

MolDraw how-to articles (part 1)

Guides and articles from the MolDraw blog.

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

Predict NMR, Mass and UV-Vis Spectra with AI: Spectroscopy Plugin

<https://www.moldraw.com/blog/ai-spectroscopy-plugin-nmr-ms-uv-prediction.html>

Draw a molecule and ask AI for a quick estimate of its ^1H or ^{13}C NMR, EI mass or UV-Vis spectrum. A practical guide to the free MolDraw Spectroscopy plugin, with honest limits.

Published: 15 Oct 2026 · Author: Scidart Academy · Reading time: ~6 min

Short answer: Install **Spectroscopy** from Settings > Plugins and add a Gemini API key in Settings > AI. Draw a molecule, then choose **Predict NMR**, **Predict MASS spectra** or **Predict UV** from the Chemistry menu, or ask the AI chat. You get a chart, a peak table and notes. Treat the numbers as AI estimates and check them against real spectra.

Why predict a spectrum before you measure one?

Spectroscopy problems start with a structure and a question: what should its spectrum look like? A rough prediction tells you where to look and what to expect. It also helps you explain why a signal appears where it does.

Each technique answers a different question:

- **NMR** shows the chemical environments of nuclei. In a ^1H spectrum, the chemical shift (in ppm) reflects the electronic surroundings of each hydrogen, the integral reflects how many hydrogens give the signal, and the splitting reflects neighbouring hydrogens. A ^{13}C spectrum shows the distinct carbon environments.
- **EI mass spectrometry** hits the molecule with energetic electrons. This removes an electron and forms a radical cation, the molecular ion. Its m/z gives the molecular mass, and the fragment peaks show which bonds break. The tallest peak is the base peak, set to 100.
- **UV-Vis** measures light absorbed by chromophores such as conjugated π systems and carbonyl groups. More conjugation usually moves the absorption maximum (λ_{max}) to longer wavelength.

The Spectroscopy plugin sends your structure to an AI language model and shows its answer. The values are estimates, not measured data. They are good for learning and discussion. They are not a reference.

What the plugin gives you

Ask the AI chat for a spectrum of the structure on the canvas. Callout 1 is the AI chat button, callout 2 the prompt box.

Spectra	^1H and ^{13}C NMR, EI mass spectrum and UV-Vis absorption.
Result window	A title, the formula and molecular weight, a stick chart of the peaks, a peak table, notes and a disclaimer.
Export	Download PNG saves the chart. Download CSV saves the table.
Needs	A free MolDraw account to install it, your own Gemini API key and an internet connection.

How to install the Spectroscopy plugin

1. Open the [MolDraw editor](#) and sign in. A free account is enough.
2. Click **Settings** (the gear), then **Plugins**.
3. Click **Install** next to Spectroscopy.
4. Open **Settings** > **AI** and paste a Gemini API key. MolDraw stores the key only in your browser.

Without a key, the plugin shows the message "Spectroscopy requires AI. Add a Gemini API key in Settings → AI."

How to predict a spectrum

From the Chemistry menu

1. Draw the molecule, or paste a SMILES.
2. Open the **Chemistry** menu in the toolbar and choose **Spectroscopy**.
3. Pick **Predict NMR** (^1H), **Predict MASS spectra** (EI) or **Predict UV**.
4. The result window opens with the chart, table and notes.
5. Use **Download PNG** or **Download CSV** to keep the result.

From the AI chat

1. Click the **AI** button to open the AI chat.
2. Type a request, for example "Predict the ^{13}C NMR spectrum of the molecule on the canvas".
3. Ask follow-up questions, such as "Why is the base peak at m/z 43?"

To focus on one part of a larger structure, select those atoms first. MolDraw still sends the whole structure, but asks the model to treat the selection as the fragment of interest.

Ways to use it in class and in the lab

- **Practice problems:** predict a spectrum, export the chart as PNG and ask students to assign each peak. Then show a real spectrum and discuss where the estimate was off.
- **Pre-lab preparation:** before you record a spectrum, get a rough idea of where the main signals should fall.
- **After the measurement:** open your real data next to the prediction. [Reference and integrate an NMR spectrum](#) in the browser. [Check a mass spectrum against its formula and isotope pattern](#). Find λ_{max} and ϵ in a UV-Vis spectrum.
- **Before and after a reaction:** predict spectra for the starting material and the expected product. Note which signals should appear or disappear, then look for them in your data.
- **Explaining fragments:** use the chat to ask why a fragment forms. Check the molecular ion with the [exact mass calculator](#).

Tips and honest limits

- Treat every value as an estimate. Compare it with experimental spectra in SDBS or NIST, or with a second prediction from the [NMR Analyser plugin](#).
- The formula and molecular weight in the result window also come from the model. Compare them with the Formula and MW values in MolDraw's status bar.
- The chart draws simple sticks with the x axis increasing from left to right. Printed NMR spectra usually run from high to low ppm. Read exact positions from the table.
- A language model can give slightly different numbers if you run the same request again.
- The model sees only the SMILES and molfile of your drawing. Check stereochemistry, charges and hydrogens before you ask.

Learn to read the plots first: see [how to read an NMR spectrum](#) and [how to read a mass spectrum](#).

Questions and answers

Does the Spectroscopy plugin cost money?

No. The plugin is free. Predictions use your own Gemini API key, which has a free tier from Google, and you need a free MolDraw account to install plugins.

Are the predicted spectra accurate enough for a lab report?

No. They are plausible estimates from a language model, useful for learning and explaining. Confirm every value with experimental spectra, for example from SDBS or NIST, before you rely on it.

Which spectra can it predict?

^1H and ^{13}C NMR, electron ionisation (EI) mass spectra and UV-Vis absorption bands.

How is it different from the NMR Analyser plugin?

NMR Analyser is a dedicated NMR tool with ^1H , ^{13}C and 2D experiments, and it does not need a Gemini key. Spectroscopy asks an AI model for NMR, mass and UV-Vis estimates. Running both gives you two independent views of the same structure.

Look Up Drug Targets and Bioactivity from Your Drawing: ChEMBL Plugin

<https://www.moldraw.com/blog/chembl-plugin-bioactivity-lookup.html>

Draw a molecule and see its ChEMBL record: approval phase, protein targets, IC50 and Ki values, and similar compounds. A practical guide to the free MolDraw ChEMBL plugin.

Published: 15 Oct 2026 · Author: Scidart Academy · Reading time: ~5 min

Short answer: Install **ChEMBL** from Settings > Plugins, draw a molecule (or type a name or ChEMBL ID), and press **Lookup**. You get the compound's ChEMBL record with its approval phase, the protein targets it was tested on, activity values such as IC50 and Ki, and similar compounds you can load back onto the canvas.

Why look up bioactivity while you draw?

A structure on its own tells you what a molecule is. Bioactivity data tells you what it does. If you are studying a drug, planning an analogue or teaching structure-activity relationships, the next question after drawing is usually "has this been tested, and against what?"

[ChEMBL](#) answers that question. It is a free, manually curated database of drug-like molecules run by EMBL-EBI, with millions of measured activity data points. The MolDraw plugin brings it next to your canvas, so you do not have to copy SMILES between browser tabs.

What the plugin shows

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

Overview	Preferred name, ChEMBL ID, molecule type, maximum development phase (for example Approved) and InChIKey.
Targets	The proteins and other targets the compound was tested against, each linked to its ChEMBL target page.
Activity	Measured values such as IC50 and Ki, with the target, assay and source.
Similar	Look-alike compounds from ChEMBL. Load any of them onto the canvas.

How to install the ChEMBL plugin

1. Open the [MolDraw editor](#) and sign in. A free account is enough.
2. Click **Settings** (the gear), then **Plugins**.
3. Click **Install** next to ChEMBL. A **ChEMBL** tab appears in the analysis panel.

How to look up a molecule

1. Draw the molecule, or leave the canvas empty if you will search by name.
2. Open the **ChEMBL** tab.
3. Press **Use canvas** to search for your drawing, or type a name (aspirin) or ChEMBL ID (ChEMBL25) in the query box.
4. Press **Lookup**.
5. Browse **Overview**, **Targets**, **Activity** and **Similar**.
6. Keep working with a hit: **Load to canvas** replaces the drawing, **Append** adds it beside your structure, and **Send to Compare** opens it in the [Compare molecules plugin](#).

Ways to use it in class and in the lab

- **Teaching drug discovery:** draw a well-known drug, show its approved status and real targets, then open Similar to discuss how small changes to a scaffold affect activity.
- **Checking an idea:** before you spend time on an analogue, see whether it or a close relative has already been tested.
- **Finding starting points:** use Similar on a hit, append a few neighbours to the canvas and compare them side by side.
- **Screening with rules of thumb:** pair the results with the [Lipinski rule of five calculator](#) and the [drug-likeness calculator](#).

Tips for reliable results

- Search by drawing uses the InChIKey, which is exact. If nothing is found, check stereocentres, charges and salt forms, or search by name.
- Activity values come from many different assays. Compare them only within the same assay and conditions; follow the assay link for details.
- The plugin reads ChEMBL live, so it needs an internet connection.

New to chemical databases? Our [free chemical databases guide](#) explains when to use ChEMBL, PubChem, ChEBI and others.

Questions and answers

What is ChEMBL?

ChEMBL is a free, manually curated database of bioactive drug-like molecules run by EMBL-EBI. It holds over two million compounds and their measured activities against biological targets.

Is the MolDraw ChEMBL plugin free?

Yes. It uses ChEMBL's public web services. You only need a free MolDraw account to install it.

Can I search ChEMBL by drawing a structure?

Yes. Use canvas looks up the drawn molecule by its InChIKey, and the Similar tab finds related structures.

Why is my drawn molecule not found?

InChIKey matching is exact, so a missing stereocentre or a different charge or salt form gives a different key. Check stereochemistry and charges, or search by name or ChEMBL ID instead.

ChemDraw vs MolDraw: Free ChemDraw Alternative (2026)

<https://www.moldraw.com/blog/chemdraw-vs-moldraw-free-alternative-guide.html>

ChemDraw vs MolDraw compared: features, file formats, price and when a free ChemDraw alternative is enough. Try MolDraw online, no install needed.

Published: 2 Mar 2026 • Updated: 12 Jun 2026 • Author: Scidart Academy • Reading time: ~8 min

You want to draw molecules in your browser, and you may not have a ChemDraw licence. This guide compares ChemDraw and MolDraw on what matters day to day: browser access, drawing, [reaction](#) drawing, exports, and how fast you can learn each one.

Short answer: MolDraw is a free browser-based chemical structure drawing app that works well for common online molecule drawing, SMILES copy/paste, 3D viewing, SVG/PNG export, and student or research communication workflows. ChemDraw remains a commercial desktop ecosystem for institutions that require its specific templates and legacy pipelines.

Want to try it now? [Draw chemical structures online](#) in MolDraw. It opens instantly in your browser as an [online ChemDraw alternative](#), with no install or account needed.

Quick Overview

ChemDraw is a long-established commercial chemistry drawing ecosystem. **MolDraw** is a browser-first, free workflow that focuses on fast structure drawing, [SMILES](#) handling, 3D visualization, and practical exports.

Decision shortcut: if your priority is a no-cost, quick-start web workflow with modern integrations, MolDraw is a strong option. If your institution already has established ChemDraw-specific pipelines, ChemDraw may remain your default.

Drawing Chemistry Online Without ChemDraw

You may need to draw a molecule now, on a computer where you cannot install desktop software. MolDraw is not ChemDraw, but it handles the same everyday tasks: open a browser, draw chemical structures, sketch reactions, copy identifiers, and export clean figures or structure files.

- **Use MolDraw for quick browser drawing:** draw structures online, paste SMILES, search known compounds, and export images.
- **Use the reaction drawer workflow:** open the [chemical reaction drawer](#) for reactants, products, arrows, reagents, and conditions.
- **Use the tools hub:** convert structures, calculate properties, search by name or formula, and support chemistry homework or lab workflows.
- **Write in LaTeX?** Paste chemfig code to edit it on the canvas, and download chemfig back for your document, as shown in the [chemfig and MolDraw guide](#).
- **Draw the lab setup too:** add flasks, condensers and heaters from the [lab apparatus library](#), and the joints and water tubing connect on the same canvas as your scheme.

MolDraw vs ChemDraw vs ChemSketch vs Marvin

In short: MolDraw is free and runs in any modern web browser. ChemDraw is paid software. ChemSketch, including its old freeware version, is no longer offered to new users since ACD/Labs joined Revvity Signals in January 2026. Marvin is now sold mainly as Marvin Cloud, a paid subscription.

Building chemistry drawing into your own software? Ketcher is an open-source editor made for that. Our [Ketcher guide covers what it does and the file formats it uses](#).

Feature	MolDraw	ChemDraw	ChemSketch	Marvin
Made by	MolDraw (Scidart Academy)	Revvity Signals	ACD/Labs	Chemaxon (Certara)
Price	Free	Paid licence (price varies)	Not sold to new users since 2026; existing licences keep working	Paid subscription (Marvin Cloud); free individual academic licences ended in 2026
Where it runs	Web browser, no install	Desktop app (Windows, macOS); web options vary	Desktop app (Windows)	Browser (Marvin Cloud) and desktop (MarvinSketch)
2D structure drawing	Yes	Yes	Yes	Yes
Reaction drawing	Yes	Yes	Yes	Yes
SMILES copy and paste	Yes	Yes	Yes	Yes
PubChem name or CAS search	Yes, built in	Varies	Varies	Varies
3D molecule view	Yes, in the browser	Varies by edition	Varies	Varies
CDXML export	Yes	Yes (native format)	Varies	Varies

Based on each maker's public product pages, checked October 2026. Prices and features change, so check the vendor's site before you buy. "Varies" means it depends on the edition, licence or add-on. ChemDraw, ChemSketch and Marvin are trademarks of their owners.

ChemDraw vs MolDraw Comparison Table

Criteria	ChemDraw	MolDraw
Pricing model	Commercial licensing (varies by edition/institution)	Free browser-based usage
Setup speed	Installed desktop workflow	Open in browser and start drawing
2D structure editing	Mature and comprehensive	Robust editor workflow for day-to-day tasks
Reaction drawing	Supported in desktop workflows	Browser reaction drawing with reaction SMILES examples and guide links
SMILES-driven workflow	Supported	Supported with quick copy/paste pipeline
3D visualization workflow	Depends on edition/ecosystem	Integrated viewer with display modes and settings
Export flexibility	Strong export ecosystem	Image + chemistry format export for common workflows
Learning curve for beginners	Moderate	Low-to-moderate (web-first UI)

Criteria	ChemDraw	MolDraw
Best fit	Enterprise/institutional legacy workflows	Students, teaching, agile research communication

Technical Content: What Actually Matters

Data Portability Prefer tools that preserve reusable identifiers (SMILES/SDF), not only screenshots. Workflow Latency Fast load + minimal friction improves throughput in assignment and reporting cycles. Export Readiness A practical stack needs publication graphics and structure exchange formats together.

In a real chemistry workflow, software value is not just about drawing quality. You also need transferability between notebooks, reports, presentations, and computational tools. That means export hygiene, reproducibility, and clean structure representation.

- Use **SVG/PNG** for report-ready visuals.
- Use **SDF/XYZ/PDB** for interoperability and downstream tooling.
- Keep **SMILES** for indexing, communication, and repeatable handoffs.

Workflow Diagram

Below is a compact pipeline you can use in class or lab [documentation](#):

1) Draw / paste SMILES in 2D editor ↓ 2) Validate name + structure consistency ↓ 3) Open 3D view and set display mode (ball-stick / surface / etc.) ↓ 4) Export target format (PNG, JPG, SDF, XYZ, PDB) ↓ 5) Insert into report / ELN / slides and keep SMILES reference attached

This process keeps visual communication and machine-readable chemistry aligned, which reduces rework later.

Who Should Use Which Tool?

Choose ChemDraw if your team already depends on deeply integrated enterprise templates or existing internal standards built around that ecosystem.

Choose MolDraw if you want a modern free ChemDraw alternative for rapid browser access, easy onboarding, and practical chemistry output formats.

FAQs: ChemDraw vs MolDraw

Is there a free ChemDraw online alternative?

Yes. MolDraw is a free browser-based chemistry drawing app for common structure drawing, SMILES workflows, 3D viewing, and exports.

Is MolDraw really a free ChemDraw alternative?

Yes. MolDraw provides a free browser workflow for structure drawing, 3D viewing, and exports without a licensing barrier.

Can I use MolDraw for assignments and teaching labs?

Yes. It is suitable for student and instructor workflows where quick access, simple UI, and reliable exports are important.

What can I use if I need ChemDraw online for free?

Use MolDraw when your goal is browser-based chemical drawing, reaction sketching, SMILES handling, 3D viewing, and export without a desktop install.

Can MolDraw draw chemical reactions?

Yes. Use the [chemical reaction drawer](#) page to open reaction examples and sketch reactants, products, arrows, reagents, and conditions.

Does MolDraw support technical export workflows?

Yes. Typical workflows include image export and chemistry-format export such as SDF/XYZ/PDB, depending on the view context.

Where can I read more about MolDraw usage?

Use the internal resources below for setup, updates, and help.

Draw Chemical Structures Online | Chemical Structure Drawing App

<https://www.moldraw.com/blog/chemical-structure-drawing-app-seo-optimized.html>

Chemical structure drawing app guide: draw chemical structures online, create clean molecule drawings, sketch reactions, export SVG/PNG/SDF, and choose browser molecule drawing software.

Published: 24 Feb 2026 • Updated: 12 Jun 2026 • Author: Scidart Academy When you choose an app to **draw chemical structures online**, look for clear drawings, naming support, easy export, and results you can reproduce. These matter more than a flashy interface.

What Is a Chemical Structure Drawing App?

A chemical structure drawing app helps you create, edit, and communicate molecules and [reactions](#). It is used in class reports, lab notebooks, publications, and collaboration.

The best tools make your structures easy to read and scientifically consistent, while supporting both quick sketches and publication-quality output.

How to Draw Chemical Structures Online

Start with a browser editor, draw atoms and bonds, verify stereochemistry and labels, then export a visual image and a machine-readable structure format. For known compounds, name or [SMILES](#) lookup can save time; for reactions, open a reaction drawer workflow that supports reactants, products, arrows, and conditions.

MolDraw supports this workflow from the main app and connects it to structure converters, formula tools, and reaction guides.

Core Features You Need

- Fast 2D structure editing with clear bond and atom tools.
- SMILES support for import/export and reproducible data exchange.
- IUPAC naming support for better communication and indexing.
- 3D visualization for geometry review and presentation.
- Export options (PNG, SVG, SDF, XYZ, OBJ/X3D) for different workflows.

A Practical Workflow

Start by drawing or pasting SMILES, verify naming and metadata, then check 3D orientation. Finally, export the format your destination requires (notebook, report, or model viewer).

For reaction work, keep naming and stoichiometry annotations consistent across all saved files.

