Animation:** [Click Clean up](#). (Animation: clicking Clean up tidies the phenol drawing) *The Clean up button. Phenol after Clean up.*
6. **Check what you drew.** Press **Ctrl+A** to select all. Click **Info** at the top. The panel shows the name, formula and weight. **Animation:** [Select all, then click Info](#). (Animation: select all, click Info, and the molecule details panel opens showing phenol) *1 Info. 2 Molecule details. 3 Copy SMILES. 4 Download. The details panel for phenol.*

Save or share your structure

- Your drawing saves in this browser by itself. Find it later in **My designs**.
- Click **Copy SMILES** to copy the structure as text.
- Click **Download** to save a PNG, SVG, PDF or MOL file. See [Download and file formats](#).

Note: The 3D panel on the right updates as you draw. Drag it to rotate the molecule. See [3D viewer](#).

Faster ways to do the same thing

- Type a name like *phenol* in the search box at the top. MolDraw draws it for you.
- Paste a SMILES such as Oc1ccccc1 with **Paste SMILES**.
- With nothing selected, press **O** to set oxygen as the atom to place.

Warning: Clean up moves atoms. If you placed things by hand on purpose, press **Ctrl+Z** to undo it.

Questions and answers

How do I draw a benzene ring in MolDraw? Click the benzene button in the ring bar at the bottom left. Then click the canvas.

How do I change a carbon to oxygen? Click **O** in the atom palette, then click the atom. You can also select the atom and type **O**.

How do I see the name of my structure? Select the molecule and click **Info** at the top. The panel shows the name, formula and molecular weight.

Do I need to save? No. MolDraw saves your drawing in the browser. Open it again from **My designs**.

The MolDraw screen

<https://www.moldraw.com/docs/get-started/moldraw-editor-interface-toolbar-and-panels-explained/>

The screen has a top bar, a tools row, a left tool rail, an atom palette, a ring bar and the canvas. A 3D panel sits on the right.

1 Ring bar. 2 Left tool rail. 3 Atom palette. 4 Canvas.

Top bar

The top bar has **My designs**, the search box, and the **Home**, **Draw** and **Info** tabs. It also has the language menu, Updates and your account.

Editor row

This row holds **File**, **Select**, **Community**, **Copy SMILES**, **Paste SMILES**, **Copy SVG**, **Paste** and **Download**.

Ribbons

Home, Draw and Style are ribbons. Only one is open at a time.

- **Home** has Clean up, hydrogens, 3D Clean Up, aromatize and zoom.
- **Draw** has the pencil, shapes, images and glassware.
- **Style** sets font, bond width and the structure look.

Left tool rail

The rail holds the tools you use most. You get select, erase, charges, lone pairs, bonds, chains, atom labels, arrows, brackets and orbitals. A small arrow under a button opens more choices.

Atom palette and ring bar

The atom palette next to the canvas has H, C, N, O, S, P, F, Cl, Br and I. The grid button opens the full periodic table. The ring bar at the bottom has rings from three to eight atoms and the Library.

Canvas and 3D panel

The canvas has no edges. Pan with the hand tool or by holding Space and dragging. The 3D panel shows your molecule in 3D. Hide it with the **3D** button.

Questions and answers

How do I hide the 3D panel? Click the 3D button in the tools row. Click it again to bring it back.

Where is the periodic table? Click the grid button in the atom palette, under I.

Save and open your work

<https://www.moldraw.com/docs/get-started/how-to-save-and-open-chemical-drawings-in-moldraw/>

MolDraw saves your drawing in your browser by itself. Open old drawings from My designs. Use File, Save to keep a .moldraw file on your computer.

Autosave

Every change saves in this browser. You do not need to press save. Your drawings stay on this device.

Open My designs

1. Click **My designs** at the top left.
2. Click a card to open that drawing.
3. Use folders to group your work.

Save a file to your computer

1. Click **File**.
2. Click **Save**, or press Ctrl+S.
3. MolDraw downloads a .mol draw file with everything on the canvas.