Quality and Reproducibility Tips

- Always keep canonical identifiers (SMILES/InChIKey) in your records.
- Use SVG for publication graphics to retain sharp scaling.
- Use local autosave to avoid accidental data loss.
- Prefer explicit stereochemistry when needed.

Why MolDraw Is Useful

MolDraw combines 2D editing, metadata display, 3D viewing, and practical microapps (like TLC and calculators) in one web workflow, making it useful for both learning and daily chemistry tasks.

Quick FAQ

Is MolDraw free? Yes, it is free to use.

Can I draw chemical structures online without installing software? Yes. MolDraw runs in the browser and supports structure drawing, SMILES workflows, 3D viewing, and exports.

Can I export structures? Yes, including SVG/PNG and chemistry formats.

Can beginners use it? Yes. The workflow is straightforward and includes guidance pages.

Chemistry Draw Online Guide | Chemical Drawing Workflows

<https://www.moldraw.com/blog/chemistry-drawing-keyword-guide.html>

Chemistry draw and chemical drawing guide for students and researchers. Learn how to draw chemical structures online, create chemistry drawings, and export clean molecule or reaction figures.

Published: 2 Mar 2026 • Updated: 12 Jun 2026 • Author: Scidart Academy

You want to draw chemistry online: make readable structures or [reactions](#) quickly, and export them without losing chemical meaning. This guide shows how, for students, teachers and lab teams.

Tip: Use consistent atom labels, explicit stereochemistry, and a clear export format strategy from the start.

Core Principles for Chemical Drawing

- Keep structure geometry readable before adding stylistic details.
- Use unambiguous notation for stereocenters and ring systems.
- Preserve machine-readable structure data alongside visuals.

Common Chemistry Drawing Tasks

Task	Goal	Best output
Class assignment drawing	Readable and accurate structures	PNG or SVG
Lab notebook record	Reproducible structure data	SDF + image snapshot

Task	Goal	Best output
3D interpretation	Visualize orientation and shape	XYZ/PDB plus screenshot
Collaboration handoff	Easy transfer between tools	SMILES + SDF

Minimal Technical Workflow

Draw structure (2D) -> Validate naming and bonds -> Open 3D view -> Select visual style -> Export PNG/SDF/XYZ/PDB -> Add to report

How to Draw Chemicals Online

A browser chemistry drawing workflow should let you draw chemical structures online, paste or copy [SMILES](#), search known molecules, sketch reactions, and export images or reusable structure files. MolDraw supports this flow from the main editor and connects it with tools for formula, mass, structure lookup, and reactions.

- For molecule sketches, start in the [MolDraw editor](#).
- For reaction schemes, use the [chemical reaction drawer](#).
- For format conversion, use the [MolDraw tools hub](#).

Quality Checklist

- Bond angles and labels are readable at report scale.
- Important stereochemistry is explicit and not implied.
- A structure file is saved with every final figure.

FAQs

What makes a chemistry drawing look professional?

Consistent bond style, readable atom labels, clear spacing, and explicit stereochemistry where required.

Is browser-based molecule drawing reliable for students?

Yes. Browser workflows reduce setup time and make chemistry drawing more accessible across devices.

Can I draw chemical reactions online?

Yes. Use a reaction drawer workflow when you need reactants, products, arrows, reagents, conditions, and labels in one scheme.

Which export format should I choose first?

Use PNG/SVG for visuals and SDF for structure portability; add XYZ/PDB for 3D-focused workflows.

[Open MolDraw Community Chemical Reaction Drawer](#) [ChemDraw vs MolDraw Chemical Structure Drawing Guide](#) [Free Chemical Drawing Software](#) [MolDraw FAQ](#) [Chemistry Tools](#)

Compare Analogues with Tanimoto Similarity: Compare Molecules Plugin

<https://www.moldraw.com/blog/compare-molecules-plugin-tanimoto-similarity.html>

Score how alike two or more molecules are. A practical guide to Tanimoto similarity, functional similarity and the free MolDraw Compare molecules plugin.

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Short answer: Install **Compare molecules** from Settings > Plugins, draw your reference molecule, open the **Compare** tab and press **Add canvas**. Paste other structures as SMILES, one per line, and press **Add SMILES**. Each row shows a structure similarity (Tanimoto) score, a functional similarity score and a short list of changes. Press **CSV** to export the table.

Why put a number on "similar"?

Chemists say two molecules are "similar" all the time. Ask three people how similar paracetamol and aspirin are, and you get three answers. A similarity score gives everyone the same yardstick.

That matters when you work through an analogue series, pick compounds to test, or teach structure-activity relationships. A score lets you rank a list instead of eyeballing it. A list of changes tells you what actually differs from the reference.

What Tanimoto similarity means

Software first turns each molecule into a **fingerprint**: a long row of on/off bits. Each bit records whether a structural feature, such as a ring or a small fragment, is present.

The **Tanimoto coefficient** compares two fingerprints. Count the bits set in both molecules and divide by the bits set in either one. If molecule A has *a* bits on, B has *b* bits on and they share *c*, then $T = c / (a + b - c)$. A score of 1 (100%) means the fingerprints are identical. A score of 0 means they share no features.

Keep three points in mind:

- The score depends on the fingerprint. The same pair can score differently in different programs, so compare numbers only within one tool.
- Fingerprints like this ignore stereochemistry. Two enantiomers get the same fingerprint.
- Similar structures often, but not always, have similar activity. A small change can switch activity off.

What the plugin shows

Chloramphenicol as the reference, next to salicylic acid and paracetamol. Each row has two scores and a list of changes.

Structure similarity	Tanimoto score on a structural fingerprint (same atoms and bonds).
Functional similarity	Similarity of pharmacophore features: H-bond donors and acceptors, aromatic rings, charges, halogens and hydrophobic groups.
Changes	Plain-language differences from the reference, such as Cl → H, plus notes such as a stereocentre or protonation difference.
2D, 3D, Properties	Side-by-side drawings with differences coloured, a 3D superposition with RMSD, and a physicochemical and drug-likeness table.
CSV	Exports the comparison table with scores, changes and property values.

How to install Compare molecules

1. Open the [MolDraw editor](#) and sign in. A free account is enough.
2. Click **Settings** (the gear), then **Plugins**.
3. Click **Install** next to Compare Molecules. A **Compare** tab appears in the analysis panel.

How to compare a series step by step

1. Draw the reference molecule on the canvas.
2. Open the **Compare** tab and press **Add canvas**. The first molecule in the list is the reference. If the canvas holds several molecules, each one is added.
3. Paste more structures in the SMILES box, one per line. You can add a name after a space, for example CC(=O)Nc1ccc(O)cc1 paracetamol.
4. Press **Add SMILES**. Every row now shows its scores against the reference.
5. Click a row to see **Reference** and **Selected** side by side. Coloured atoms mark **Stereo**, **Charge** and **Not shared** differences. When the two share a core, tick **Overlay** to draw one on top of the other.
6. Switch to **3D** and press **Run 3D comparison** to superimpose conformers, or to **Properties** for a side-by-side property table.
7. Click the star on any row to make it the new reference. Press **CSV** to save the table, or **Clear** to start again.

Ways to use it in class and in the lab

- **Teaching stereoisomers:** compare a molecule with its enantiomer. The Tanimoto score is 100%, yet the note says the structures differ at a stereocentre. This shows students why a fingerprint is not the whole story.
- **Acids and their salts:** compare a carboxylic acid with its carboxylate. The plugin reports that the skeleton is the same and the charge or protonation differs.
- **Analogue series:** paste a list of analogues and read the changes column. You see at a glance which ring position or substituent each one changes.
- **Scaffold hops:** a low structure score with a higher functional score can hint that a new scaffold keeps similar features, such as donors, acceptors and aromatic rings.
- **Database hits:** in the [ChEMBL plugin](#), use Send to Compare to add a compound straight to the table.

Tips and honest limitations

- Read the notes column, not only the score. A 100% Tanimoto score can still hide stereo or charge differences.
- Draw wedges where stereochemistry matters, so the plugin compares the configurations you intend.
- Similarity scores do not predict activity. Use them to organise a series, then check the data.
- Property values in the Properties tab are estimates. Rows marked with an asterisk use a stand-in descriptor.
- Need SMILES from names? Use the [name to SMILES converter](#), then paste the results.

Screening a series for drug-likeness? Pair the table with the [Lipinski rule of five calculator](#).

Questions and answers

What does a Tanimoto score of 100% mean?

The two fingerprints are identical. That does not always mean the molecules are identical, because the fingerprint ignores stereochemistry. The plugin reports stereocentre and charge differences separately in the notes.

What is the difference between structure and functional similarity?

Structure similarity is a Tanimoto score on a structural fingerprint, so it rewards the same atoms and bonds. Functional similarity compares pharmacophore features: H-bond donors and acceptors, aromatic rings, charges, halogens and hydrophobic groups.

Can I change the reference molecule?

Yes. The first molecule you add is the reference. Click the star on any row to make that molecule the reference, and the scores are recalculated against it.

Is the Compare molecules plugin free?

Yes. You install it with a free MolDraw account.

Read Cyclic Voltammograms Online: $E_{1/2}$, ΔE_p , HOMO/LUMO and Scan Rate

<https://www.moldraw.com/blog/cyclic-voltammetry-viewer-guide.html>

A practical guide to the free MolDraw cyclic voltammetry viewer: open potentiostat files, read E_{pa} , E_{pc} , $E_{1/2}$ and ΔE_p , convert reference electrodes, estimate HOMO/LUMO and run a Randles-Ševčík analysis.

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Short answer: Open the [cyclic voltammetry viewer](#), press **Open CV file(s)** or drop a CSV, CH Instruments, BioLogic, Gamry or Autolab export onto the page. Pick a cycle and read E_{pa} , E_{pc} , $E_{1/2}$, ΔE_p and i_{pa}/i_{pc} , with a short note on what they mean. The same page converts reference electrodes, estimates HOMO and LUMO from onset potentials and runs a Randles-Ševčík scan-rate analysis. Your files stay on your device.

Try the CV viewer here

Press **Ferrocene (reversible)** in the live viewer to load a worked example.

Click to load the live viewer in this page, or [open the full cyclic voltammetry viewer](#). Your files stay on your device.

Why use a browser CV viewer?

Potentiostat software usually runs on one lab computer and reads one vendor's files, so collaborators often cannot open your data. Reading peaks by hand from a plot is slow and error-prone. The MolDraw viewer reads the common exports, overlays them and measures the standard values the same way every time.

Cyclic voltammetry in brief

The working electrode potential is swept linearly to a vertex and back while the current is recorded. The **anodic peak** (E_{pa} , current i_{pa}) comes from oxidation. The **cathodic peak** (E_{pc} , current i_{pc}) comes from reduction.

For an electrochemically reversible couple, $E_{1/2} = (E_{pa} + E_{pc})/2$ is close to the formal potential. The peak separation ΔE_p is about 59/n mV at 25 °C, where n is the number of electrons, and it does not change with scan rate. A ratio i_{pa}/i_{pc} near 1 means both forms are stable during the scan. A wider ΔE_p points to slower electron transfer or uncompensated resistance. A missing return peak means the product reacts away.

A potential only has meaning against a **reference electrode**. Aqueous work often uses SCE or Ag/AgCl. In organic solvents, IUPAC recommends reporting potentials against the ferrocene/ferrocenium couple (Fc/Fc+) measured in the same cell.

For organic semiconductors, the **onset** potentials of oxidation and reduction vs Fc/Fc+ give rough frontier orbital energies: $E(\text{HOMO}) \approx -(E_{\text{ox, onset}} + 4.8)$ eV, and the same with the reduction onset for LUMO. The 4.8 eV value is a convention, not a constant.

The **Randles-Ševčík** equation links peak current to scan rate. For a reversible wave of a dissolved species at 25 °C, $i_p = 2.69 \times 10^5 n^{3/2} A D^{1/2} C v^{1/2}$. So i_p grows with $v^{1/2}$. For a species fixed on the electrode, i_p grows with v instead.

Files the viewer opens

CSV or TXT	Potential and current columns, with optional time and cycle columns. Current units (A, mA, μ A, nA) are read from the header.
Instrument exports	CH Instruments text exports, BioLogic EC-Lab .txt exports, Gamry .DTA files and Autolab NOVA ASCII exports.
Scan rate	Read from the header or a time column, or typed in mV/s next to the file name.
Cycles	Taken from a cycle column, or found from the turning points of the sweep.

How to analyse a CV step by step

1. Press **Open CV file(s)**, or drop files on the box. To explore first, press an example such as **Quasi-reversible** or **Irreversible oxidation**.
2. Under **Reference and units**, set **Data vs** to the electrode you measured against and **Show vs** to the one you want to report. If you ran ferrocene in the same cell, type its $E_{1/2}$ in **Ferrocene $E_{1/2}$ vs data ref (V)**.
3. Choose a cycle in the **Peaks** menu. Read the table and the "What it means" note under it.
4. For energy levels, open **HOMO / LUMO from onset potentials**. Tick **Use oxidation onset**, **Use reduction onset** or both, and **Mark onsets** to see them on the plot.
5. For a scan-rate series, select several files at once, or tick **Add to the plot instead of replacing**. Check each scan rate, open **Scan-rate analysis (Randles-Sevcik)**, and enter **Electrons n** and **Concentration (mM)**.
6. Save your work with **Export PNG**, **Export CSV** or **ip plot PNG**.

What the viewer does

- **Overlays:** each file gets its own colour. Show, hide or remove files, and choose which cycles to draw.

- **Plain-language verdict:** the note calls ΔE_p up to 75 mV reversible and up to 200 mV quasi-reversible. Peaks more than 0.8 V apart are treated as separate processes, so $E_{1/2}$ and ΔE_p are not given.
- **References and signs:** convert between SCE, two Ag/AgCl electrodes, SHE, NHE, Hg/HgO and Fc/Fc⁺. Oxidation is plotted up (IUPAC); tick **US convention** to flip it.
- **Scan-rate analysis:** ipa against $\sqrt{v}$ with a fitted line and R^2 , the slope of log ip against log v , a diffusion or surface verdict, and the diffusion coefficient D when n , area and concentration are set.
- **Current density:** set **Electrode area (cm²)** and tick **Current density** to plot j instead of I .

Ways to use it in class and in the lab

- **Teaching reversibility:** load **Ferrocene (reversible)**, **Quasi-reversible** and **Irreversible oxidation** in turn and compare ΔE_p , ipa/ipc and the return peak.
- **Reporting a new compound:** enter your ferrocene $E_{1/2}$ and quote $E_{1/2}$ vs Fc/Fc⁺, which other groups can compare directly.
- **Organic electronics:** estimate HOMO, LUMO and the electrochemical gap from a film CV, then compare the gap with the optical gap from the [UV-Vis spectrum viewer](#).
- **Mechanism checks:** run a scan-rate series to tell a diffusing species from one adsorbed on the electrode.

Tips and limits

- Files rarely record the reference electrode, so check **Data vs** every time.
- The conversions use fixed aqueous values vs SHE. In organic solvents an internal ferrocene standard is more reliable.
- The scan-rate analysis uses the first cycle of each file. D assumes a reversible, diffusion-controlled wave at 25 °C.
- HOMO and LUMO values are estimates. Compare only values made with the same Fc/Fc⁺ level and the same method (onset or $E_{1/2}$).
- With overlapping waves, check that the E_p and E_{pc} markers sit on the peaks you mean.

The [tools page](#) lists all the free MolDraw data viewers.

Questions and answers

Why is my ΔE_p larger than 59 mV for a couple that should be reversible?

Uncompensated resistance and slow electron transfer both widen ΔE_p . Run ferrocene in the same cell. If it also shows a large ΔE_p , the cell is the cause.

Can I report potentials vs Fc/Fc⁺ if I measured against Ag/AgCl?

Yes. Set Data vs to your Ag/AgCl electrode, type the ferrocene $E_{1/2}$ measured in the same cell, and set Show vs to Fc/Fc⁺. Without it, the viewer assumes +0.40 V vs SCE (acetonitrile), which is only approximate.

How many files do I need for the scan-rate analysis?

At least three CVs at different scan rates. If a file does not give its scan rate, type it in mV/s next to the file name.

Does the viewer handle files with several cycles?

Yes. Pick the cycle to analyse in the Peaks menu and tick which cycles to show on the plot.

Download MolDraw for Windows (Free) | Official Install Guide

<https://www.moldraw.com/blog/download-moldraw-windows.html>

Download MolDraw for Windows: free installer for the MolDraw molecule editor and 3D viewer. System requirements, install steps, and safe official links from Scidart Academy.

Published: 29 Mar 2026 • Scidart Academy **Official Windows installer:** MolDraw is free chemistry software for drawing structures, running IUPAC-oriented workflows, and viewing molecules in 3D. Use the button below for the current Windows setup. You can always use the full app in your browser at moldraw.com without installing anything. [Download Windows setup](#) [Launch web app](#)

What you get with MolDraw

- 2D structure editing in a focused MolDraw workspace.
- Integrated 3D visualization for geometry review and teaching.
- Practical exports (for example PNG, SVG, and chemistry-friendly formats where supported).
- Access to the same learning resources as the web app, including the [course](#) and [FAQ](#).

System requirements (typical)

Windows 10 or later is recommended. The desktop build is a standard Windows installer; allow the installer to complete and start MolDraw from the Start menu or desktop shortcut if one is created. If SmartScreen appears, confirm you trust the publisher and source link you used (this page and moldraw.com).

Install steps

1. Click **Download Windows setup** above.

2. Run the downloaded installer and follow the prompts.
3. Open MolDraw from the Start menu or desktop shortcut when the installer creates one.
4. For the newest fixes without waiting for an installer refresh, keep using the [web version](#).

Prefer not to install?

The browser app at moldraw.com is the reference experience and updates continuously. The Windows package is ideal when you want a desktop shortcut and a more app-like window.

FAQ

Is MolDraw free? Yes. MolDraw is free to use; see site terms for redistribution.

Is there a Mac or Linux build? Use the web app today; other desktop platforms may be added later.

Is this the official download page? This article is published by Scidart Academy on the official MolDraw blog. The download button uses the same official redirect as the in-app “Download Windows Setup” control.

Embed MolDraw on Your Site | Free Molecule Editor Iframe

<https://www.moldraw.com/blog/embed-moldraw.html>

Embed the MolDraw editor on your site. Copy one iframe, paste it into a blog, course, docs page, or app, and set the frame height. Includes a live preview.

Published: 18 Sep 2026 · Author: Scidart Academy

Add a live molecule editor to a chemistry blog, lesson, lab page, docs article, or app. Copy one iframe, paste it where the drawing should appear, and set the height so the canvas fits your layout.

Short version: click Copy embed code, paste the snippet into your HTML, and start with a height of 640 pixels. Readers draw in place. Open in MolDraw opens the full editor in a new tab.

Who it is for

Use the embed when a reader should try a structure next to your explanation, not only look at a picture.