Open a file

Click **File**, then **Open**. You can open MolDraw, MOL, CDX and CDXML files.

Warning: Drawings live in this browser only. If you clear browser data, they are gone. Save a .mol draw file for anything important.

Questions and answers

Where are my drawings saved? In your browser on this device. Open them from My designs.

Can I open ChemDraw files? Yes. Use File, Open for CDX and CDXML files.

Do I need an account to save? No. Local saving works without an account.

Keyboard shortcuts

<https://www.moldraw.com/docs/get-started/mol draw-keyboard-shortcuts-list/>

Press ? in the editor to see every shortcut. The most used are Ctrl+Z to undo, Ctrl+C to copy, 1, 2 and 3 for bond types, and letters like O or N to pick an element.

On a Mac, use ⌘ where this page says Ctrl. Change any shortcut in **Settings, Shortcuts**.

Editing

Action	Keys
Cancel edit / clear selection / close menus	Esc
Erase selected object	Delete or Backspace
Undo	Ctrl Z
Redo	Ctrl Y or Ctrl Shift Z
Select all	Ctrl A
Copy fragment	Ctrl C
Paste fragment	Ctrl V
Save entire canvas (.mol draw)	Ctrl S

Selection (Select menu)

Action	Keys
Deselect	Ctrl Shift A
Invert selection	Ctrl Shift I
Select connected	Ctrl Shift C
Grow selection	Ctrl Shift G
Same as selection	Ctrl Shift S
Select all rings	Ctrl Shift R
Select heteroatoms	Ctrl Shift H
Chain atoms	Alt Shift C
Longest path	Alt Shift L
Side chains	Alt Shift S
All 5-rings	Alt Shift 5
All 6-rings	Alt Shift 6
Aromatic atoms	Alt Shift A
Charged atoms	Alt Shift Q
Wedge / dash atoms	Alt Shift W
CIP R / S centers	Alt Shift R
Aliases / R-groups	Alt Shift G
Bonds in selection	Alt Shift B
All bonds	Ctrl Alt B
Select tool	V
Lasso select tool	L

Navigation

Action	Keys
Pan canvas (hand tool)	Hand drag
Temporary pan (hold, then drag)	Space drag
Pan	Middle-click drag
Pan vertically	Scroll wheel
Pan horizontally	Shift Scroll
Zoom toward pointer	Ctrl Scroll or % Scroll
Zoom in	Ctrl = or Ctrl +
Zoom out	Ctrl -
Reset zoom (100%)	Ctrl 1

Action	Keys
Fit all objects	Ctrl 0
Pinch zoom	Two-finger pinch
Two-finger pan	Two-finger drag
Touch pan on empty canvas	Touch drag

Tools

Action	Keys
Single bond	1
Double bond	2
Triple bond	3
Benzene ring	B
Select tool	V
Lasso select tool	L
Open this shortcuts panel	? or Shift /

Atom labels (placement element when no atom selected)

Action	Keys
Carbon	C
Nitrogen	N
Oxygen	O
Sulfur	S
Phosphorus	P
Fluorine	F
Hydrogen	H
Chlorine	Shift C
Bromine	Shift B
Iodine	I

Type-to-rename (one atom selected)

Action	Keys
Open inline label editor seeded with letter	A to Z
Multi-char symbols (Cl, Si, Br): keep typing	C + l
Abbreviations (Me, Et, Ph, Boc, OMe, NH ₂ , ...)	type group
Accept suggestion	Tab or Enter
Commit current text	Enter

Action	Keys
Cancel	Esc
Quick rename (select tool)	Double-click atom

3D Structure Perspective

Action	Keys
3D Clean Up (canvas pose: then drag to rotate)	Ctrl Shift D or ⌘ Shift D
Perspective tool / toggle depth shading	Alt D

Modifiers & canvas

Action	Keys
Select entire connected molecule (atom or bond)	Ctrl click or ⌘ click
Add / toggle atom or bond in selection	Shift click
Esc priority: alias editor → deselect text → deselect arrow → clear atoms → close menu → select tool	Esc
Select tool on empty canvas: drag rectangle (marquee); Shift+drag for lasso	Shift drag
Rebind shortcuts in Settings → Shortcuts	Settings
Undo / redo / copy / paste use Ctrl on Windows/Linux or ⌘ on macOS	Ctrl

Tip: Shortcuts do not fire while you type in a text box or label.

Questions and answers

How do I see all shortcuts in the app? Press ? in the editor.

Can I change shortcuts? Yes. Open Settings, then Shortcuts.

Draw atoms

<https://www.moldraw.com/docs/drawing/how-to-draw-atoms-and-change-elements/>

Pick an element in the atom palette, then click the canvas or the end of a bond.
Click an atom to change it. Use the periodic table for other elements.

1. Click an element in the atom palette, for example **N**.
2. Click an empty spot to place it. Or click an atom to change it.
3. For other elements, click the grid button and pick from the periodic table.

Keyboard tricks

- With nothing selected, press a letter like N or O to set the element.
- With one atom selected, type a symbol to rename it. Type Cl or Br for two letters.
- Type groups like Me, Ph or OMe too.

Change an atom

Right click an atom. You can set the element, isotope, charge, explicit H, lone pairs and radicals.

Tip: The **A** button places an "any atom". It is the same as * in SMILES.

Questions and answers

How do I add a chlorine atom? Click Cl in the atom palette and click the atom. Or select the atom and type Cl.

How do I add an isotope like deuterium? Right click the atom and pick Isotope.

Draw bonds

<https://www.moldraw.com/docs/drawing/how-to-draw-single-double-triple-and-wedge-bonds/>

Pick a bond type in the left rail and drag from atom to atom. Click a bond to change its type. Press 1, 2 or 3 for single, double or triple bonds.

1. Click the bond button in the left rail. Open the small arrow for more types.
2. Drag from an atom to draw a bond. Or click an atom to grow a bond from it.
3. Click an existing bond to switch it to the chosen type.

Bond types

Single, double, triple, aromatic, wedge, hash, wavy, bold, dative, hydrogen bond (dotted), cis/trans, any and centroid bonds are all in the bond menu.

Shortcuts

- 1 single, 2 double, 3 triple.
- B benzene ring.

Tip: The **Chain** tool draws a zigzag chain in one drag. Watch the count as you drag.

Questions and answers

How do I draw a double bond? Pick the double bond in the bond menu, or press 2, then click the bond.

How do I draw a wedge bond? Open the bond menu and pick Wedge up or Hash down. Drag from the stereo center outward.

Rings and structures

<https://www.moldraw.com/docs/drawing/how-to-draw-benzene-cyclohexane-and-fused-rings/>

Use the ring bar at the bottom to place rings from 3 to 8 atoms. Click a ring atom or bond to fuse a new ring. Clean up tidies the shape.

1. Click a ring in the ring bar, such as benzene or cyclohexane.
2. Click empty canvas to place it.
3. Click an atom or bond of a ring to fuse or attach another ring.
4. Click **Clean up** to even out bonds and angles.

Special rings

- The small arrow under cyclohexane gives chair and boat shapes.
- The arrow under benzene gives a tilted arene for metal complexes.
- Cyclopentadiene has a Cp option.

Select and move

Drag a box with the select tool. Hold Shift and drag for a lasso. Use the handles to rotate or resize.

Questions and answers

How do I draw naphthalene? Place a benzene ring. Then click one of its bonds with the benzene tool to fuse a second ring.

How do I draw a chair cyclohexane? Open the small arrow under the cyclohexane button and pick Chair.

Atom labels and R-groups

<https://www.moldraw.com/docs/drawing/how-to-add-atom-labels-and-r-groups/>

Pick the atom label tool (A) and click an atom. Type a label like Ph, COOH or R1. MolDraw can expand known labels into full structures.