- **Chemistry bloggers** — a working canvas under a reaction or structure post.
- **Educators and LMS authors** — a drawing box on a lesson, lab manual, or problem set.
- **Docs authors** — an editor beside a format, SMILES, or workflow note.
- **App builders** — a ready editor frame inside a page that already has its own interface.

You do not host the editor. The frame loads it from <https://www.moldraw.com/embed>. Your page stays yours.

Copy and paste

Copy embed code puts this snippet on your clipboard. Paste it into the HTML of your page, an LMS HTML block, or the markup of your app.

```
<iframe src="https://www.moldraw.com/embed" title="MolDraw editor" width="100%" height="640" style="border:0;border-radius:12px" loading="lazy" referrerpolicy="strict-origin-when-cross-origin"></iframe>
```

If the frame is blank, your site or course tool may block embeds. Use an HTML or embed block that allows iframes. If the platform still removes the frame, link to www.moldraw.com instead.

Preview

This is the same player the snippet loads. Draw a bond or pick a template. The bar at the top is part of the embed.

Size the frame

Width is 100% so the editor fills the column you drop it into. Height is 640 pixels, enough for the toolbar and a small structure. Raise the height number for a larger canvas. Drop it toward 480 on a short page, or use about 800 when readers need more room.

On a phone, a tall frame means more scrolling. Match the height to the task: a quick sketch can stay shorter; a [reaction scheme](#) needs more space.

Open in MolDraw

Inside the player, **Open in MolDraw** opens the full editor at www.moldraw.com in a new tab. Your page stays open. Tell readers once: sketch here, and use Open in MolDraw if you want the full screen.

FAQ

Who is this for?

Chemistry bloggers, educators, LMS authors, docs writers, and app builders who want a molecule editor beside their own text. It is a poor fit if you only need a logo or a screenshot. In that case, link to MolDraw or use an image.

Do readers need an account?

No. They can draw in the frame without signing up on your site. Open in MolDraw is there when they want the full editor.

Can I change the size after I paste it?

Yes. Edit height in the snippet. Leave width="100%" unless your layout needs a fixed width. The preview on this page is 640 pixels tall on a wide screen and shorter on a phone.

The frame is blank. What now?

A blank frame usually means the host blocks iframes. Switch to the platform's HTML or embed block. If that still fails, send readers to www.moldraw.com with a normal link.

Free Chemical Databases: PubChem, ChEMBL & More

<https://www.moldraw.com/blog/free-chemical-databases-guide.html>

Compare 12 free chemical databases (PubChem, ChEMBL, ChEBI, ZINC, PDB, UniChem and more) with verified sizes, licences and real API queries.

Published: 6 Oct 2026 · By [Rafeeqe Mavoor](#) · Category: Guides · Data checked: October 2026

Short answer: The most useful free chemical databases are **PubChem** (the largest general compound database), **ChEMBL** (curated bioactivity data for drug discovery), **ChEBI** (a curated dictionary of small molecules), **ZINC** (billions of purchasable compounds for virtual screening) and the **RCSB PDB** (3D protein-ligand structures). For spectra, use **nmrshiftdb2** (**NMR**), **MassBank** (MS/MS) and the **NIST Chemistry WebBook**; for natural products, **COCONUT**; for patents, **SureChEMBL**; and **UniChem** links the identifiers between them.

Chemistry students meet the same problem sooner or later: you have a molecule, and you need its properties, its biological activity, a crystal structure, a reference spectrum or a patent. Each of those questions lives in a different database. This guide explains what each major free chemical database is, what it is good for, how big it is, what the licence allows, and how to query it, with real example URLs that we tested before publishing.

All figures below were **checked in October 2026** against the official sites or APIs. Database sizes change every release, so treat them as snapshots, not constants.

Free chemical databases grouped by data type: compounds, bioactivity, screening, natural products, 3D structures, spectra and patents, linked by UniChem.

What is a chemical database?

A **chemical database** is a searchable collection of chemical structures linked to data about them: names, identifiers, calculated properties, experimental measurements, biological activities, 3D coordinates, spectra or the documents where they were reported. Most modern databases can be searched by name, by identifier (CAS number, InChIKey, [SMILES](#)) or by drawing a structure, and many offer a free REST API for programmatic access.

The key thing to understand is that **no single database does everything**. They differ in focus:

- **Compound encyclopedias** (PubChem, ChEBI) answer "what is this molecule?"
- **Bioactivity databases** (ChEMBL, DrugBank) answer "what does this molecule do to a protein?"
- **Screening libraries** (ZINC) answer "what similar molecules can I buy or dock?"
- **Structural databases** (RCSB PDB) answer "how does this molecule sit in its target?"
- **Spectral databases** (nmrshiftdb2, MassBank, NIST WebBook) answer "what should its spectrum look like?"
- **Specialist collections** (COCONUT for natural products, SureChEMBL for patents) cover niches the big ones miss.

How do the free chemical databases compare?

Database	Focus	Size (checked Oct 2026)	Best for	API	Licence
PubChem	General compounds, substances, bioassays	~124 M compounds, ~349 M substances	Identifiers, properties, broad lookups	PUG-REST, PUG-View	Free; reuse terms vary by depositor
ChEMBL	Curated bioactivity	2.92 M compounds, 24.5 M activities, 18,552 targets (ChEMBL 37)	SAR, potency, drug targets	REST (JSON/XML)	CC BY-SA 3.0
ChEBI	Curated small-molecule dictionary + ontology	201,471 entries, 61,961 fully curated (release 244)	Definitions, classes, biological roles	REST (ChEBI 2.0)	CC BY 4.0

Database	Focus	Size (checked Oct 2026)	Best for	API	Licence
ZINC-22	Purchasable "make-on-demand" compounds	~54.9 B (2D), ~5.9 B (3D)	Virtual screening, analogue buying	Web (CartBlanche), bulk download	Free to use; no redistribution of major portions without permission
RCSB PDB	3D macromolecular structures	260,724 entries	Protein-ligand complexes, docking prep	Data API, Search API	CC0 1.0
UniChem	Identifier cross-mapping	25 sources	Converting IDs between databases	REST	Free (EMBL-EBI terms); source licences apply
nmrshiftdb2	NMR spectra + prediction	271,817 structures, 70,030 measured spectra	¹ H/ ¹³ C NMR reference and prediction	Web; new REST interface	Open content licence
MassBank (Europe)	Experimental mass spectra	139,006 records	MS/MS matching, metabolomics	REST	Per-record Creative Commons
COCONUT 2.0	Natural products	738,829 unique molecules, 71 collections	Natural product discovery	REST (login required)	CC0 (data)
SureChEMBL	Chemistry from patents	116.6 M patent documents (May 2025)	Prior art, patent landscaping	REST	CC BY 4.0
DrugBank	Drugs and drug targets	n/a (not checked)	Approved-drug details	Paid API	Free academic, CC BY-NC 4.0; commercial licence needed
NIST Chemistry WebBook	Thermochemistry, IR, EI-MS	n/a (not checked)	Reference IR/MS, physical data	Web only	NIST Standard Reference Data (copyrighted)

What is PubChem? The largest free chemical database

PubChem is the world's largest free chemistry database, run by the US National Center for Biotechnology Information (NCBI). It aggregates data from more than a thousand contributors into linked collections: Substance (what depositors submitted), Compound (unique standardized structures), BioAssay, Protein, Gene, Pathway and Patent.

- **Size:** about 124 million compounds and 349 million substances on the PubChem homepage (checked October 2026). The peer-reviewed [PubChem 2025 update](#) reported 118.6 million compounds as of September 2024.
- **Used for:** looking up names, synonyms, CAS numbers, formulas, computed properties (XLogP, TPSA), safety data, suppliers and literature.
- **Who uses it:** students, teachers, analytical chemists, toxicologists, cheminformaticians and anyone who needs a quick, reliable identifier.
- **Access:** web search with a structure drawer, and the free PUG-REST API. PubChem asks programmatic users to stay below **5 requests per second**.
- **Licence:** free to use; reuse rights follow each data source, so check the source before redistributing data.

Plain-language query: "Give me the formula, [molecular weight](#), SMILES and InChIKey of aspirin."

```
https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/property/MolecularFormula,MolecularWeight,SMILES,InChIKey/JSON
```

Real response (trimmed):

```
{
  "PropertyTable": {
    "Properties": [
      {
        "CID": 2244,
        "MolecularFormula": "C9H8O4",
        "MolecularWeight": "180.16",
        "SMILES": "CC(=O)OC1=CC=CC=C1C(=O)O",
        "InChIKey": "BSYNRYMUTXBXSQ-UHFFFAOYSA-N"}
    ]
  }
}
```

Heads-up: PubChem has renamed its SMILES properties. Asking for the old CanonicalSMILES still works, but the answer now comes back labelled ConnectivitySMILES (no stereochemistry). Ask for SMILES if you want the full, stereo-aware string.

More tested PubChem queries:

- InChIKey to CID: <https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/inchikey/BSYNRYMUTXBXSQ-UHFFFAOYSA-N/cids/JSON> returns 2244.
- 2D similarity (≥90%) to cetirizine:
https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/fastsimilarity_2d/cid/2678/cids/JSON?Threshold=90&MaxRecords=10
- Substructure search from SMILES:
[https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/fastsubstructure/smiles/c1ccc\(cc1\)C\(c1ccc\(Cl\)cc1\)N1CCNCC1/cids/MaxRecords=10](https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/fastsubstructure/smiles/c1ccc(cc1)C(c1ccc(Cl)cc1)N1CCNCC1/cids/MaxRecords=10)

What is ChEMBL? The go-to bioactivity database

ChEMBL is a manually curated database of bioactive, drug-like molecules, maintained by EMBL's European Bioinformatics Institute (EMBL-EBI). Its core is measured activity data, such as IC50, Ki and EC50 values, extracted from journal articles and deposited datasets, each linked to a compound, an assay and a biological target.

- **Size (ChEMBL 37, May 2026):** 2,921,148 distinct compounds, 24,527,044 activities, 18,552 targets and 101,100 publications, as reported by the ChEMBL API status endpoint.
- **Used for:** structure-activity relationships (SAR), finding known actives for a target, building machine-learning training sets, and checking drug approval phase.
- **Who uses it:** medicinal chemists, pharmacologists, computational chemists and data scientists.
- **Licence:** CC BY-SA 3.0. ChEMBL asks that ChEMBL IDs and the release number be preserved when you reuse its data.

<https://www.ebi.ac.uk/chembl/api/data/molecule/search.json?q=aspirin>

Plain-language query: "What potency values does ChEMBL hold for cetirizine (ChEMBL1000) on the human histamine H1 receptor (ChEMBL231)?"

```
{
  "activities": [
    {
      "standard_type": "Ki",
      "standard_value": "14.0",
      "standard_units": "nM",
      "pchembl_value": "7.85",
      "target_pref_name": "Histamine H1 receptor"},
    {
      "standard_type": "Ki",
      "standard_value": "5.89",
      "standard_units": "nM",
      "pchembl_value": "8.23",
      "target_pref_name": "Histamine H1 receptor"}
  ]
}
```

PubChem is broad; ChEMBL is deep. PubChem tries to include every chemical anyone has deposited, so it is the best place to identify a compound. ChEMBL contains far fewer compounds but curates their biological activity in a consistent format (standard units, pChEMBL values, mapped targets), so it is the better place to ask "how potent is it, and on what?" In practice you use both: PubChem to confirm the structure and identifiers, ChEMBL to read the pharmacology.

ChEBI (Chemical Entities of Biological Interest) is a manually curated dictionary and ontology of small molecules, run by **EMBL-EBI**. Curated entries have a definition, structure, synonyms and ontology links that say what the molecule *is* (e.g. "a member of the class of benzoic acids") and what *role* it has (e.g. "non-steroidal anti-inflammatory drug").

Plain-language query: "What is CHEBI:15365?"

What is ZINC? Billions of compounds for virtual screening

ZINC is a free database of commercially available ("tangible") compounds prepared for virtual screening, built by the Irwin and Shoichet labs at UCSF. ZINC-22 focuses on huge make-on-demand catalogues from Enamine, WuXi and Mcule, while its sister database ZINC20 covers smaller in-stock catalogues. ZINC15 is the older generation, which many [tutorials](#) still mention.

Plain-language query: "Find purchasable compounds similar to cetirizine." Paste the SMILES

What is the RCSB PDB? 3D structures of proteins and ligands

The Protein Data Bank (PDB) is the single global archive of experimentally determined 3D structures of proteins, nucleic acids and their complexes; RCSB PDB is its US data centre and search portal. For chemists, its value is the bound ligands: you can

see exactly how a small molecule sits in its binding pocket.

- **Size:** 260,724 current entries (RCSB holdings API, checked October 2026).
- **Used for:** studying binding modes, preparing receptors for docking, teaching protein structure, and finding every structure that contains a given ligand.
- **Access:** web, the Data API (data.rcsb.org) and the Search API (search.rcsb.org), which supports text, sequence and chemical searches.
- **Licence:** PDB data are released under CC0 1.0 (public domain).

Plain-language query: "Show me the ligand record for aspirin (component ID AIN)."

```
https://data.rcsb.org/rest/v1/core/chemcomp/AIN
```

This returns the name 2-(ACETYLXY)BENZOIC ACID and formula C₉ H₈ O₄.

Plain-language query: "Which PDB entries contain aspirin?" (Search API; paste it into a browser, which URL-encodes the JSON for you):

```
https://search.rcsb.org/rcsbsearch/v2/query?json={\"query\":{\"type\":\"terminal\",\"service\":\"text\",\"parameters\":{\"attribute\":\"rcsb_nonpolymer_instance_annotation.comp_id\",\"operator\":\"exact_match\",\"value\":\"AIN\"}},\"return_type\":\"entry\"}
```

Real response (trimmed): "total_count": 8, with entries such as 10XR, 1TGM and 3GCL. A chemical search posted with the SMILES of aspirin (service: "chemical") also returned AIN as the top match. You can load any of these entries by its PDB ID in the [MolDraw protein viewer](#) or open it at rcsb.org.

What is UniChem? Translating IDs between databases

UniChem is EMBL-EBI's identifier cross-referencing service: give it one structure identifier and it returns the matching IDs in other databases. It links records through the standard InChI/InChIKey, so it works whenever two databases hold the same structure.

- **Size:** 25 sources listed by the UniChem API, including ChEMBL, PubChem, ChEBI, DrugBank, RCSB PDB, PDBe, SureChEMBL, HMDB, BindingDB and nmrshiftdb2 (checked October 2026).
- **Used for:** merging datasets, jumping from a ChEMBL ID to a PDB ligand code, and checking where else a compound appears.
- **Access:** web and REST API ([/unichem.org/api/v1/](https://unichem.org/api/v1/)).
- **Licence:** free to use under EMBL-EBI's terms of use; the data behind each mapped ID keeps its source's licence.

Plain-language query: "Where else does aspirin's InChIKey appear?"

```
curl -X POST https://www.ebi.ac.uk/unichem/api/v1/compounds \
-H "Content-Type: application/json" \
-d '{\"type\":\"inchikey\",\"compound\":\"BSYNRYMUTXBXSQ-UHFFFAOYSA-N\"}'
```

The response maps it to ChEMBL25, ChEBI:15365, PubChem CID 2244, DrugBank DB00945, PDB ligand AIN and Guide to Pharmacology 4139, among others.

UniChem maps aspirin's InChIKey to its IDs in ChEMBL, ChEBI, PubChem, RCSB PDB, DrugBank and Guide to Pharmacology.

What is nmrshiftdb2? A free NMR spectra database

nmrshiftdb2 is an open, peer-reviewed web database of organic structures and their NMR spectra, with built-in ¹H and ¹³C shift prediction. Its core is fully assigned spectra, many with raw data.

- **Size:** 271,817 structures, 70,030 measured spectra and 396,583 calculated spectra (homepage counter, checked October 2026).
- **Used for:** checking an assignment, finding reference shifts for a compound class, and teaching NMR interpretation.
- **Access:** web search by structure, substructure, spectrum and other properties; the site announced a new REST interface in June 2026 (we did not test it).
- **Licence:** the software is open source and the data are published under an open content licence.

Plain-language query: "Find measured ¹³C spectra of compounds containing a 4-chlorobenzhydryl group." Draw the fragment in the nmrshiftdb2 search tab and run a substructure search. For a quick estimate before you search, MolDraw's [structure to NMR](#) tool predicts a spectrum from your drawing.

What is MassBank? Experimental MS/MS spectra

The examples here use MassBank Europe (massbank.eu). Each record describes one spectrum: compound, instrument, ionisation, collision energy and the peak list.

- **Size:** 139,006 records (MassBank API count, checked October 2026).
- **Used for:** identifying unknowns in LC-MS/MS and metabolomics, comparing fragmentation patterns, and teaching mass spectrometry.
- **Access:** web search (name, formula, peaks) and a REST API.
- **Licence:** each record carries its own Creative Commons licence (CC BY by default, but some are CC0, CC BY-SA or non-commercial), so check the license field before reuse.

Plain-language query: "List MassBank spectra for caffeine."

```
https://massbank.eu/MassBank-api/records/search?compound_name=caffeine
```

This returned 134 record accessions. Fetching one, https://massbank.eu/MassBank-api/records/MSBNK-ACES_SU-AS000088, gives an LC-APCI Orbitrap MS2 spectrum of [M+H]⁺ with the precursor at *m/z* 195.088 and a major fragment at *m/z* 138.067, licensed CC BY.

What is COCONUT? The open natural products database

COCONUT (COLlection of Open NatUral productTs) is the largest open collection of natural product structures, curated by the Steinbeck group at Friedrich Schiller University Jena. Version 2.0 links each molecule to its source organisms, literature and stereochemical variants.

- **Size:** 738,829 unique molecules from 71 collections, with 73,137 organisms (COCONUT statistics page, checked October 2026). The [COCONUT 2.0 paper](#) reported 695,133 at its September 2024 release.
- **Used for:** natural-product dereplication, scaffold ideas, and building screening sets.
- **Access:** web search (name, structure, substructure, similarity) and full SDF/SQL downloads. The REST API exists but requires a free account login, so we did not run it for this guide.
- **Licence:** data CC0; code MIT.

Plain-language query: "Show natural products similar to caffeine." Paste caffeine's SMILES CN1C=NC2=C1C(=O)N(C(=O)N2C)C into the structure search at coconut.naturalproducts.net.

What is SureChEMBL? Chemistry from patents

SureChEMBL is EMBL-EBI's free patent chemistry database: it text- and image-mines patent documents and extracts the chemical structures they mention. It is the easiest free way to ask "which patents contain this structure?"

- **Size:** SureChEMBL 2.0 (May 2025) covers about 116.6 million patent documents from five authorities (CNIPA, EPO, JPO, USPTO, WIPO); USPTO alone contributed about 19.9 million unique compounds.
- **Used for:** prior-art checks, patent landscaping, and spotting compound series before they appear in journals.
- **Access:** web search by structure or keyword, a REST API, and bulk Parquet files updated every two weeks.
- **Licence:** CC BY 4.0.