1. Click the **Atom label** tool in the left rail.
2. Click an atom.
3. Type a label, such as Ph, COOH, Boc or R1.
4. Press Enter.

Expand or collapse a label

Right click a label. Pick **Expand** to show every atom. Pick **Collapse** to go back to the short label.

Tip: Labels MolDraw does not know stay as text. They still show on your figure.

Questions and answers

How do I add an R group? Use the atom label tool, click an atom and type R, R1 or R2.

Stereochemistry

<https://www.moldraw.com/docs/drawing/how-to-draw-stereochemistry-wedge-hash-and-r-s-labels/>

Use wedge and hash bonds for 3D centers. Open Chemistry and pick Show CIP labels to see R and S. Right click to invert a center.

1. Pick **Wedge up** or **Hash down** in the bond menu.
2. Drag from the stereo center to the outer atom.
3. Open **Chemistry** and click **Show CIP labels** to see R, S, E and Z.

More stereo tools

Right click a suitable atom, bond or ring. You can invert a center or make Newman, Fischer, chair and boat views.

Warning: Wedges point away from the stereo center. Draw from the center outward.

Questions and answers

How do I show R and S labels? Open the Chemistry menu and click Show CIP labels.

How do I flip a stereocenter? Right click the atom and pick Invert.

Lone pairs, radicals and charges

<https://www.moldraw.com/docs/drawing/how-to-add-lone-pairs-radicals-and-formal-charges/>

Pick the lone pair tool and click an atom to add a pair of dots. Use the radical tool for one dot. Charge tools add plus and minus marks you can drag around the atom.

1. Click the **Lone pair** tool in the left rail.
2. Click an atom. A pair of dots appears.
3. Drag the dots around the atom to a free side.
4. For a radical, open the small arrow and pick the radical tool.

Charges

Use + and – in the rail. Click again for +2 or –2. The rail also has circled charges and $\delta+$ and $\delta-$.

When to show lone pairs

Show lone pairs when you draw mechanisms. A curved arrow should start at a lone pair or a bond. Oxygen in water has two pairs. Nitrogen in ammonia has one.

Tip: Check that charges match electrons. Oxygen with three bonds and one lone pair is +1.

Questions and answers

How do I add a lone pair in MolDraw? Pick the Lone pair tool in the left rail and click the atom. Drag the dots to move them.

How do I add a radical? Open the small arrow under the lone pair tool, pick the radical, and click the atom.

Polymer brackets

<https://www.moldraw.com/docs/drawing/how-to-draw-polymer-repeat-unit-brackets/>

Select the repeat unit, then click the Brackets tool. Click the small n to change the number of units.

1. Select two or more atoms of the repeat unit.
2. Click **Brackets** in the left rail.
3. Click the subscript to type n, m or a number.

Click Brackets again for more types. You get polymer n, copolymer m and parenthesis (CH₂)_n. Brackets move with the structure.

Questions and answers

How do I draw a polymer repeat unit? Select the unit and click Brackets. Then edit the subscript.

Text, shapes and images

<https://www.moldraw.com/docs/drawing/how-to-add-text-shapes-images-and-lab-glassware/>

Open the Draw ribbon to add text, shapes, images and glassware. Click the canvas to place them and drag to move.

Add text

1. Click the **Text** button (T) in the tools row.
2. Click empty canvas and type.
3. Press Esc when you are done.

Shapes, images and glassware

- **Shapes** gives arrows, boxes and outlines.
- **Image** adds PNG, JPEG, WebP, GIF or SVG files.
- **Glassware** adds lab apparatus as clean line drawings. Choose **Premium** in the apparatus library or in **Color and style** for soft 3D shading.
- Drag the small grip on the liquid surface to set the level. Turn a vessel with its rotate handle and the liquid stays level. Tip it past the lip and it pours into any vessel below.