Plain-language query: "Resolve the name cetirizine to a SureChEMBL compound."

```
https://www.surechembl.org/api/chemical/name/cetirizine
```

Real response (trimmed): "chemical_id": "4176", "inchi_key": "ZKLPARSLTMPFCP-UHFFFAOYSA-N". You can then search for patents containing that structure in the web interface.

What about DrugBank and the NIST Chemistry WebBook?

DrugBank is a detailed knowledge base of approved and investigational drugs, their targets, metabolism and interactions. It is free to browse, but downloads require an account; academic datasets are licensed CC BY-NC 4.0 for non-commercial use, and commercial use needs a paid licence. Treat it as "free to read, not free to reuse."

The NIST Chemistry WebBook (NIST Standard Reference Database 69) offers thermochemical data, gas-phase IR spectra and electron-ionisation mass spectra for many small molecules. It is free to search online, for example <https://webbook.nist.gov/cgi/cbook.cgi?Name=caffeine&Units=SI>, but the data are copyrighted and bulk redistribution needs permission from NIST.

Which chemical database should I use?

Your question	Start with	Then try
What is this compound? Name, formula, CAS, properties	PubChem	ChEBI
How potent is it, and on which target?	ChEMBL	PubChem BioAssay
What class is it, and what is its biological role?	ChEBI	PubChem
Which similar compounds can I buy or dock?	ZINC-22	PubChem (vendors)
How does a ligand bind its protein?	RCSB PDB	ChEMBL (target data)
I have an ID from database A; what is it in database B?	UniChem	PubChem cross-references
What should its ¹ H/ ¹³ C NMR look like?	nmrshiftdb2	MolDraw NMR prediction
Does my MS/MS spectrum match a known compound?	MassBank	NIST WebBook (EI-MS)
Is it a natural product, and from which organism?	COCONUT	ChEBI
Is this structure in a patent?	SureChEMBL	PubChem Patent
Details on an approved drug?	DrugBank (browse)	ChEMBL
Thermochemistry or reference IR?	NIST WebBook	PubChem

How do I use these databases with MolDraw?

Most databases search best with a machine-readable identifier rather than a name. MolDraw gives you those identifiers straight from a drawing:

1. **Draw** the structure in the [MolDraw editor](#) (or paste a name with [name to structure](#)).

2. **Copy SMILES** from the top options row. *Copy as...* in the context menu also gives InChI and MOL formats (see the [SMILES chapter of the MolDraw course](#)).
3. **Make an InChIKey** with the [SMILES to InChIKey converter](#). InChIKeys are the most reliable exact-match key across PubChem, ChEMBL, ChEBI and UniChem.
4. **Query**: paste the SMILES into a database's structure search, or drop the InChIKey into one of the REST URLs above.
5. **Bring results back**: convert a PubChem CID with the [CID to SMILES converter](#) or an InChIKey with [InChIKey to SMILES](#), then paste it into MolDraw to edit.

Workflow: draw in MolDraw, copy SMILES or make an InChIKey, query a database, read the results.

Worked example: how do I compare cetirizine analogues?

Suppose you are studying the antihistamine **cetirizine** and want to know which close analogues exist, how potent they are, and whether you could buy new ones. Here is a three-database workflow; every number comes from the live queries we ran.

Step 1: Identify it in PubChem. Draw cetirizine in MolDraw, copy the SMILES, and look it up:

```
https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/cetirizine/property/MolecularFormula,MolecularWeight,InChIKey,XLogP,TPSA/JSON
```

PubChem returns CID 2678, C₂₁H₂₅ClN₂O₃, MW 388.9, XLogP 1.7, TPSA 53 and InChIKey ZKLPARSLTMPFCP-UHFFFAOYSA-N.

Step 2: Find analogues in PubChem. The 2D similarity query (threshold 90) returns relatives including hydroxyzine (CID 3658, cetirizine's parent drug) and levocetirizine (CID 1549000, its single enantiomer), plus their salts. A substructure search on the chlorobenzhydryl-piperazine core adds chlorcyclizine, meclizine and buclizine.

Step 3: Compare activity in ChEMBL. Look up the InChIKey in ChEMBL:

```
https://www.ebi.ac.uk/chembl/api/data/molecule.json?molecule_structures__standard_inchi_key=ZKLPARSLTMPFCP-UHFFFAOYSA-N
```

This gives ChEMBL1000 (max phase 4, first approved 1995). Its activity records include human H1 receptor Ki values between 5.89 and 79 nM (pChEMBL 7.1–8.2) and a much weaker hERG (KCNH2) IC₅₀ of about 30 μM (pChEMBL about 4.5). That window of roughly three orders of magnitude is the kind of selectivity comparison ChEMBL makes easy. A similarity search, <https://www.ebi.ac.uk/chembl/api/data/similarity/ZKLPARSLTMPFCP-UHFFFAOYSA-N/80.json>, lists levocetirizine and cetirizine salt forms to compare in the same way.

Step 4: Look for purchasable analogues in ZINC. Paste the SMILES into CartBlanche22's similarity search to see make-on-demand compounds that vary the acid side chain or the aryl rings. Then check any interesting hit's properties in MolDraw, for example with the [Lipinski rule calculator](#).

Interpretation tip: activity values from different papers are measured in different assays. Compare pChEMBL values for the same target and assay type, and treat single measurements with caution.

How do I search chemical databases well?

- **Prefer InChIKeys for exact matches** and SMILES for similarity or substructure searches. Names are ambiguous ("vitamin C", salts, brand names).
- **Watch for salts and stereoisomers.** Cetirizine, cetirizine dihydrochloride and levocetirizine are different records in every database.
- **Note the release or date.** Cite ChEMBL with its release number and record the date you queried PubChem.
- **Respect rate limits.** PubChem asks for no more than 5 requests per second; batch large jobs or download the bulk files.
- **Check the licence before you redistribute.** Browsing is free everywhere in this guide; republishing data is not always.

Key takeaways

- **PubChem** is the largest free chemical database and the best first stop to identify a compound.
- **ChEMBL** is the best free bioactivity database: curated potency data linked to targets.
- **ChEBI** classifies molecules; **UniChem** translates IDs between databases.
- **ZINC-22** is for virtual screening and buying analogues; **RCSB PDB** is for 3D binding modes.
- **nmrshiftdb2**, **MassBank** and the **NIST WebBook** cover NMR, MS/MS and IR/thermochemistry.
- **COCONUT** covers natural products and **SureChEMBL** covers patents.
- Draw in MolDraw, copy the SMILES, generate an InChIKey, and you can query all of them.

FAQ

What is the largest free chemical database?

PubChem is the largest free chemical database, with about 124 million unique compounds and 349 million deposited substances (checked October 2026). ZINC-22 lists more molecules (about 54.9 billion), but most of them are virtual make-on-demand compounds for screening rather than characterised substances.

What is the difference between PubChem and ChEMBL?

PubChem is a broad aggregator that tries to cover every deposited chemical, so it is best for identification and properties. ChEMBL is smaller but manually curated for bioactivity, with standardised potency values linked to targets, so it is best for structure–activity and drug-discovery questions.

Is ZINC free for commercial use?

According to the UCSF ZINC licence, ZINC is free to use and download for everyone, including companies. The restriction is redistribution: you may not redistribute major portions of ZINC without written permission from the ZINC team. The compounds themselves must be bought from the listed vendors.

Which free database has NMR spectra?

nmrshiftdb2 is the main free NMR database, with 70,030 measured spectra for 271,817 structures (checked October 2026) and built-in ^1H and ^{13}C prediction. PubChem compound pages also link to spectra from other sources, and the NIST Chemistry WebBook covers IR and mass spectra rather than NMR.

Which free database has mass spectra?

MassBank holds 139,006 experimental mass spectrum records (checked October 2026), mostly MS/MS spectra of small molecules, under per-record Creative Commons licences. The NIST Chemistry WebBook offers electron-ionisation mass spectra for many small molecules online.

Can I search chemical databases by structure?

Yes. PubChem, ChEMBL, ChEBI, ZINC, RCSB PDB, nmrshiftdb2, COCONUT and SureChEMBL all support structure search, usually by drawing or pasting SMILES. You can draw the molecule in MolDraw, copy its SMILES, and paste it into the database's structure search, or use exact, substructure or similarity queries through their APIs.

Which chemical database is best for students?

Start with PubChem for names, properties and safety data, ChEBI for definitions and compound classes, and the RCSB PDB for 3D structures. All three are free, need no account and have clear web interfaces. Add ChEMBL when you study pharmacology, and nmrshiftdb2 when you learn NMR.

What is a bioactivity database?

A bioactivity database stores measured effects of compounds on biological targets, such as IC₅₀, K_i or EC₅₀ values, linked to the assay and protein. ChEMBL is the leading free bioactivity database; PubChem BioAssay holds screening results deposited by laboratories and screening centres.

Is DrugBank free?

DrugBank is free to browse online, and academic users can download datasets under a CC BY-NC 4.0 licence after registering. Commercial use, including use in commercial products or services, requires a paid licence from DrugBank.

How do I convert a PubChem CID into a ChEMBL ID?

Use UniChem. Look up the compound's InChIKey (PubChem shows it on every compound page), then send it to the UniChem compounds API, which returns the matching ChEMBL, ChEBI, DrugBank, PDB and other identifiers. For aspirin, InChIKey `BSYNRYMUTXBXSQ-UHFFFAOYSA-N` maps CID 2244 to ChEMBL25.

Sources

- PubChem: pubchem.ncbi.nlm.nih.gov · [PUG-REST documentation](#) · Kim S. *et al.* PubChem 2025 update, *Nucleic Acids Res.* 2025, doi:10.1093/nar/gkaf1059
- ChEMBL: ebi.ac.uk/chembl · [API documentation](#) · [Licence and about](#) · [ChEMBL 37 release post](#)
- ChEBI: ebi.ac.uk/chebi · [ChEBI 2.0 launch](#) · ChEBI: re-engineered for a sustainable future, *Nucleic Acids Res.* 2026, academic.oup.com/nar/article/54/D1/D1768/8349173
- ZINC: [CartBlanche22](#) · Tingle B. I. *et al.* ZINC-22, *J. Chem. Inf. Model.* 2023, doi:10.1021/acs.jcim.2c01253 · [UCSF ZINC licence](#)
- RCSB PDB: rcsb.org · [Data API](#) · [Search API](#) · [Usage policy](#)
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- COCONUT: coconut.naturalproducts.net · Chandrasekhar V. *et al.* COCONUT 2.0, *Nucleic Acids Res.* 2025, doi:10.1093/nar/gkaf1063
- SureChEMBL: surechembl.org · [SureChEMBL 2.0 announcement](#) · [FAQ and licence](#)
- DrugBank: go.drugbank.com · [Academic licensing](#)
- NIST Chemistry WebBook: webbook.nist.gov/chemistry · [NIST SRD licensing](#)

Related MolDraw tools and guides

[MolDraw editor](#) [Structure to SMILES](#) [SMILES to InChIKey](#) [InChIKey to SMILES](#) [CID to SMILES](#) [CAS to SMILES](#) [Name to structure](#) [Structure to NMR](#) [Mass spectrum predictor](#) [Lipinski calculator](#) [Protein viewer](#) [Aspirin molecule page](#) [Free chemistry tools guide](#) **Rafeeqe Mavoor**, product and development lead at MolDraw. Figures were checked against official sites and live APIs in October 2026; see our [editorial guidelines](#).

Free Chemical Drawing Software and Chemistry Drawing Program

<https://www.moldraw.com/blog/free-chemical-drawing-software-iupac-guide.html>

Free chemical drawing software guide focused on MolDraw: browser chemistry drawing software, free chemistry drawing software, chemical drawing program workflows, exports, and ChemDraw alternative use cases.

Published: 12 Mar 2026 • Updated: 12 Jun 2026 • Author: Scidart Academy MolDraw is free chemical drawing software that combines 2D structure drawing, reaction drawing, metadata support, SMILES workflows, and 3D visualization in one browser workflow.

Why Free Chemical Drawing Software Matters

Students, educators, and early-stage labs often need fast structure communication without expensive licenses. A free tool should still support professional workflows such as clean diagrams, reproducible identifiers, and useful export options.

MolDraw is designed for that exact use case: practical daily chemistry work without a paywall for core tasks.

Chemical Drawing Software vs Chemistry Drawing Program

Searches like **chemical drawing software**, **chemistry drawing software**, and **chemical drawing program free** usually describe the same need: a reliable editor for molecular structures, [reaction schemes](#), labels, and export-ready figures. A browser workflow makes that easier because students and collaborators can open the same tool without installing a desktop program.

MolDraw is best for fast no-install chemical drawing, common export formats, teaching examples, and handoffs that need [SMILES](#) or structure files.

Key MolDraw Features

- **Fast 2D structure editor** for sketching molecules and reaction ideas quickly.
- **Chemical reaction drawer** workflow for reactants, products, arrows, and conditions.
- **SMILES-friendly workflow** for copy/paste and reproducible communication.
- **IUPAC support for many known compounds** through public chemistry data integrations.
- **Integrated 3D viewer** for fast visual inspection of molecular geometry.
- **Export coverage** across image and chemistry formats for reports and downstream tools.

No free workflow guarantees strict IUPAC naming for every arbitrary structure. For strict “any structure” coverage, use MolDraw with an optional commercial naming fallback.

Recommended Workflow in MolDraw

For consistent results in daily chemistry tasks:

- Draw or paste a structure (SMILES or direct canvas editing).
- Validate naming and identifiers for clarity in notes and reports.
- Inspect 3D quickly to catch obvious geometry communication issues.
- Export the right format for your destination (coursework, lab note, manuscript, or modeling tool).

This workflow keeps your chemistry communication fast, readable, and reproducible while staying inside a free chemical drawing software stack.

Who Should Use MolDraw

Students: learn structure representation and submission-ready formatting without software cost barriers.

Educators: share visual examples and lightweight assignments with browser-friendly access. Teaching on a touch screen? [Sketch structures by hand with the Smart Draw plugin](#) and convert them when the drawing is done.

Researchers: capture fast drafts, communicate structures in teams, and export for downstream workflows.

Quick FAQ

Is MolDraw really free? Yes, core MolDraw usage is free.

Can I use MolDraw as a free chemistry drawing program? Yes. It works in the browser for structure drawing, reaction sketching, SMILES workflows, 3D viewing, and exports.

Is MolDraw good for coursework and reports? Yes, especially with its export and readability-focused workflow.

Can MolDraw support naming workflows? Yes, for many compounds via integrated/public data, with optional advanced fallback if required.

Free Chemistry Tools and Calculators

<https://www.moldraw.com/blog/free-chemistry-tools-and-calculators.html>

Free chemistry tools and calculators by MolDraw: mass spectrum predictor, XYZ/Gaussian to 2D structure, name to structure, formula to structure, SMILES converters, formula and mass tools, grams to moles, percent yield, pKa, Lipinski, druglikeness, LogP, TPSA, Lewis structures, TLC, periodic table, and molecule utilities.

MolDraw includes a growing tools hub for chemistry students, educators, researchers, and lab teams. This guide gathers the most useful converters, calculators, structure tools and teaching tools on one page, so you can find the right one quickly.

Published: 6 Jun 2026 · Category: Tools · Publisher: Scidart Academy

Overview

Use the [MolDraw Tools Hub](#) when you need quick chemistry utilities without leaving the browser. The tools are grouped around common workflows: converting identifiers, preparing solutions, drawing structures, balancing equations, making TLC diagrams, and checking [periodic table](#) data.

Short answer: MolDraw tools cover chemistry converters, concentration calculators, structure utilities, periodic table lookup, TLC diagrams, and file-format helpers for everyday chemistry work. For the full linked list of every tool, see the [complete MolDraw tools guide](#).

Chemistry Converters

Converter pages help move between common chemical identifiers and file formats. They are useful when a database, notebook, docking workflow, or drawing tool expects a specific format.

SMILES and structure converters

Convert between [SMILES](#), 2D structures, XYZ/Gaussian coordinates, MOL, SDF, MOL2, PDB, and PDBQT formats.

[SMILES to structure](#) [SMILES to 3D XYZ / Gaussian to 2D](#) [SMILES to MOL](#) [SMILES to SDF](#) [SMILES to PDB](#) [SMILES to PDBQT](#)

Identifier converters

Resolve and convert InChI, InChIKey, [IUPAC](#), CID, compound names, formulas, and SMILES identifiers.

[Name to structure](#) [Formula to structure](#) [search SMILES to InChI](#) [SMILES to InChIKey](#) [InChI to SMILES](#) [InChIKey to SMILES](#) [IUPAC to SMILES](#) [SMILES to IUPAC](#) [CID to SMILES](#)

Chemistry Calculators

Calculator tools support routine classroom and wet-lab calculations such as molarity, molality, dilution, formula mass, stoichiometry, druglikeness property checks, and solution preparation.

Formula and mass tool cluster

Use these tools when you need molecular formula, [molecular weight](#), molar mass, monoisotopic exact mass, or isotope pattern prediction from a formula or SMILES string.

[Formula and mass tools](#) [Molecular weight calculator](#) [SMILES to molecular formula](#) [SMILES to molecular weight](#) [Exact mass calculator](#) [Mass spectrum predictor](#) [Grams to moles calculator](#) [Formula to structure](#) [search Molarity calculator](#) [Molality calculator](#) [Dilution calculator](#) [Solution preparation calculator](#) [Chemical equation balancer](#) [Limiting reagent calculator](#) [Percent yield calculator](#) [pH calculator](#) [pKa calculator](#)

Druglikeness and property calculators

Use these pages for early medicinal chemistry triage from SMILES or compound names: Lipinski Rule of Five, combined druglikeness, LogP, and TPSA.

[Lipinski rule calculator](#) [Druglikeness calculator](#) [LogP calculator](#) [TPSA calculator](#)

Drawing and Structure Tools

The main [MolDraw editor](#) is the fastest route for drawing molecules, visualizing 3D structures, and exporting chemistry formats. Use the [chemical reaction drawer](#) when you need to draw chemical reactions online with reactants, products, arrows, reagents, and conditions. The linked tools support format conversion, structure lookup, XYZ to SMILES conversion, and downstream workflows.

[MolDraw editor](#) [Chemical reaction drawer](#) [Tools hub](#) [Free chemistry tools directory](#) [Lewis structure generator](#) [XYZ to SMILES converter](#) [Protein viewer](#) [Molecule reference pages](#) [Reaction guide pages](#)

Learning and Classroom Tools

MolDraw also includes teaching-friendly pages for chemical structure drawing, reaction examples, TLC diagrams, and periodic table lookup.

[TLC diagram tool](#) [Interactive periodic table](#) [MolDraw course](#) [How to add lone pairs](#) [Chemical drawing guide](#) [Chemistry drawing guide](#)

FAQ

What is the best starting point?

Start with the [Tools Hub](#) for browsing, or open the [MolDraw editor](#) if you already have a molecule to draw or paste.