Questions and answers

Can I add lab glassware to my figure? Yes. Open the Draw ribbon and click Glassware.

Style and display

<https://www.moldraw.com/docs/drawing/how-to-change-structure-style-colors-and-display/>

Open Color and style to change colors, font, bond width and the structure look. Settings control hydrogens, labels, grid and snap.

1. Select what you want to change, or nothing for the whole drawing.
2. Click **Color and style** in the tools row.
3. Pick colors, label style or the **Look**, such as Ball and stick.

Settings

Click **Settings** (gear). You can change implicit hydrogens, colored atom labels, grid and snap. You can also save style presets.

Tip: For ACS style in a paper, pick a style preset in Settings, then export SVG.

Questions and answers

How do I color an atom? Select it, open Color and style, and pick a color.

Reaction arrows

<https://www.moldraw.com/docs/reactions/how-to-draw-reaction-arrows-with-reagents/>

Pick the Reaction arrow tool and drag between molecules. Choose the arrow kind in the top bar. Type reagents above or below the arrow.

1. Click **Reaction arrow** in the left rail.
2. Drag from the starting material to the product.
3. In the top bar, pick the kind: straight, equilibrium, retrosynthetic and more.
4. Click above or below the arrow to type reagents and conditions.

Tip: Open **Chemistry** and click **Automap** to match atoms across the arrow.

Questions and answers

How do I add reagents to an arrow? Click the slot above or below the arrow and type.

How do I draw an equilibrium arrow? Draw an arrow, then pick Equilibrium in the top bar.

Build a reaction scheme

<https://www.moldraw.com/docs/reactions/how-to-make-a-chemical-reaction-scheme/>

Draw the reactants and products, add an arrow, then add reagents. Export as RXN, SVG or PNG. Start from a named reaction in the Library to save time.

1. Draw the starting material.
2. Draw the product to the right.
3. Add a reaction arrow between them.
4. Type reagents on the arrow.
5. Download the scheme as SVG, PNG or RXN.

Start from a template

Open **Library** and pick a named reaction. Edit it to match your work.

Note: You can paste a reaction SMILES like CCO>>CC=O. MolDraw draws both sides and the arrow.

Questions and answers

Can I paste a reaction SMILES? Yes. Use Paste SMILES with A>>B format.

Library and templates

<https://www.moldraw.com/docs/library/how-to-use-the-structure-library-and-templates/>

Open Library in the ring bar to place ready-made structures. It has functional groups, ligands, amino acids, polymers, COFs, MOFs and named reactions.

1. Click **Library** at the end of the ring bar.
2. Search or pick a category.
3. Click an item, then click the canvas to place it.

Library is not the same as **My designs**. My designs holds your own saved drawings.

Questions and answers

Where are amino acid templates? Open Library and pick Amino acids.

Copy and paste SMILES

<https://www.moldraw.com/docs/import-export/how-to-copy-and-paste-smiles-inchi-and-mol/>

Click Copy SMILES to copy your structure as text. Click Paste SMILES to draw from a SMILES string. Right click for more formats like InChI and MOL.

1. Select a molecule, or nothing for the whole canvas.

2. Click **Copy SMILES** in the editor row.
3. To draw from text, click **Paste SMILES** and paste the string.

More copy formats

Right click and open **Copy as**. You get SMILES, InChI, InChIKey, MOL V2000, MOL V3000, CDXML, SVG, PNG, SLN, HELM, FASTA and BILN.

Tip: Ctrl+C copies an SVG picture. Paste it straight into Word or PowerPoint.

To learn SMILES, read the [SMILES notation guide](#).

Questions and answers

How do I get the SMILES of my drawing? Click Copy SMILES in the editor row.

Can I paste a MOL file? Yes. Copy the MOL text and click Paste.

Download and file formats

<https://www.moldraw.com/docs/import-export/how-to-export-png-svg-pdf-mol-and-cdxml-files/>

Click Download and pick a format. Use SVG or PDF for papers, PNG for slides, and MOL, SDF or CDXML to move to other chemistry software.