Are these tools free?

Yes. MolDraw's core browser-based tools and calculators are free to use.

Which tool should I use for a molecule identifier?

Use SMILES, InChI, InChIKey, IUPAC, and CID converter pages depending on the identifier you have and the format you need.

How to Add Lone Pairs in MolDraw

<https://www.moldraw.com/blog/how-to-add-lone-pair-in-moldraw.html>

Add lone pairs in MolDraw one click at a time, fill a whole molecule at once, switch between dots and lines, move or remove pairs, and use them with curved arrows and Lewis structures.

Published: 12 Mar 2026 • Updated: 15 Oct 2026 • Author: Scidart Academy

Short answer

Short answer: Pick the **Lone pair** tool in the left toolbar and click the centre of an atom. Each click adds one pair. When the atom is full, the next clicks take pairs off again. To fill a whole molecule in one step, open the tool's menu and choose **Add all lone pairs**.

Quick steps

1. Draw your structure, for example water as H-O-H.
2. Click the **Lone pair** tool (the icon with two dots) in the left toolbar, next to the charge tools.
3. Click the centre of the oxygen atom. A pair appears in the largest free space between the bonds.
4. Click again to add the second pair. Stop when you have the number you need.
5. To do every atom at once, click the Lone pair button a second time (or its small arrow) to open the menu, then choose **Add all lone pairs**. Select some atoms first if you only want pairs on those atoms.

When the pointer is over an existing pair, the pair lights up. A click there picks up that pair so you can move it. To add a pair, click the middle of the atom.

Every option in the lone pair tool

The Lone pair button has a menu. Click the button once to choose the tool. Click it again, or click its small arrow, to open the menu. On a touch screen, press and hold the button. The menu holds these options, in this order:

Lone pair	The click tool. Click an atom's centre to add one pair. Clicks keep adding until the atom is full. After that, each click removes one pair until none are left, and then clicks add again. Shift-click or Alt-click always removes one pair.
Free radical	Click an atom to add one unpaired electron (a single dot). Click the atom again, or click the dot, to remove it. The Erase tool removes it too.
Dots (classic)	Draws each pair as two dots. This becomes the style for new pairs. Pairs on the selected atoms change to dots. With nothing selected, every pair in the drawing changes.
Line (bar)	Draws each pair as a short bar, as many textbooks do. It works the same way as Dots: new pairs use it, and existing pairs in the selection (or the whole drawing) switch.
Add one lone pair to all	Adds a single pair to every atom that still has room. Run it again to add the next pair. It skips hydrogen and neutral carbon. With atoms selected, it only works on those atoms.
Add all lone pairs	Fills every atom to its maximum in one step. It skips hydrogen and neutral carbon, but a charged carbon, such as a carbanion, gets its pair. With atoms selected, it only fills those atoms.
Remove lone pairs	Removes every lone pair from the selected atoms. With nothing selected, it clears the whole drawing. Radical dots stay.

You can reach some of these from other places too:

- **Right-click menu:** right-click an atom or a selection and choose **Add all lone pairs**. When there are pairs to remove, you also see **Remove lone pairs** (with a selection) or **Remove all lone pairs** (without one).
- **Touch menu:** select atoms that have pairs and choose **Remove lone pairs** from the quick menu.
- **Settings:** Settings > General > Drawing > **Lone pair style** sets Dots or Line for new pairs. It does not change pairs you have already drawn. Use the tool menu for that.

The Lone pair tool has no keyboard shortcut. Undo (Ctrl+Z, or ⌘+Z on a Mac) reverses any of these actions.

Moving and removing pairs

Move a pair

Drag a pair with the Lone pair tool or the Select tool. The pair moves around its atom and stays where you let go. The other pairs on that atom do not move. Running Cleanup puts pairs back into the gaps between bonds but keeps their style.

Remove one pair

- With the Lone pair tool, Shift-click or Alt-click the atom or one of its pairs.
- With the Erase tool, click a pair.
- On a full atom, a plain click with the Lone pair tool also removes a pair.

Remove all pairs

Choose **Remove lone pairs** in the tool menu or the right-click menu. Select atoms first to clear only those.

Lone pairs with charges and radicals

MolDraw will not let you draw more pairs than an atom's electrons allow. It works the number out like this:

1. Start with the element's valence electrons (N has 5, O has 6, Cl has 7).
2. Add one for each negative charge, or take one away for each positive charge.
3. Take away one for each bond, including hydrogens hidden in a label (OH, NH₂, or a lone O for water). A double bond counts as two.
4. Halve what is left and round down. That is the maximum number of pairs.

So set the charge before you add pairs. The [charge tools add +, -, +2, circled charges and δ+ or δ-](#).

Water, H-O-H	6 – 2 bonds = 4 electrons, so oxygen gets 2 pairs .
Ammonia, NH₃	5 – 3 bonds = 2 electrons, so nitrogen gets 1 pair .
Chloride, Cl⁻	7 + 1 for the charge = 8 electrons, so chlorine gets 4 pairs .
Hydroxide, HO⁻	6 + 1 – 1 bond = 6 electrons, so oxygen gets 3 pairs .
Hydronium, H₃O⁺	6 – 1 – 3 bonds = 2 electrons, so oxygen gets 1 pair .
Ammonium, NH₄⁺	5 – 1 – 4 bonds = 0, so nitrogen gets no pairs . The atom flashes red if you click it.
Carbonyl oxygen, C=O	6 – 2 (one double bond) = 4 electrons, so oxygen gets 2 pairs .

Set the charge first. A negative charge makes room for another pair, so add it before the pairs. If you change the charge later, MolDraw removes any pairs that no longer fit.

Radicals. When an odd number of electrons is left, one electron cannot form a pair. MolDraw rounds down, so draw that last electron as a single dot with **Free radical**. For the hydroxyl radical drawn as O-H: 6 – 1 = 5 electrons, which is 2 pairs and one dot. The **Radical cation (•+)** and **Radical anion (•-)** tools in the  charge menu set the dot and the charge in one click.

Using lone pairs with curved arrows

Lone pairs are where many mechanism arrows begin. To draw one:

1. Add the lone pairs first.
2. Open the reaction arrow menu and pick **Electron flow (2e⁻)** for a pair of electrons or **Fishhook (1e⁻)** for one electron. Both are in the Mechanism group.
3. Start the arrow on a lone pair. The tail attaches to the pair, and a highlight shows what it has snapped to.
4. End the arrow on an atom or a bond. The head snaps there.

An attached arrow moves with the molecule when you drag or tidy it. Hold Alt while drawing to place an end freely. To turn snapping off, go to Settings > General > Canvas > **Snap curved arrows**. It is on by default.

Lewis structure view and free sketch mode for teaching

Two settings under Settings > General > Teaching change how lone pairs behave.

Structure display: Lewis structure

Set **Structure display** to **Lewis structure**. MolDraw then shows every atom, every hydrogen and the lone pairs as dots, without you adding them. It counts hidden hydrogens and radical dots correctly. Only the view changes: your drawing stays the same, and you can switch back to **Skeletal formula** at any time.

If you place pairs on an atom yourself, MolDraw shows your pairs on that atom instead of the automatic ones. The automatic pairs are not saved in the drawing. To keep pairs in the skeletal view, add them with **Add all lone pairs**.

Free sketch mode: Allow any number of lone pairs

Turn on **Free sketch mode** to draw structures that break the usual rules, for example to show a student's mistake. The option **Allow any number of lone pairs** is then on by default. It lets the click tool put up to four pairs on any atom, whatever its electron count. **Add all lone pairs** and **Add one lone pair to all** still follow the normal electron count.

Two other free sketch options matter here. **No valence correction** means edits, such as changing a charge, never remove pairs. **No automatic hydrogens** means the Lewis view shows only the atoms and pairs you drew. Both are on by default when free sketch mode is on.

Troubleshooting

- **The tool will not add another pair.** The atom is at its maximum. Check the charge and the bonds. For example, chloride needs its –1 charge before it can take a fourth pair.
- **A click removes a pair instead of adding one.** The atom was full, so the tool is now counting down. Keep clicking until the pairs are gone and it adds again. Also check that you are not holding Shift or Alt.

- **The atom flashes red.** There is no room for a pair at all, as on the nitrogen of NH_4^+ , or you tried to remove a pair from an atom that has none.
- **A pair moved when I wanted to add one.** You clicked on or next to an existing pair, which picks it up. Click the exact centre of the atom instead. Zoom in on crowded structures.
- **Add all lone pairs skipped a carbon.** Neutral carbon is skipped on purpose. A charged carbon gets its pairs.
- **Pairs vanished after I changed a charge.** MolDraw removed pairs that no longer fit. In free sketch mode with No valence correction, they stay.
- **A curved arrow will not attach to a pair.** Check that Snap curved arrows is on and that you are not holding Alt.

FAQ

How do I add lone pairs in MolDraw?

Choose the Lone pair tool in the left toolbar and click the centre of an atom. Each click adds one pair. To fill every atom at once, open the tool's menu and choose Add all lone pairs.

Why can't I add another lone pair to an atom?

The atom already has as many pairs as its electrons allow. MolDraw works this out from the element, its charge and the bonds drawn to it. On a full atom, the next click removes a pair instead. Free sketch mode lifts the limit to four pairs.

How do I draw lone pairs as lines instead of dots?

Open the Lone pair tool menu and choose Line (bar). New pairs use lines, and the pairs on the selected atoms change too. With nothing selected, every pair in the drawing changes. Choose Dots (classic) to go back.

How do I remove lone pairs?

With the Lone pair tool, Shift-click or Alt-click an atom to remove one pair. You can also click a pair with the Erase tool. To clear them all, choose Remove lone pairs in the tool menu or in the right-click menu.

Can a curved arrow start from a lone pair?

Yes. Pick Electron flow ($2e^-$) or Fishhook ($1e^-$) in the arrow menu and start the arrow on a lone pair. The tail attaches to the pair and moves with the molecule. Hold Alt to place an end freely.

How to Turn On the Grid in MolDraw (Interactive Demo)

<https://www.moldraw.com/blog/how-to-turn-on-the-grid-in-moldraw.html>

Turn on the canvas grid in MolDraw in one click: the top-bar grid button, Settings, or Ctrl+K. Plus Snap to grid. Follow along with an interactive step-by-step demo.

Published: 15 Oct 2026 • Author: Scidart Academy • 1 minute

A background grid makes it easier to line up rings, chains, reaction arrows and labels. In MolDraw it takes one click. Watch the demo below, or use the steps under it. Press **Pause** or the arrows to go at your own pace, or press **Try it yourself** to do the same steps in the real editor.

Way 1: the grid button (computer)

1. Open the [MolDraw editor](#).
2. In the top bar, next to the theme switch, find the **grid** button. Its tooltip says **Show canvas grid**.
3. Click it. A light grid appears behind your drawing. Click it again to hide the grid.

Way 2: Settings (computer, phone and tablet)

1. Click the **gear** in the toolbar to open **Settings**. On a phone or tablet, tap the gear at the top.
2. In **General**, find the **Canvas** group.
3. Switch on **Show grid**. The top-bar button and this switch are the same setting.

Snap to grid

In the same **Canvas** group, switch on **Snap to grid**. Molecules and reaction arrows you drag then land on the grid, so schemes line up neatly. Hold Shift while dragging to move something freely.

Way 3: the command palette

1. Press Ctrl + K (⌘ + K on a Mac).
2. Type **grid**.
3. Press Enter on **Show or hide grid**.

The grid is only a guide on the canvas. Exported PNG, SVG and PDF files, and copies you paste into Word or PowerPoint, stay clean.

Questions

Does MolDraw remember the grid setting?

Yes. It is saved in your browser and applies the next time you open MolDraw.

How do I turn on the grid on a phone or tablet?

Tap the gear at the top to open Settings, then switch on **Show grid** under **Canvas**. The top-bar grid button is on larger screens only. The demo above shows the phone steps when you open this page on a phone or tablet.

Read and Compare IR Spectra in Your Browser

<https://www.moldraw.com/blog/ir-spectrum-viewer-guide.html>

A practical guide to the free MolDraw IR viewer: open JCAMP-DX, CSV or SPC files, switch %T and absorbance, correct the baseline, pick peaks, see likely functional groups and overlay two spectra.

Published: 15 Oct 2026 · Author: Scidart Academy · Reading time: ~6 min

Short answer: Open the free [MolDraw IR viewer](#) and drop in a JCAMP-DX, CSV/TXT or SPC infrared file. Switch between %T and absorbance, correct a sloping baseline, pick peaks and read the likely functional group for each one. You can overlay a second spectrum and export a PNG or CSV. The file is read in your browser and is not uploaded.

Try the IR viewer here

Click to load the live viewer in this page, or [open the full IR viewer](#). Your files stay on your device.

Why use a browser IR viewer?

IR is often the quickest check in an organic lab. Did the ester form? Is the starting alcohol gone? The answer is in a few bands, but the spectrum usually arrives as a file from the FTIR software, and that software is only on the instrument PC.

A browser viewer lets you open that file anywhere, find the peaks and see which groups they fit. You can also put two spectra on one plot to see what changed during a reaction.

What an IR spectrum tells you

Bonds absorb infrared light at frequencies that depend on bond strength and atom mass. The x axis is wavenumber in cm^{-1} , drawn from high to low.

%T and absorbance show the same data. Transmittance T is the fraction of light that passes through. Absorbance is $A = -\log_{10}(T)$. In %T, bands point down. In absorbance, they point up, and band height scales with concentration (Beer-Lambert law). That makes absorbance the better choice for comparing intensities.

Key regions to learn first:

- O-H: a broad band near $3200\text{--}3550\text{ cm}^{-1}$ in alcohols. Carboxylic acids show a very broad O-H that runs from about 3300 down to 2500 cm^{-1} .
- C-H: just below 3000 cm^{-1} for sp^3 carbons, just above 3000 cm^{-1} for alkene and aromatic C-H.
- $\text{C}\equiv\text{N}$ and $\text{C}\equiv\text{C}$: near $2100\text{--}2260\text{ cm}^{-1}$, where little else appears.
- $\text{C}=\text{O}$: a strong band near $1650\text{--}1800\text{ cm}^{-1}$. Esters sit near $1735\text{--}1750$, ketones near 1715 and amides lower, near $1650\text{--}1690$.
- C-O: strong bands near $1000\text{--}1300\text{ cm}^{-1}$ in alcohols, ethers and esters.

Below about 1500 cm^{-1} is the fingerprint region. It is unique to each compound but hard to assign band by band.

Bonds that barely change the dipole, such as the $\text{C}=\text{C}$ of a symmetric alkene, give weak IR bands or none. They are often strong in Raman, so when an expected band is missing here, [clean up and read a Raman spectrum](#) of the same sample.

Which files it opens

JCAMP-DX	.jdx, .dx or .jcamp files, including compressed data.
CSV or TXT	Two columns: wavenumber and intensity.
SPC	Thermo/Galactic SPC in the common new format. Old-format and multi-x SPC files are not supported; save those as JCAMP-DX or CSV.

The viewer works out whether your y values are %T, transmittance (0-1) or absorbance. An x axis in micrometres is changed to cm^{-1} .

How to work through a spectrum

- Press **Open IR file** or drop the file on the box. To practise, press **Ethanol** or **Benzoic acid**.
- Choose **%T** or **Absorbance** for the y axis.
- If the background slopes or curves, tick **Baseline correction**. The plot is then labelled Baseline corrected.
- Move the **Threshold** slider until the real bands are picked and the noise is not, then press **Pick peaks**. Choose **Add peak** to add a weak band by hand.
- Read the peak table. Each row gives the wavenumber, strength, best match with its usual range and reason, and other options. Tap a row to shade its band on the plot.

- To compare, press **Open 2nd file** or pick from **or an example....** Press **Swap** to make the second trace the main one.
- Export with **Export PNG**, **Export CSV** or **Peak list CSV**.

What the viewer does

Y axis	%T or absorbance, converted with $A = -\log_{10}(T)$.
Baseline	Rubber-band baseline fitted in absorbance and subtracted.
Peaks	Automatic picking with a threshold, Add peak by tapping, and strength marked s, m or w.
Groups	Best match and other options for each peak from the same correlation table as the IR spectroscopy chart . Matches that fail a whole-spectrum check are marked possible. A summary lists the groups that look present.
Compare	Overlay a second file or example in a different colour, Swap, or Remove 2nd.
Export	PNG of the plot, CSV of the data in the current y mode, and a peak list CSV with assignments.

Ways to use it in class and in the lab

- Teaching labs:** after an esterification, students open their product and check for an ester C=O near 1740 cm^{-1} and a strong C-O band. The **Ethyl acetate** example shows what to look for.
- Reaction checks:** overlay product and starting material. A lost O-H band or a new C=O band is easy to see on one plot.
- Teaching group frequencies:** load **Ethanol**, **Acetone** and **Benzoic acid** in turn to compare an alcohol, a ketone and a carboxylic acid.
- Reports:** export a PNG and the peak list CSV for a results table.

Tips and limits

- Group hints are a starting point, not an assignment. Check each one against the structure you expect.
- A low threshold picks noise and water vapour bands. Raise it, then add weak bands you trust by hand.
- Baseline correction changes band heights. Say so if you report a corrected spectrum.
- For SPC files with several subfiles, only the first is read.
- IR alone rarely proves a structure. Use it with NMR and mass spectra.

New to IR? Our guide on [how to read an IR spectrum](#) walks through each region with examples.

Questions and answers

Should I show %T or absorbance in a report?

Both are common. Organic chemistry reports often use %T, with peaks pointing down. Absorbance is better when you compare band heights, because it scales with concentration. Label the axis so readers know which one you used.

Will the viewer tell me what my compound is?

No. It suggests a functional group for each peak and checks those groups against the rest of the spectrum. It does not name compounds. Use NMR and mass spectra to work out a structure.

Why is the region below 1500 cm^{-1} hard to assign?

This fingerprint region holds many overlapping bending and skeletal bands. It is very useful for matching a sample to a known reference, but single bands there rarely prove a functional group on their own.

How can I show that a reaction worked?

Open the product as the main spectrum and the starting material under Compare with. Look for bands that appear or disappear, such as a new C=O stretch near 1700 cm^{-1} after an alcohol is oxidised to a ketone.

Ketcher Online Molecule Editor Guide | Chemical Structure Drawing

<https://www.moldraw.com/blog/ketcher-online-molecule-editor-guide.html>

Detailed Ketcher guide for chemistry students and researchers: what Ketcher is, common molecule drawing workflows, file formats, limits, alternatives, and browser-based structure editing tips.

Ketcher is one of the best-known names in browser-based chemical structure editing. This guide explains what Ketcher is, what a chemical structure editor should do, which file formats matter, and how to choose a practical drawing workflow for class, research, or computational chemistry.

Published: 11 Jun 2026 · Category: Drawing guides · Publisher: Scidart Academy

Overview

You probably came to Ketcher because you want a fast way to draw molecules online. The task is often simple: sketch a structure, fix atoms and bonds, copy a [SMILES](#) string, export an image, or prepare a molecule for another chemistry tool.