1. Click **Download** in the editor row.
2. Pick a format.
3. For PNG and JPEG, set size and background in the dialog.

Which format to pick

Format	Use it for
SVG	Papers and posters. Sharp at any size.
PDF	Journals and printing.
PNG / PNG (white)	Slides, Word and the web.
JPEG	Small photos.
SMILES (.smi)	Text, databases, code.
MOL / SDF	Other chemistry software. SDF keeps 3D coordinates.
CDXML / CDX	ChemDraw.
RXN	Reactions.
InChI	Database lookup.
SMARTS	Substructure search.
CML, XYZ	Other tools and 3D programs.
GLB, OBJ, X3D	3D models from the 3D panel.

Save the whole canvas

Click **File**, then **Save**. You get a .molDraw file with structures, arrows, text and images.

Questions and answers

What format should I use for a journal figure? Use SVG or PDF. They stay sharp at any size.

Can I export to ChemDraw? Yes. Download CDXML or CDX.

Search PubChem

<https://www.moldraw.com/docs/import-export/how-to-search-pubchem-by-name-or-cas-number/>

Type a name or CAS number in the search box at the top. MolDraw draws the structure from PubChem.

1. Click the search box at the top left.
2. Type a name like *caffeine* or a CAS number.
3. Pick a result. MolDraw places the structure on the canvas.

The PubChem panel also does advanced search and batch SMILES import. Batch import lays molecules out on a grid.

Questions and answers

Can I search by CAS number? Yes. Type the CAS number in the search box.

Names, formula and properties

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

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 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? Select the molecule and click Info. The IUPAC name is in the panel.

3D viewer

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

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? Drag inside the 3D panel.

AI assistant

<https://www.moldraw.com/docs/ai/how-to-use-the-ai-chemistry-assistant/>

Click AI in the tools row to open the chat. Add your Gemini API key once. Ask it to draw, name or edit structures.

1. Click **AI** in the tools row.
2. Paste your Gemini API key in the panel or in **Settings, AI**.
3. Type a request, such as "Draw aspirin".
4. The assistant can place structures on the canvas.

Note: Your key stays in your browser. Google's free tier is enough to try it.

For spectra, see [AI Spectroscopy](#).

Questions and answers

Do I need to pay for the AI assistant? No. You use your own Gemini key. Google has a free tier.

Plugins overview

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

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, ¹³C, 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.
- **Symmetry and Point Groups**: Find the point group of any molecule, see every axis and mirror plane, and play each symmetry operation in 3D.
- **pKa and Microspecies**: Estimate pKa values, the main charged form and the share of each microspecies at any pH, right in your browser.

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

Questions and answers

Are plugins free? Yes. All plugins are free. Most need a free account.

Where do plugin panels open? Most open as tabs next to Structure in the right panel.

NMR Analyser plugin

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

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 ^{13}C 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 **^{13}C** 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

- Pick your magnet size under Spectrometer (60 to 1200 MHz). On a small magnet the multiplets look wider, because the splitting is J in Hz divided by MHz.
- 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 CDCl_3 -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? Typical ^1H predictions fall within about 0.2 to 0.3 ppm and ^{13}C within a few ppm for common organic molecules. Exchangeable OH/NH protons and unusual ring systems can deviate more, so treat predictions as a guide, not a measured spectrum.

Does the NMR Analyser need an account? Yes. Plugins are installed to your free MolDraw account. For a no-login quick check, use the free structure to NMR tool.

Can it predict 2D NMR? Yes: COSY, HSQC and HMBC are drawn as contour plots alongside the 1D ¹H and ¹³C spectra.

Can I export the spectrum? Yes. Download the plot as PNG or SVG and the peak table as CSV.

ChEMBL plugin

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

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

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 K_i.
- **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? A free, manually curated database of bioactive drug-like molecules maintained by EMBL-EBI, with over two million compounds and their measured activities against biological targets.