Short answer: Ketcher is an open-source chemical structure editor for drawing molecules in a web browser. If you need a free browser editor to draw, view, search and export molecules, you can also try [MolDraw](#).

What Is Ketcher?

Ketcher is an open-source chemical structure editor created for drawing and editing molecular structures in a web environment. It is commonly discussed in the context of molecule sketchers, cheminformatics interfaces, ELN systems, database search forms, and chemistry web apps.

A Ketcher-style editor normally focuses on precise 2D chemical drawing rather than artistic illustration. The main goal is to create chemically meaningful structures that can be converted into machine-readable formats such as SMILES, MOL, or [reaction](#) formats.

Why chemists use Ketcher

- They need a free molecule editor that works in a browser.
- They want to draw a compound and copy SMILES or MOL data.
- They need reaction sketching for organic chemistry workflows.
- They want to compare Ketcher with ChemDraw, Marvin and newer browser tools.
- They want a quick editor for teaching, assignments, lab notes, or database lookup.

How an Online Molecule Editor Workflow Works

A good online molecule editor should let users move from a rough chemical idea to a usable digital structure without installing desktop software. The typical workflow is:

1. Draw atoms, bonds, rings, charges, stereochemistry, and functional groups.
2. Clean up the layout so the structure is readable.
3. Generate or copy a chemical identifier such as SMILES or InChI.
4. Export an image or chemistry file for reports, slides, notebooks, or downstream tools.
5. Optionally view the structure in 3D or run related converters.

If your goal is not to study Ketcher itself but to draw chemistry quickly, open [MolDraw](#) and start with a structure, name search, SMILES, or file export workflow.

Important Features in a Ketcher-Style Editor

2D structure drawing

Atoms, single/double/triple bonds, rings, charges, aromatic structures, templates, and stereochemical wedges are the foundation of any serious molecule editor.

Identifier support

SMILES, InChI, InChIKey, common names, and [IUPAC](#) workflows help connect drawings to databases and computational tools.

Export formats

Useful editors support image export plus chemistry formats such as MOL, SDF, RXN, PDB, and sometimes docking or quantum chemistry files.

Browser convenience

The main advantage of an online editor is speed: open the page, draw, copy, export, and continue without license setup or desktop installation.

Formats People Use With Ketcher and Online Editors

Chemical drawing is most useful when the structure can leave the editor in a format another tool understands. These are the common formats users should know:

Format	Best use
SMILES	Compact molecule identifiers for databases, search, scripts, and quick sharing.
MOL / SDF	Structure files with atom and bond blocks, useful for cheminformatics and batch workflows.
RXN	Reaction structures with reactants, agents, and products.
SVG / PNG	Images for presentations, papers, reports, and teaching slides.
PDB / PDBQT	3D coordinate and docking workflows, especially for structural biology and docking preparation.

[SMILES to structure](#) [SMILES to IUPAC](#) [SMILES to SDF](#) [PDB to PDBQT](#) [Interactive periodic table](#)

Ketcher Alternatives and Browser Drawing Options

Ketcher is not the only way to draw chemistry online. Depending on your task, you can also use free chemistry drawing software, ChemDraw alternatives, structure converters, molecule viewers, or lightweight browser editors.

MolDraw is useful when you want an online structure drawing workspace with integrated 3D viewing, PubChem-style name search, copy/export options, molecule references, reaction guides, and chemistry converters.

If you need a drawing box inside your own page, course or app without hosting an editor, you can [embed the MolDraw editor with one iframe](#).

[Open MolDraw editor](#) [Free chemical drawing software](#) [ChemDraw alternative guide](#) [Molecule pages](#) [Reaction guides](#) [Tools hub](#)

Ketcher FAQ

What is Ketcher used for?

Ketcher is used for drawing and editing chemical structures, reactions, atoms, bonds, stereochemistry, templates, and structure files in web-based chemistry workflows.

Is Ketcher the same as ChemDraw?

No. Ketcher and ChemDraw are different tools. ChemDraw is a commercial desktop suite, while Ketcher is known as an open-source chemical structure editor for web workflows.

Can I draw molecules online without installing software?

Yes. Browser tools such as [MolDraw](#) let users draw molecules online, view structures, use converters, and export common chemistry formats without installing a desktop program.

What should I use if I need an editor right now?

If your immediate goal is to draw or edit a molecule, open the [MolDraw editor](#). If your goal is format conversion, use the [MolDraw Tools Hub](#).

chemfig Mechanism Samples: Multi-Step, Curly Arrows and Radical Fish-Hooks

<https://www.moldraw.com/blog/chemfig-mechanism-samples.html>

Five worked chemfig examples with `\chemmove` curly arrows and fish-hooks: radical chlorination, anti-Markovnikov HBr addition, aldol, E1 and aromatic bromination. Download each `.tex` file, see the compiled PDF, and edit it in MolDraw.

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Short answer: below are five complete mechanisms written in chemfig: two radical chain reactions drawn with one-electron **fish-hooks** and three polar mechanisms drawn with two-electron **curly arrows**. Each one is a `.tex` file you can download and compile with pdf_lat_ex (run it twice). To change one, paste the file onto the [MolDraw canvas](#), edit it with the mouse, and choose **Download → chemfig (.tex)**.

The five samples

Radical chlorination of methane	Initiation, two propagation steps and termination, under step headings. Homolysis, fish-hooks that meet in a new bond. radical-chlorination-of-methane.tex
Anti-Markovnikov addition of HBr	The peroxide effect in four steps: peroxide homolysis, bromine atom formation, addition to propene and H abstraction. Radical dots on skeletal carbons. anti-markovnikov-hbr-addition.tex
Base-catalysed aldol addition	Enolate formation (equilibrium), C-C bond formation and protonation. Arrows from charges and π bonds. base-catalysed-aldol-addition.tex
E1 dehydration of tert-butanol	One scheme that wraps over four rows, with conditions over each arrow and a carbocation. e1-dehydration-of-tert-butanol.tex
Bromination of benzene	Electrophilic aromatic substitution through the σ -complex, with a catalyst over the arrow. bromination-of-benzene.tex

Each step below has three parts: its chemfig code (use the **Copy** button), the PDF that pdf_lat_ex makes from that code, and the drawing MolDraw makes when you paste the same code. Both pictures are made from exactly the code shown, so you can check that a paste gives you the layout, spacing and curly arrows of the PDF.

How curly arrows are written in chemfig

chemfig draws arrows between atoms with TikZ, in three parts:

1. **Name the ends.** Put `@{a1}` in front of an atom, or inside a bond's options (`-[@{b1}:0]`), to give it a name.
2. **Draw in `\chemmove`.** After the scheme, `\chemmove{ \draw[...] (a1) to[bend left=50] (a2); }` draws the arrow from one name to the other.
3. **Compile twice.** chemfig saves the positions of the named atoms in the first run and uses them in the second.

The samples use these rules, which match how the arrows look on the MolDraw canvas:

Two electrons	A full arrow head: <code>-\Stealth[length=4pt,inset=1.5pt]</code> .
One electron	A fish-hook, which is half an arrow head: <code>-\Straight Barb[left,length=4pt]</code> . <code>[left]</code> or <code>[right]</code> keeps only the barb on the outside of the curve.
Where the tail starts	On the lone pair, the negative charge, the radical dot or the middle of the bond that gives the electrons. <code>[shift={(...em,...em)}]</code> moves the tail from the atom's centre to that spot.

Where the head stops	Just short of the atom that receives the electrons, or between two atoms when a new bond forms.
Scale	<code>\setchemfig{atom sep=2.5em, ...}</code> sets the bond length. Every shift in em is measured against it, so keep the line when you copy code.
Curve	<code>bend left / bend right</code> with an angle, plus looseness for deep curves. The angle is relative to the line between the ends, so the curve keeps its shape if chemfig spaces the scheme differently from the canvas.

All five files load the same two lines, which you also need if you copy the code into your own document:

```
\usepackage{chemfig}
\usetikzlibrary{arrows.meta,decorations.pathmorphing}
```

1. Radical chlorination of methane

The standard first example of a radical chain reaction, in four steps:

- **Initiation:** light breaks the Cl-Cl bond evenly (homolysis). Two fish-hooks leave the bond, one to each chlorine.
- **Propagation 1:** a chlorine atom takes a hydrogen from methane. One electron from Cl• and one from the C-H bond form the new H-Cl bond; the other C-H electron stays on carbon as the methyl radical.
- **Propagation 2:** the methyl radical takes a chlorine atom from Cl₂ and gives back Cl•, which starts the cycle again.
- **Termination:** two radicals pair up, here CH₃• and Cl•.

Download [radical-chlorination-of-methane.tex](#)

Each step is its own `\schemestart ... \schemestop`. The termination step shows the part that is hardest to write by hand: two fish-hooks that meet in the middle of the bond they make.

Initiation

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}Cl-[@{b1}:0]@{a2}Cl}
\arrow{->[h$\nu$]}
\chemfig{\charge{90=\.}{Cl}}
\+
\chemfig{\charge{90=\.}{Cl}}
\schemestop
\chemmove{
\draw[-{Straight Barb[left,length=4pt]}]([shift={{(0.25em,-0.27em)}}b1] to[bend left=77,looseness=1.4] ([shift={{(0.23em,-0.63em)}}a1];
\draw[-{Straight Barb[left,length=4pt]}]([shift={{(-0.25em,0.27em)}}b1] to[bend left=77,looseness=1.4] ([shift={{(-0.23em,0.63em)}}a2];
}
```

chemfig, compiled with pdf_latex

MolDraw, after pasting the same code

Propagation 1: hydrogen abstraction

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}\charge{90=\.}{Cl}}
\+
\chemfig{@{a2}H-[@{b1}:0]@{a3}CH_3}
\arrow{->}
\chemfig{HCl}
\+
\chemfig{\charge{90=\.}{C}H_3}
\schemestop
\chemmove{
\path (a2) -- (a1) coordinate[pos=0.5] (m1);
\draw[-{Straight Barb[left,length=4pt]}]([shift={{(0em,1.71em)}}a1] to[bend left=65,looseness=1.2] ([shift={{(0em,1.64em)}}m1];
\path (a2) -- (a1) coordinate[pos=0.5] (m2);
\draw[-{Straight Barb[left,length=4pt]}]([shift={{(0em,-0.33em)}}b1] to[bend left=57,looseness=1.1] ([shift={{(0em,-1.64em)}}m2];
\draw[-{Straight Barb[left,length=4pt]}]([shift={{(-0.45em,0.33em)}}b1] to[bend left=65,looseness=1.2] ([shift={{(-0.83em,0.78em)}}a3];
}
```

chemfig, compiled with pdf_latex

MolDraw, after pasting the same code

Propagation 2: chlorine transfer

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}\charge{90=\.}{C}H_3}
\+
\chemfig{@{a2}Cl-[@{b1}:0]@{a3}Cl}
\arrow{->}
\chemfig{H_3C-[:0]Cl}
\+
\chemfig{\charge{90=\.}{Cl}}
\schemestop
\chemmove{
\path (a2) -- (a1) coordinate[pos=0.5] (m1);
```

```
\draw[-{Straight Barb[left,length=4pt]}]([shift={(-0.55em,1.36em)})a1] to[bend left=57,looseness=1.1] ([shift={(0em,0.87em)})m1];
\path (a2) -- (a1) coordinate[pos=0.5] (m2);
\draw[-{Straight Barb[left,length=4pt]}]([shift={(0em,-0.27em)})b1] to[bend left=57,looseness=1.1] ([shift={(0em,-0.87em)})m2];
\draw[-{Straight Barb[left,length=4pt]}]([shift={(-0.45em,0.27em)})b1] to[bend left=77,looseness=1.4] ([shift={(-0.23em,0.63em)})a3];
}
```

chemfig, compiled with pdf_latex

MolDraw, after pasting the same code

Termination

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}\charge{90=\.}{C}H_3}
\+
\chemfig{@{a2}\charge{90=\.}{Cl}}
\arrow{->}
\chemfig{H_3C-[:0]Cl}
\schemestop
\chemmove{
\path (a2) -- (a1) coordinate[pos=0.58] (m1);
\draw[-{Straight Barb[left,length=4pt]}]([shift={(-0.55em,1.36em)})a1] to[bend left=57,looseness=1.1] ([shift={(0em,0em)})m1];
\path (a1) -- (a2) coordinate[pos=0.5] (m2);
\draw[-{Straight Barb[right,length=4pt]}]([shift={(0em,1.37em)})a2] to[bend right=57,looseness=1.1] ([shift={(0em,1.31em)})m2];
}
```

chemfig, compiled with pdf_latex

MolDraw, after pasting the same code

In the termination code, the `\path ... coordinate` lines make a point between the two radicals. Because it is a fraction of the distance between them, the fish-hooks still meet in the gap if you change `+ sep left` or the bond length. A fixed offset from one atom would miss the gap as soon as the spacing changes.

The radical dots are written with `\charge{90=\.}{Cl}`: a single electron at 90°, above the atom. For $\text{CH}_3\cdot$ the dot goes on the carbon, `\charge{90=\.}{C}H_3`, not on the whole group.

2. Anti-Markovnikov addition of HBr (peroxide effect)

With a peroxide present, HBr adds to propene the "wrong" way round: bromine ends up on the end carbon. The reason is that the chain is carried by $\text{Br}\cdot$, which adds where it leaves the more stable secondary radical.

- **Initiation 1:** di-tert-butyl peroxide splits at the weak O–O bond.
- **Initiation 2:** the tert-butoxyl radical takes H from HBr and frees $\text{Br}\cdot$.
- **Propagation 1:** $\text{Br}\cdot$ adds to the CH_2 end of the $\text{C}=\text{C}$. One π electron goes to the new C–Br bond and the other stays on the middle carbon.
- **Propagation 2:** that secondary radical takes H from HBr, gives 1-bromopropane and makes $\text{Br}\cdot$ again.

[Download anti-markovnikov-hbr-addition.tex](#)

Initiation: peroxide homolysis

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{[-:23](-[:69]@{a2}0-[@{b1}:-3]@{a1}0-[:52](-[:43])(-[:75])(-[:161])(-[:47])-[:133])}
\arrow{->[h$\nu$ or $\Delta$]}[1.3]
\chemfig{\charge{90=\.}{O}(-[:12](-[:36])(-[:82])-[:122])}
\+
\chemfig{\charge{90=\.}{O}(-[:12](-[:36])(-[:82])-[:122])}
\schemestop
\chemmove{
\draw[-{Straight Barb[left,length=4pt]}]([shift={(-0.24em,0.28em)})b1] to[bend left=77,looseness=1.4] ([shift={(-0.23em,0.62em)})a1];
\draw[-{Straight Barb[left,length=4pt]}]([shift={(0.24em,-0.28em)})b1] to[bend left=77,looseness=1.4] ([shift={(0.23em,-0.62em)})a2];
}
```

chemfig, compiled with pdf_latex

MolDraw, after pasting the same code

Initiation: bromine atom formation

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}\charge{90=\.}{O}(-[:12](-[:36])(-[:82]@{a3})-[:122])}
\+
\chemfig{@{a2}H-[@{b1}:0,0.8]@{a4}Br}
\arrow{->}
\chemfig{H0-[:12](-[:36])(-[:82])-[:122]}
\+
\chemfig{\charge{90=\.}{Br}}
\schemestop
\chemmove{
\path (a2) -- (a3) coordinate[pos=0.7] (m1);
\draw[-{Straight Barb[left,length=4pt]}]([shift={(0em,1.36em)})a1] to[bend left=65,looseness=1.2] ([shift={(-0.08em,-0.19em)})m1];
\path (a2) -- (a1) coordinate[pos=0.5] (m2);
\draw[-{Straight Barb[right,length=4pt]}]([shift={(0em,0.27em)})b1] to[bend right=57,looseness=1.1] ([shift={(0em,0em)})m2];
}
```

```
\draw[-{Straight Barb[right,length=4pt]}]([shift={(-0.36em,-0.27em)})b1] to[bend right=77,looseness=1.4] ([shift={(-0.11em,-0.63em)})a4];
}
```

chemfig, compiled with pdflatex

MolDraw, after pasting the same code

Propagation 1: Br• adds to the less substituted carbon

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}\charge{90=\.}{Br}}
\+
\chemfig{@{a2}=[@{b1}:0]{a3}-[: -60]}
\arrow{->}
\chemfig{-[:0]\charge{90=\.}{-[: -60]-[:0]Br}}
\schemestop
\chemmove{
\path (a2) -- (a1) coordinate[pos=0.5] (m1);
\draw[-{Straight Barb[left,length=4pt]}]([shift={ (0em,1.37em)})a1] to[bend left=65,looseness=1.2] ([shift={(-0.12em,0.87em)})m1];
\path (a2) -- (a1) coordinate[pos=0.5] (m2);
\draw[-{Straight Barb[right,length=4pt]}]([shift={ (0em,0.48em)})b1] to[bend right=57,looseness=1.1] ([shift={(-0.12em,0.87em)})m2];
\draw[-{Straight Barb[right,length=4pt]}]([shift={(-0.45em,-0.48em)})b1] to[bend right=65,looseness=1.2] ([shift={(-0.44em,-0.53em)})a3];
}
```

chemfig, compiled with pdflatex

MolDraw, after pasting the same code

Propagation 2: hydrogen abstraction from HBr

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{-[:0]{a1}\charge{90=\.}{-[: -60]-[:0]Br}}
\+
\chemfig{@{a2}H-[@{b1}:0,0.8]{a3}Br}
\arrow{->}
\chemfig{-[:0]-[: -60]-[:0]Br}
\+
\chemfig{\charge{90=\.}{Br}}
\schemestop
\chemmove{
\path (a2) -- (a1) coordinate[pos=0.58] (m1);
\draw[-{Straight Barb[left,length=4pt]}]([shift={ (0em,1.36em)})a1] to[bend left=57,looseness=1.1] ([shift={ (0em,0em)})m1];
\path (a2) -- (a1) coordinate[pos=0.5] (m2);
\draw[-{Straight Barb[right,length=4pt]}]([shift={ (0em,0.27em)})b1] to[bend right=57,looseness=1.1] ([shift={ (0.05em,0.43em)})m2];
\draw[-{Straight Barb[right,length=4pt]}]([shift={(-0.36em,-0.27em)})b1] to[bend right=77,looseness=1.4] ([shift={(-0.11em,-0.63em)})a3];
}
```

chemfig, compiled with pdflatex

MolDraw, after pasting the same code

The radical in propagation 2 sits on a skeletal carbon, which has no letter to hang a dot on. chemfig handles this with `\charge{90=\.}{}`: `\charge` on an empty atom, so the bonds still meet at the vertex.

A fish-hook can start on a bond as well as on a dot. In propagation 1 the arrows start on the C=C bond, named with `[@{b3}:0]`.

3. Base-catalysed aldol addition

A polar mechanism with two-electron arrows, in three steps:

1. Hydroxide removes an α -hydrogen from acetone to give the enolate. This step is an equilibrium (`\arrow{<=>}`).
2. The enolate carbon attacks the carbonyl carbon of acetaldehyde, and the C=O π electrons move onto oxygen.
3. The alkoxide takes a proton from water, giving the β -hydroxy ketone and hydroxide again.

[Download base-catalysed-aldol-addition.tex](#)

1. Enolate formation

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{@{a1}HO^{\scriptstyle -}}
\+
\chemfig{-[:0](-[: -60]{a3}-[@{b1}:0,0.8]{a2}H)=[:60]O}
\arrow{<=>}
\chemfig{-[:0](-[: -60]\charge{300:4pt=\scriptstyle -}{})=[:60]O}
\+
\chemfig{H_2O}
\schemestop
\chemmove{
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={ (1.88em,0em)})a1] to[bend right=47] ([shift={(-0.69em,-0.4em)})a2];
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={ (0.2em,0.27em)})b1] to[bend right=65,looseness=1.2] ([shift={ (0.17em,0.47em)})a3];
}
```

chemfig, compiled with pdflatex

MolDraw, after pasting the same code

2. Nucleophilic addition to the aldehyde

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{-[:0](-[:60]@{a1}\charge{300:4pt=$\scriptstyle-$)}=[:60]O}
\+
\chemfig{@{a3}O=[@{b1}:60]@{a2}-[:0]}
\arrow{->}
\chemfig{O=[[:0](-[:60])]-[:60]-[:0](-[:60])-[:60]O^{\scriptstyle-}}
\schemestop
\chemmove{
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={(-0.39em,1.07em)})a1] to[bend left=57,looseness=1.1] ([shift={(-0.65em,0.38em)})a2];
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={(-0.64em,0.15em)})b1] to[bend left=77,looseness=1.4] ([shift={(-0.64em,0em)})a3];
}
```

chemfig, compiled with pdflatex

MolDraw, after pasting the same code

3. Protonation of the alkoxide

```
\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{O=[:0](-[: -60])-[[:60]-[:0](-[:60])]-[: -60]@{a1}O^{\-}}
\+
\chemfig{@{a3}HO-[@{b1}:90,0.8,2]@{a2}H}
\arrow{->}
\chemfig{O=[:0](-[: -60])-[[:60]-[:0](-[:60])]-[: -60]OH}
\+
\chemfig{HO^{\-}}
\schemestop
\chemmove{
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={ (0.62em,1.07em)}]a1) to[bend left=40] ([shift={ (-0.72em,0.26em)}]a2);
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={ (0.27em,0.36em)}]b1) to[bend left=77,looseness=1.4] ([shift={ (1.01em,0.11em)}]a3);
}
```

chemfig, compiled with pdflatex

MolDraw, after pasting the same code

Every arrow here has a full head. Each step has two arrows: one makes a bond, and one breaks a bond and takes its electrons onto an atom. The second kind starts on the bond (b1) and ends on the atom.

The enolate's negative charge sits on a skeletal carbon. It is written the same way as the radical in sample 2, with \charge on an empty atom, so the bond is not cut short around a "-" label.

4. E1 dehydration of tert-butanol: one scheme over several rows

The first three samples put each step under its own heading. You can also draw the whole mechanism as one continuous scheme that wraps onto new rows, as in many textbooks:

1. The OH group takes a proton from H_3O^+ .
2. Water leaves and gives the tert-butyl cation. This is the slow step.
3. Water removes a proton from the carbon next to C^+ , and the C-H electrons form the C=C bond of 2-methylpropene.

[Download e1-dehydration-of-tert-butanol.tex](#)

In chemfig each row is a separate scheme that begins with its arrow, so the conditions stay with the arrow they belong to:

The whole scheme

```

\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
{\centering\textbf{Acid-catalysed dehydration of tert-butanol (E1)}\par}
\par\bigskip
\vspace{0.9em}
\schemestart
\chemfig{@{a1}H\charge{90=\:, -90=\:}{0}-[: -12](-[: -36])(-[: 82]) -[: -122]}
\+
\chemfig{@{a3}H_20^{+}-[@{b1}:90,0.8,2]@{a2}H}
\schemestop
\par\bigskip
\schemestart
\arrow{->[protonation]}{,1.6}
\chemfig{@{a4}H_20^{+}-[@{b2}:-12](-[: -36])(-[: 82]) -[: -122]}
\+
\chemfig{H_20}
\schemestop
\par\bigskip
\schemestart
\arrow{->[-$\mathscr{H}_2$]$0}[slow]}
\chemfig{-[:0]\charge{120:4pt=\scriptstyle+}{\cdot}(-[@{b4}:-60]-[@{b3}:0,0.8]@{a6}H)-[:60]}
\+
\chemfig{@{a5}H_2\charge{90=\:, -90=\:}{0}}
\schemestop
\par\vspace{1.2em}
\par\bigskip
\schemestart

```

chemfig, compiled with pdflatex
MolDraw, after pasting the same code

Two details worth copying:

- `[,1.6]` makes the arrow 1.6 times its normal length, so the word *protonation* fits above it instead of running into the next structure.
- The carbocation is `\charge{120:4pt=$\scriptstyle+$}`: a small "+" 4 pt from the vertex, in the widest gap between the bonds.

5. Electrophilic bromination of benzene

Benzene's π electrons attack bromine (activated by FeBr_3) to give the σ -complex. Bromide then removes the proton from the sp^3 carbon, and the C-H electrons restore the aromatic ring.

[Download bromination-of-benzene.tex](#)

1. Attack on bromine (σ -complex)

```

\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{?{a} - [:90] = _[@{b1}:30] - [: -30] = _[: -90] - [: -150]?{a, {=}_}}
\+
\chemfig{@{a1}Br - [@{b2}:0]@{a2}Br}
\arrow{->[FeBr$_{3}$]}{,1,1}
\chemfig{?{a} = _[:90] - [:30] ( - [:90]Br) - [: -30]\charge{30:4pt=$\scriptstyle+$}{-} - [: -90] = _[: -150]?{a}}
\+
\chemfig{Br^{ - }}
\schemestop
\chemmove{
\draw[ - {Stealth[length=4pt,inset=1.5pt]}]([shift={(-0.13em,0.23em)})b1] to[bend left=74,looseness=1.34] ([shift={(-0.13em,0.73em)})a1];
\draw[ - {Stealth[length=4pt,inset=1.5pt]}]([shift={(-0.25em,-0.27em)})b2] to[bend right=77,looseness=1.4] ([shift={(-0.23em,-0.63em)})a2];
}

```

chemfig, compiled with pdflatex
MolDraw, after pasting the same code

2. Loss of H^+ restores the ring

```

\setchemfig{atom sep=2.5em, + sep left=0.7em, + sep right=0.7em, compound sep=4em, arrow offset=6pt}
\schemestart
\chemfig{?{a}=[:90]-[:30](-[:90]Br)(-[@{b2}:-30]\charge{30:4pt=$\scriptstyle+$}{-[:90]=[[:150]?{a}]-[@{b1}:30,0.8]@{a2}H}
\+
\chemfig{@{a1}Br^{--}}
\arrow{->}
\chemfig{?{a}[:90]=[[:30](-[:90]Br)-[:30]=[[:90]-[:150]?{a},{=}]}}
\+
\chemfig{HBr}
\schemestop
\chemmove{
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={{(-1.55em,0em)}}a1) to[bend right=51]([shift={{(0.73em,0.13em)}}a2);
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={{(-0.04em,-0.33em)}}b1) to[bend left=51]([shift={{(0.51em,-0.02em)}}b2);
}

```

chemfig, compiled with pdflatex
MolDraw, after pasting the same code

Rings are written with absolute bond angles and hooks (`{[a]}`) rather than `*6(...)`, so each ring has exactly the orientation it has on the canvas and every ring bond can carry an `@{...}` name for an arrow. The subscript in FeBr_3 is typed as `FeBr3` in MolDraw and exported as `FeBr$_{3}$`.

Make your own mechanism

1. Draw the species and reaction arrows in the [MolDraw editor](#), or start from one of these files: open it, copy everything and paste it onto the canvas with **Ctrl+V**.
2. Pick the curly arrow tool. Drag from a lone pair, charge, radical dot or bond to the atom or bond that receives the electrons. For one-electron steps choose **Fishhook (1e⁻)** in the arrow options.
3. Add step headings with the text tool, above each row.
4. Choose **Download → chemfig (.tex)**, or **Copy as chemfig (LaTeX)** to paste the code into your own document.
5. Compile twice.

You can also ask the AI assistant in the editor, for example: *"Draw the radical bromination of toluene at the benzylic position with fish-hook arrows, initiation, propagation and termination under headings."* It draws the steps on the canvas, and you can export them the same way.

When you paste chemfig back in, MolDraw reads which atom or bond each `\chemmove` arrow starts and ends on, whether it has a full head or a fish-hook, the side its bend curves to and how deep the curve is. A head that ends on a `\path ... coordinate` point between two atoms becomes a bond-forming arrow, so fish-hooks meet in the gap again. The spacing comes from `\setchemfig` (atom sep, compound sep, + sep left/right, arrow offset), and text and lines are drawn in a LaTeX-like serif at chemfig's thin line width. MolDraw still fits each arrow to its own rules, so a hand-written `\draw` does not have to be perfect.

Adjusting the exported code by hand

- **Flatter or deeper curve:** change the bend angle (`bend left=40` instead of 57), or remove `looseness`.
- **Curve on the other side:** swap `bend left` and `bend right`. For a fish-hook, swap `[left]` and `[right]` in the tip as well, so the barb stays outside.
- **Move a tail or head:** edit the shift in em. `(0em,1em)` is 1 em above the atom's centre.
- **Where fish-hooks meet:** change `pos=0.58`. 0.5 is exactly half-way between the two atoms.
- **Room above a row:** the `\vspace{...em}` before each scheme leaves space for arrows that bow upward. Make it larger if an arrow touches the heading.

Questions and answers

How do I draw a fish-hook arrow in chemfig?

Name the two ends with `@{...}` and draw the arrow in `\chemmove` with a half arrow tip: `\draw[-{Straight Barb[left,length=4pt]] (a1) to[bend left=50] (a2);` Use `[left]` or `[right]` so the barb sits on the outside of the curve. Load the TikZ library `arrows.meta`.

How do I make two fish-hooks meet in the middle of a new bond?

Make a point between the two atoms with `\path (a1) -- (a2) coordinate[pos=0.5] (m1);` inside `\chemmove`, then end both fish-hooks at `(m1)`. The point moves with the atoms however chemfig spaces the scheme.

How do I put a radical dot on a skeletal carbon in chemfig?

Use `\charge` on an empty atom: `\charge{90=\.}{}`. The bonds still meet at the vertex and the dot sits above it. For a labelled atom write `\charge{90=\.}{Cl}`.

Why are the curly arrows in the wrong place in my PDF?

`\chemmove` uses positions saved in the first LaTeX run. Compile the file a second time.

Can I edit these samples?

Yes. Open the `.tex` file, copy its contents and paste them onto the MolDraw canvas. Change the structures or arrows with the mouse, then download chemfig `(.tex)` again.

Are the samples free to use?

Yes. Use them in notes, problem sets, theses and papers.

chemfig and MolDraw: Paste chemfig, Edit Visually, Export LaTeX

<https://www.moldraw.com/blog/chemfig-latex-moldraw-guide.html>

A guide for chemfig and LaTeX users: paste \chemfig code into MolDraw to see and edit the structure, then download it back as a .tex file that compiles with pdflatex. Works for schemes and curly arrows.

Published: 17 Oct 2026 · Author: Scidart Academy · Reading time: ~9 min

Short answer: Copy your `\chemfig{...}` code (or a whole `\schemestart ... \schemestop` scheme, or the full `.tex` file), open the [MolDraw editor](#) and press **Ctrl+V**. MolDraw draws it, curly arrows included. Edit it with the mouse, then choose **Download → chemfig (.tex)** for a file that compiles with `pdflatex`, or **Copy as chemfig (LaTeX)** for code to paste into your thesis or paper.

Who this is for

chemfig is the standard way to draw molecules inside LaTeX. The output is beautiful and it lives in the same file as your text, but writing it is slow. You type `-[:30]` and `=[::-60]`, compile, look, and adjust an angle. Fixing someone else's chemfig is harder still, and a curly arrow in `\chemmove` can take many attempts.

MolDraw now reads and writes chemfig. You keep chemfig as your format and use a canvas for the drawing:

- **See** what a chemfig snippet draws without compiling.
- **Fix** it with the mouse: move an atom, flip a double bond, add a charge or a curly arrow.
- **Get chemfig back** that compiles with `pdflatex`, with the same angles you see on screen.
- **Start from other formats** (SMILES, MOL, ChemDraw files, a compound name) and get chemfig out.

Everything runs in your browser. Your code is not sent to a server to be converted.

Paste chemfig onto the canvas

A chemfig scheme pasted with Ctrl+V. The names, the arrow text and both curly arrows come through.

1. Copy the code from your editor or Overleaf. A single `\chemfig{...}`, several of them, a `\schemestart ... \schemestop` block or a complete document all work.
2. Open the [MolDraw editor](#), click an empty part of the canvas and press **Ctrl+V** (**Cmd+V** on a Mac). You can also use the **Paste** button or right-click → Paste.
3. The drawing appears selected, beside anything already on the canvas. Drag it where you want it.

Try it with this scheme:

```
\schemestart
\chemname{\chemfig{*6(==--)}{benzene}}
\+
\chemfig{Br-Br}
\arrow{->[FeBr$_3$][CH$_2$Cl$_2$]}
\chemname{\chemfig{*6(==(-Br)-)}{bromobenzene}}
\schemestop
```

MolDraw keeps the bond angles and lengths you wrote, so the drawing has the same shape as your PDF. Labels such as H₃C, NH₂ or CO₂Me, charges, lone pairs from `\lewis` or `\charge`, and `@{name}` nodes all carry over.

Edit it like any drawing

The pasted drawing is a normal MolDraw structure, so every tool works on it:

- drag atoms, or select a group and rotate it;
- hover a bond and press **1**, **2** or **3** to make it single, double or triple, and click a double bond with the double-bond tool to move its second line to the other side;
- add charges, lone pairs and radicals from the toolbar or the right-click menu;
- draw curly arrows and fish-hooks with the arrow tool. They attach to lone pairs, bonds and charges and stay attached when you move atoms;
- edit the text above and below a reaction arrow by double-clicking it.

You also get the chemistry checks that chemfig cannot give you: valence warnings, the formula and mass, SMILES, and a 3D view of each structure.

Export chemfig back to LaTeX

Download → chemfig (.tex), at the end of the Text group.

There are two ways out:

- **Download → chemfig (.tex)** saves a complete, standalone LaTeX file. Compile it on its own to get a PDF of the drawing, or include that PDF in your document with `\includegraphics`.
- **Copy as chemfig (LaTeX)** (in the Copy menu and in the right-click **Copy as** menu) copies only the drawing code, with no `\documentclass`. Paste it straight into your thesis or paper.

For copied code, add these two lines to your preamble once:

```
\usepackage{chemfig}
\usetikzlibrary{arrows.meta,decorations.pathmorphing}
```

If a drawing has curly arrows or polymer brackets, **compile twice**. chemfig draws those from positions it saves in the first run. If you select part of the canvas first, only the selection is exported.

What the exported code looks like

This is the file MolDraw writes for the SN2 scheme in the first screenshot:

```
% Exported from MolDraw – compile with pdflatex / lualatex (twice: arrows and brackets use positions from the first run)
\documentclass[border=22pt,varwidth=60cm]{standalone}
\usepackage{chemfig}
\usetikzlibrary{arrows.meta,decorations.pathmorphing}
\begin{document}
\setchemfig{+ sep left=2em, + sep right=2em, arrow offset=6pt}
{\centering \textbf{SN2 of bromomethane}\par}
\par\bigskip
\schemestart
\chemname[2em]{\chemfig{@{a1}H0^{}}{hydroxide}}
\+
\chemname[2em]{\chemfig{@{a2}-[@{b1}:90]{a3}Br}}{bromomethane}
\arrow{->[SN2][acetone]}
\chemname[2em]{\chemfig{[:90,,,1]OH}}{methanol}
\+
\chemfig{Br^{}}
\schemestop
\chemmove{
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={(1.07em,0.77em)}]a1) to[bend right=47]([shift={(-0.39em,-0.23em)}]a2);
\draw[-{Stealth[length=4pt,inset=1.5pt]}]([shift={(0.21em,-0.36em)}]b1) to[bend right=77]([shift={(0.64em,-0.23em)}]a3);
```

```
}
\end{document}
```

A few things to notice:

- Bonds use **absolute angles** (`-[:90]`), so each bond points the same way as on the canvas. A bond that is not the standard length gets a length factor such as `-[:30,1.2]`.
- Atoms and bonds that a curly arrow touches get **node names** (`@{a1}`, `@{b1}`). `\chemmove` draws each arrow between them, with a bend angle that matches the curve on the canvas.
- Compound names sit under the structures, with room left for curly arrows that bow underneath.
- Ring bonds are closed with hooks (`?[a]`), and each double bond gets `=^` or `=_` so its second line is on the same side as in MolDraw, inside the ring for rings.

An E2 elimination on the canvas (top) and the exported chemfig compiled with pdflatex (bottom).

Get chemfig from SMILES, MOL or ChemDraw files

Because MolDraw reads many formats, it also works as a **converter to chemfig**:

1. Bring the structure in: paste SMILES or InChI, search a compound name in the PubChem box, or open a MOL, SDF, RXN, CDXML or CDX (ChemDraw) file.
2. Tidy it if needed. Clean-up and rotation are in the toolbar.
3. Choose **Download → chemfig (.tex)**.

This is the quickest way to move a set of ChemDraw figures into a LaTeX thesis: open each file and download it as chemfig.

Reaction mechanisms and curly arrows

Curly arrows are the hardest part of chemfig to write by hand. In MolDraw you draw them with the mouse, or ask the AI assistant to draw a mechanism, and the export writes the `@{...}` names and the `\chemmove` block for you.

When you paste chemfig that already has `\chemmove` arrows, MolDraw reads which atoms or bonds each arrow joins and which side its bend curves to. It then places the arrow by its own drawing rules: the tail starts on the lone pair, charge or bond, and the head stops just short of its target. You do not have to copy the exact TikZ curve.

For complete worked examples, see the [chemfig mechanism samples](#): radical chain reactions with fish-hooks and multi-step polar mechanisms, each as a .tex file you can download.

Ask the AI assistant

The chat assistant in the editor knows chemfig. For example, you can ask:

- *"Export this as chemfig."* It returns the code for what is on the canvas.
- *"Draw this: `\chemfig{H_3C-C(=[:60]O)-[: -60]OH}`."* It puts the structure on the canvas.
- *"Draw the mechanism of acid-catalysed ester hydrolysis, then give me the chemfig."*

What carries over in both directions

Each item below is exported, compiled with pdflatex, read back into MolDraw and checked against the original drawing.