Is the ChEMBL plugin free? Yes. It uses ChEMBL's public web services and needs only a free MolDraw account to install.

Can I search by structure? Yes. Use canvas looks up the drawn molecule by InChIKey; the Similar tab finds related structures.

Electrostatic Potential (MEP) plugin

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

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

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 positive or negative the electric potential is at the surface of a molecule. Red regions attract positive charges (lone pairs, electronegative atoms); blue regions are electron-poor.

How is the MEP calculated in MolDraw? From Gasteiger partial atomic charges mapped onto a solvent-accessible surface. It is an approximation, not a quantum-chemical ESP.

Is it free? Yes, with a free MolDraw account.

Compare Molecules plugin

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

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

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? The number of fingerprint bits two molecules share divided by the number set in either. 1 means identical fingerprints; above about 0.7 is usually considered similar.

How many molecules can I compare? You can add many rows at once by pasting a list of SMILES; the first molecule added is the reference.

Does it detect stereoisomers? Yes, stereocentre differences are reported separately because fingerprints ignore stereochemistry.

Protein Viewer plugin

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

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? No. The Protein Viewer is installed by default and works without signing in.

Which file formats can I open? PDB IDs are fetched directly; local PDB and mmCIF files can be opened from your computer.

Can I show a ligand as sticks? Yes. Select the residue or ligand in the sequence strip and change its style.

Smart Draw plugin

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

Install Smart Draw, pick the Smart Draw pencil in the left toolbar, sketch, then press Convert or Enter when the drawing is finished.

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. Check the preview and the read-out in the Smart Draw bar. Use **Undo stroke** (Ctrl+Z) or **Clear** (Esc) to fix mistakes.
6. Press **Convert** or **Enter** to turn the strokes into a structure. Turn on **Auto** in the bar if you prefer converting after a 2.5 s pause.
7. Write a letter at a bond end to place a heteroatom, or switch to the normal tools to refine.
8. 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? Yes. Stroke recognition runs locally in the browser; no data is sent to a server.

Can I draw on a phone or tablet? Yes, with a finger or stylus. A stylus gives the cleanest strokes.

What can it recognise? Single bonds, chains, rings (3 to 8 members), connections to existing atoms and simple atom labels.

AI Spectroscopy plugin

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

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? The plugin is free; requests use your own Gemini API key, which has a free tier from Google.

Are AI-predicted spectra accurate? They are plausible estimates for teaching. Always confirm with experimental data or rule-based predictors.

Which spectra can it predict? $^1\text{H}/^{13}\text{C}$ NMR, mass spectra (EI) and UV-Vis absorption.

Themes (Ball-and-Stick) plugin

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

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? No, it is a 2D drawing style with shaded spheres. Use the 3D viewer for rotatable models.

Does it need an account? No. Themes is installed by default.

Which colours are used? Standard CPK colours: C grey, H white, O red, N blue, S yellow, Cl green, Br dark red.

Symmetry and Point Groups plugin

<https://www.moldraw.com/docs/plugins/symmetry-plugin-point-group-finder-3d-symmetry-operations/>

Install Symmetry from Settings, Plugins, open the Symmetry tab in the 3D panel, then press Use my drawing or pick an example.

PCl5 is D3h. The C3 axis is vertical, three C2 axes lie in the equatorial plane, and the list on the right names every element.

1. Point group badge with the group order.
2. 3D viewer with axes, planes and the inversion centre.
3. Source: use your drawing or a built-in example.
4. Tabs: elements, operations, character table and projection.
5. Layer chips to show or hide each kind of element.

What it does

The plugin centres the molecule at its centre of mass, classifies its moments of inertia, and tests candidate rotations, reflections, inversion and improper rotations by checking that every atom lands on an atom of the same element within a tolerance. The group is then rebuilt from ideal operations and the coordinates are symmetrised. Character tables follow Cotton and Harris and Bertolucci, with Mulliken axis conventions.

Who it is for

Students learning group theory and spectroscopy, teachers who want to show operations live, and chemists checking the symmetry of a structure.

How to use it

1. Open the [MolDraw editor](#) and sign in. Click **Settings**, then **Plugins**, then **Install** next to Symmetry and Point Groups.
2. Draw a molecule, or pick an example such as water, benzene or C60.
3. Open the **Symmetry** tab (callout 4) and press **Use my drawing** (callout 3).
4. Read the point group in the badge (callout 1).
5. Hover an element in the list to highlight it in 3D (callout 2).
6. Click an element or an operation to play it. Atoms move and land on equivalent atoms.
7. Open **Character table** for irreducible representations and their functions.

Tips

- Use Tight tolerance for accurate structures and Loose for rough drawings.
- For C2v the B1 and B2 labels depend on which plane is called xz. The plugin puts the molecular plane in yz and says so.
- Turn on Numbers to follow each atom through an operation.

Questions and answers

How does MolDraw find the point group? It tests every candidate symmetry operation by mapping atoms onto atoms of the same element within a distance tolerance, following the standard Schoenflies flowchart, including linear, cubic and icosahedral groups.

Which point groups are supported? All molecular point groups are detected, from C1 to Ih and the linear groups. Character tables are stored for 43 common groups.

Is it free? Yes, with a free MolDraw account.

pKa and Microspecies plugin

<https://www.moldraw.com/docs/plugins/pka-plugin-microspecies-protonation-states-at-any-ph/>

Install pKa and Microspecies from the + menu next to the Structure tab, draw a molecule, then set the pH.

Cetirizine at pH 7.4. The chart shows each charged form from pH 0 to 14 and the Sites table lets you type in a measured pKa.

1. Chart of every microspecies from pH 0 to 14.
2. pH controls with a slider and presets.
3. Summary: major species, net charge, isoelectric point and pKa values.
4. Sites table with the estimate and a box for your own value.

What it does

MolDraw finds each acidic or basic group, starts from a measured value for that type of group, and adjusts it for nearby groups using the Hammett and Taft equations. Groups that

sit close together affect each other. Every protonation state is then weighted at your pH to give the percentages. No server and no AI model are used.

All values are estimates. On about 2,000 test molecules the tool never saw during tuning, the average error is 0.92 pKa units and 71% of values are within 1 unit. For common drugs the average error is about 0.45. Acids, amines and phenols do well. Some ring systems, tautomers, amidines, enols and C-H acids can be off by 2 units or more.

The test data comes from the SAMPL6, SAMPL7 and SAMPL8 challenges (MIT licence), the AvLiLuMoVe, DataWarrior and Novartis sets shared by Baltruschat and Czodrowski (CC BY 4.0), and literature drug values.

Who it is for

Students learning acids and bases, medicinal chemists checking charge at blood pH, and anyone who needs protonation states for docking or a figure.

How to use it

1. Open the [MolDraw editor](#) and sign in. Click **Settings**, then **Plugins**, then **Install** next to pKa and Microspecies.
2. Draw a molecule, or select one if the canvas has several.
3. Click **+** next to the Structure tab and install pKa and Microspecies. You can also right-click a molecule and choose **pKa and microspecies**.
4. Set the pH with the slider or a preset (callout 2).
5. Read the major species and the percentages (callouts 1 and 3).
6. To use a measured value, open **Sites** and type it in (callout 4).
7. Press **Insert major species** or **Replace drawing** to put the charged form on the canvas.

Tips

- Leave a Your pKa box empty to keep the estimate.
- Click the chart to jump to that pH.
- Switch to Major at pH to see the charged structure.

Questions and answers

How accurate is it? It is an estimate. The average error on held-out test molecules is about 0.9 pKa units, and about 0.5 for common drugs.

Does it send my molecule anywhere? No. Everything runs in your browser.

Is it free? Yes, with a free MolDraw account.