Bonds	Single -, double =, triple ~; aromatic rings in Kekulé form; the side of a double bond's second line (<code>=^</code> / <code>=_</code>); wedge and hash bonds with their direction (<code><></code> <code><:</code> <code>>:</code>).
Bond styles	Wavy, bold, dotted and dative bonds, and bond colours, written as TikZ options on the bond.
Atoms	Labels with implicit H, condensed groups (<code>CO_2Me</code> , <code>Ph</code>), charges, circled charges (<code>\oplus</code>), isotopes, D and T, lone pairs and radical dots (<code>\charge</code> , <code>\lewis</code>), atom colours.
Rings	Any ring and fused rings; on import also <code>*6(...)</code> , <code>**6(...)</code> and nested rings.
Schemes	<code>-></code> , <code><-</code> , equilibrium <code><=></code> , half equilibrium <code><-></code> , resonance <code><-></code> , retrosynthesis arrows; conditions above and below on several lines; <code>\+;</code> <code>\chemname</code> ; schemes wrapped onto several rows.
Text	A title above the scheme and notes below it.
Brackets	Transition-state brackets with <code>\chemleft[... \chemright]</code> and polymer repeat units (<code>\polymerdelim</code>).
Curly arrows	Two-electron arrows and one-electron fish-hooks between named atoms and bonds (<code>\chemmove</code>).

When you paste, MolDraw also understands `\definesubmol` with `!{name}`, a starting angle such as `\chemfig{[:30]...}`, invisible bonds (`draw=none`), arrows at an angle such as `\arrow{->}[-90]` (the next compound goes below), `\subscheme`, and colour names such as `red` and `blue`.

What chemfig cannot hold

Some things on a MolDraw canvas have no chemfig form: pasted images, shapes and lab glassware, freehand strokes, orbitals, ring fills and highlights. They are left out of the export, and the hint bar tells you what was left out after each download or copy, so nothing disappears without notice.

Curved or S-shaped scheme arrows become straight chemfig arrows. Text placed beside the drawing (not above or below it) is kept as a % comment in the file.

chemfig quick reference

The pieces of chemfig syntax you will meet most often, and what MolDraw draws for each:

<code>A-B=C-D</code>	Single, double and triple bonds. With no angle, bonds go to the right.
<code>-[2], -[:30], -[:60]</code>	Angle in steps of 45°, an absolute angle, or an angle relative to the previous bond.
<code>-[:30,1.5]</code>	Angle and length factor (1.5 times the normal bond length).
<code><<: >>:</code>	Wedge and hash bonds. < is narrow at the atom you start from.
<code>C(-[2]H)(-[6]H)</code>	Branches in parentheses.
<code>*6(==--==)</code>	A six-membered ring, here benzene. <code>**6(-----)</code> draws a circle inside; MolDraw reads it as a benzene ring with alternating double bonds.
<code>?[a] ... ?[a]</code>	A hook: bonds the two atoms that carry the same letter (closes a ring).
<code>=^, =_</code>	Double bond with the second line on the left or on the right of the direction of travel.
<code>\charge{90=:\:}{0}</code>	A lone pair at 90° on O. \. is a single electron.
<code>@{a1}</code>	Names an atom or bond so \chemmove can draw an arrow to it.
<code>\arrow{->[above] [below]}</code>	A scheme arrow with text above and below.

Troubleshooting

- **Nothing happens when I paste.** The text must contain `\chemfig` or `\schemestart`. Click the canvas first, so the paste goes to the drawing and not to a text box.
- **Curly arrows are in the wrong place in the PDF.** Compile a second time.
- **"I do not know the key /tikz/Stealth".** Add `\usetikzlibrary{arrows.meta,decorations.pathmorphing}` to your preamble.
- **A structure looks squashed after pasting.** If the chemfig puts two atoms on the same spot, MolDraw lays the structure out again and says so in the hint bar. Use the clean-up button to tidy it.
- **"B" or "D" turned into boron or deuterium.** MolDraw reads atom labels as chemistry. Placeholder letters from the chemfig manual are read as elements where one exists.

Questions and answers

Can I convert chemfig code into a drawing?

Yes. Paste `\chemfig{...}` code, a `\schemestart` scheme or a whole .tex file onto the MolDraw canvas. MolDraw reads the bonds, angles, rings, charges, lone pairs, arrows, compound names and `\chemmove` curly arrows and draws them.

Can MolDraw export chemfig code?

Yes. Download → chemfig (.tex) saves a standalone LaTeX file, and Copy as chemfig (LaTeX) copies only the drawing code for your own document. The code compiles with `pdflatex` and `lualatex`.

Which LaTeX packages do I need?

chemfig, plus the TikZ libraries `arrows.meta` and `decorations.pathmorphing`: `\usepackage{chemfig}` and `\usetikzlibrary{arrows.meta,decorations.pathmorphing}`. The downloaded file already contains these lines.

Why are my curly arrows in the wrong place after compiling?

chemfig's `\chemmove` draws curly arrows from positions saved in the first LaTeX run. Compile the file a second time and the arrows land on their atoms and bonds.

Can I turn a ChemDraw or MOL file into chemfig?

Yes. Open the MOL, SDF, CDXML or CDX file in MolDraw, or paste SMILES, then choose Download → chemfig (.tex).

What does not convert to chemfig?

Images, shapes and glassware, freehand strokes, orbitals, ring fills and highlights have no chemfig form. MolDraw lists anything it left out in the hint bar after you download or copy.

Is it free?

Yes. Pasting chemfig and editing it is free in the browser. Downloading files needs a free MolDraw account.

Draw Lab Glassware and Apparatus Setups: The MolDraw Apparatus Library

<https://www.moldraw.com/blog/lab-glassware-apparatus-library-guide.html>

Draw reflux, distillation and filtration setups in your browser. A guide to the free MolDraw apparatus library: 125 pieces, joints that snap together, liquid levels, pouring and bendable tubing.

Published: 15 Oct 2026 · Author: Scidart Academy · Reading time: ~8 min

Short answer: In the [MolDraw editor](#), click **Apparatus** at the right end of the tools row. A library of 125 pieces opens beside the canvas and stays open. Click a card to add it, or drag it onto the canvas. Joints snap together on their own: a condenser fits on a flask neck, and a flask sits on a heating mantle. Use **Tubing** to connect hose barbs with a hose that you can bend. Then download the drawing as PNG, SVG or PDF.

Why draw apparatus in a structure editor?

Lab manuals, theses, slides and exam papers often need a reaction scheme and a picture of the setup. People usually draw the scheme in one program and the glassware in another, or paste in clip art that does not match. The flasks are the wrong size, the joints do not line up and the water lines are straight sticks.

The MolDraw apparatus library keeps everything on one canvas. The glassware is drawn in the same line weight as your structures, it knows where its joints and hose barbs are, and the pieces connect the way real glassware does. You can draw a full reflux or distillation setup in about a minute, next to the reaction that runs in it.

Open the apparatus library

The Apparatus button opens a docked panel that stays open while you add pieces.

1. Open the [editor](#). On a computer, click **Apparatus** (the flask icon) at the right end of the tools row, next to **Image**.
2. The panel docks on the left, beside the tool rail. It stays open while you work, so you can add a flask, a condenser and a heater one after another. Close it with the x in its header or by clicking **Apparatus** again.
3. Type in the search box to find a piece by name, such as “Dean-Stark” or “Büchner”, or pick a category chip.

On a phone, the library opens as a full-screen sheet. The pieces and features are the same.

What is in the library

There are 125 pieces in nine categories:

Flasks & vessels	Round-bottom flasks with one to four necks, pear-shaped, conical, Schlenk and volumetric flasks, beakers, test tubes, jacketed and pressure reactors.
Funnels & filtration	Filter, separatory, dropping and Büchner funnels, Büchner flasks and filtration setups.
Condensers & columns	Straight, Allihn and Dimroth condensers, Vigreux and chromatography columns.
Distillation & rotovap	Distillation heads, receiving flasks, Dean-Stark traps, short-path distillation and a rotary evaporator.
Adapters & closures	Claisen, bent, reducing, vacuum and thermometer adapters, stoppers and septa.
Vacuum, gas & tubing	Schlenk lines, gas bubblers, gas inlet adapters, gas cylinders, vacuum and coolant tubing.
Heating & cooling	Heating mantles, hotplate stirrers, oil, sand, ice and dry-ice baths, chillers.
Stands, clamps & tools	Retort stands, clamps, rings, spatulas, mortar and pestle.
Measuring & analysis	Graduated cylinders, burettes, Pasteur pipettes, thermometers, an analytical balance and TLC chambers.

Hover over a card to see a large preview. The preview also lists the piece's connections: its **joints** (for example the neck of a flask), its **hose barbs** (for example the water inlet and outlet of a condenser) and what it **fits on**.

Line, Premium and Illustrated styles

- **Line** draws clean outlines in the same ink as your structures. It suits exam papers, worksheets and journal figures, and it follows the light or dark theme.
- **Premium** adds soft 3D shading, reflections and glass tint. It suits slides and posters.
- **Illustrated** places full-colour drawings as pictures. They do not snap or hold liquid, but they are useful for instruments that are not in the line set.

You can switch one piece between Line and Premium later in the format panel.

Click or drag to add pieces

- **Click a card** to add the piece. If a glassware piece is selected and one of its openings fits, the new piece goes straight onto it. For example, select a flask and click **Condenser**, and the condenser lands on the flask neck. If nothing is selected, the piece appears in the middle of the visible canvas, and the next one is placed a little offset so pieces do not stack.
- **Drag a card** onto the canvas to drop the piece exactly where you want it. If you drop it near a free joint, it snaps on.
- The new piece is selected after you add it, so the next click on a card builds on top of it. This makes it quick to stack a flask, a Claisen adapter and a condenser.

How joints snap together

While you drag, a green ring shows the joint the piece will snap to.

Each piece knows where its openings are and which way they face. When you drag a piece close to a matching opening, MolDraw lines the two up, turning the piece slightly if needed, and shows a green ring at the joint. Release the mouse to fit it.

Openings	A flask neck, a condenser end or an adapter port connects to another opening that faces it.
Bottoms on seats	The bottom of a flask or beaker sits on a seat: a heating mantle, hotplate stirrer, ring, bath, balance pan or stand platform. A flask never snaps by its bottom onto another flask's neck.
Hose barbs	Barbs do not snap to glass. Connect them with tubing (see below).
Reach	Snapping works within about 20 screen pixels when you drag and 28 when you place a piece, and only if the piece has to turn less than 50°. Zooming in gives finer control.
Turn it off	Hold Alt while you drag to move a piece freely.

Moving a whole selected setup also snaps, but only by sliding it. The setup is never turned, so it stays the way you built it.

Step by step: a reflux setup

The finished reflux setup. Water flows in at the lower barb and out at the upper one.

1. Open **Apparatus** and click **Heating mantle** under Heating & cooling.
2. With the mantle selected, click **Round-bottom flask**. The flask sits in the mantle.
3. With the flask selected, click **Condenser**. It fits on the flask neck.
4. Drag a **Chiller** from the panel to the right of the setup.
5. Click **Tubing** in the panel. Drag from the chiller's outlet to the condenser's *lower* barb, then from the condenser's *upper* barb back to the chiller's inlet. Both ends fit on the barbs, and the tubes become water lines.
6. Select the flask and drag the grip on the liquid surface to set the level. Add the reaction scheme beside it and export.

The same steps build a distillation (flask, distillation head, condenser, receiving flask), a vacuum filtration (Büchner funnel on a Büchner flask, tubing to a vacuum line) or a Dean-Stark setup.

Liquids: level, colour, tilting and pouring

- **Level:** select a vessel and drag the small grip on the liquid surface up or down.
- **Colour and layers:** in the format panel, set the liquid colour and opacity. Add a second layer to show two immiscible liquids, for example in a separatory funnel.
- **Tilting:** turn a vessel with its rotate handle. The liquid surface stays level and the liquid moves to the low side, as it would in a real flask.
- **Pouring:** tip a vessel past its lip and the excess pours out in a straight vertical stream. If another vessel is below, the liquid is added to it.

Tubing: connect hoses and water lines

A selected tube shows its two ends and its curve handles.

Tubes are drawn as smooth curves (cubic Bézier curves) that leave each barb in the direction the barb points, and hang slightly as a real hose does.

1. Click **Tubing** in the apparatus panel, or pick the tubing tool in the draw panel.
2. Drag from one hose barb to another. An end fits on a free barb within reach. An end released away from a barb stays free and shows an open cut end.
3. Select the tube to edit it:
 - Drag an **end** (round handle) to move it to another barb, or away to free it. Filled handles are fitted on a barb.
 - Drag a **curve handle** (diamond) to change how the tube leaves that end.
 - Drag the **body** of the tube to bend the whole curve.
4. In the format panel, choose the style: **rubber** (red vacuum hose), **water** (water line with blue water inside) or **clear**. You can also change the outline colour and the thickness.

Tubes stay attached. When you move, turn, resize or flip a piece, every tube fitted on it follows. If you delete the piece, the tube ends become free.

Customise the look

Select any piece and open the format panel to change:

- the outline colour and line width, or leave the outline to follow the light or dark theme;
- Line or Premium style, glass tint and reflection highlights;
- graduation marks on cylinders, beakers and burettes;
- the liquid colour, opacity, level and a second layer.

Pieces can be resized, turned, flipped, grouped, duplicated (Ctrl-drag) and nudged with the arrow keys, like any other object.

Export and reuse

- **Download** the canvas as PNG for slides, SVG for editing in a vector program, or PDF for print.
- **Copy** the drawing and paste it into a document or presentation.
- Save it as a design to keep editing later. The setup keeps its joints, liquids and tubes.

Tips

- Build from the bottom up: heater, then flask, then adapters and condenser. Each click attaches to the selected piece.
- Zoom in when you fit small pieces such as stoppers and septa.
- Hold **Alt** to place a piece beside a setup without it snapping on.
- Use the Line style for printed exam papers. It prints sharply in black and white.
- Put the scheme and the setup in one drawing. Learn how to draw the scheme in [how to draw benzene, cyclohexane and fused rings](#).

Everything runs in your browser. The apparatus drawings are part of MolDraw and are not fetched from an outside service.

Questions and answers

Is the apparatus library free?

Yes. All 125 line-art pieces, the Premium shading, snapping, liquids and tubing are free in the MolDraw editor. You do not need an account to draw with them.

How do I stop a piece from snapping?

Hold Alt while you drag. The piece then moves freely and does not snap to nearby joints.

Why does my flask not snap onto the condenser?

Joints only snap when the two openings are within reach and nearly lined up. Drag the flask so its neck is close to the bottom of the condenser and turn it upright if it is tilted. Bottoms only sit on seats such as a heating mantle, a hotplate stirrer or a ring.

Do tubes follow the glassware when I move it?

Yes. A tube end that is fitted on a hose barb stays on that barb when you move, turn, resize or flip the piece. A free end stays where you left it.

Can I change the colour of the liquid?

Yes. Select the vessel and use the format panel to set the liquid colour and opacity, or add a second layer for two immiscible liquids. Drag the small grip on the liquid surface to change the level.

Which formats can I export?

Download the drawing as PNG, SVG or PDF, or copy it to paste into slides, a report or a lab manual.

Does it work on a phone or tablet?

Yes. On a phone the library opens as a full-screen sheet instead of the docked panel. Tap a piece to add it, then drag it into place.

Check Isotope Patterns, Adducts and ppm Error in Your Browser

<https://www.moldraw.com/blog/mass-spectrum-viewer-guide.html>

A practical guide to the free MolDraw mass spectrum viewer: open JCAMP-DX, CSV, mzML or mzXML files, overlay the isotope pattern of a formula, check adducts and ppm error, and read neutral losses.

Published: 15 Oct 2026 · Author: Scidart Academy · Reading time: ~6 min

Short answer: Open the free [MolDraw mass spectrum viewer](#) and drop in a JCAMP-DX, CSV/TXT, mzML or mzXML file. Type the formula, SMILES or peptide you expect and pick the ion. The viewer overlays the theoretical isotope pattern, lists which common adducts are present, works out the ppm error and labels neutral losses. Export a PNG or CSV. The file is read in your browser and is not uploaded.

Try the mass spectrum viewer here

Click to load the live viewer in this page, or [open the full mass spectrum viewer](#). Your files stay on your device.

Why use a browser mass spectrum viewer?

A mass spectrum answers two questions: is the mass right, and does the pattern fit the formula? Instrument software can answer both, but it is often locked to one PC. Students may only get a printout or an exported file.

This viewer puts the measured spectrum and the theory on one plot. You can see at a glance whether a chlorine pattern is there, whether your main ion is [M+H]⁺ or [M+Na]⁺, and how far the measured mass is from the calculated one.

Mass spectrometry basics you need here

m/z is the ion mass divided by its charge. For singly charged ions it equals the ion mass. A 2+ ion appears at about half its mass, and its isotope peaks sit 0.5 apart.

Ionisation decides what you see. Electron ionisation (EI) gives a radical cation $M+\bullet$ and many fragments. Electrospray (ESI) is softer and mostly gives $[M+H]^+$, $[M+Na]^+$ or $[M-H]^-$. A sodium adduct sits about 22 above $[M+H]^+$, so a pair of peaks 22 apart is a common clue.

Isotope patterns help confirm the formula. Each carbon adds about 1.1% to the M+1 peak. Chlorine (^{35}Cl and ^{37}Cl) gives M and M+2 in about a 3:1 ratio. Bromine (^{79}Br and ^{81}Br) gives about 1:1.

ppm error compares a measured and a calculated m/z: $(\text{measured} - \text{theoretical}) / \text{theoretical} \times 10^6$. For caffeine $[M+H]^+$ at m/z 195.0877, an error of 1 mDa is about 5 ppm. This only makes sense for high-resolution data.

Which files it opens

JCAMP-DX	.jdx, .dx or .jcamp mass spectra, as peak tables or continuous data.
CSV or TXT	Columns of m/z and intensity.
mzML and mzXML	The first spectrum in the file. Compressed (zlib) arrays work in current browsers.

How to check a spectrum against a formula

1. Press **Open mass spectrum** or drop the file on the box. To practise, press **Caffeine ESI $[M+H]^+$** .
2. Check the line above the plot. It says whether the data is profile or centroid and whether it is unit or high resolution.
3. In **Formula, SMILES or peptide**, choose the input type and type your compound, for example C₈H₁₀N₄O₂.
4. Pick the **Ion**, such as $[M+H]^+$ for ESI or $M+\bullet$ (EI) for EI. Leave **Pattern** on Auto resolution unless you need another setting.
5. Press **Zoom to ion**. Compare the red theoretical sticks with your peaks, and read the Theory % and Found % columns.
6. Tap the measured peak, or its row under **Main peaks**, to fill **Measured m/z**. Read the ppm error.
7. Scan the **Common adducts** table for other ions that are present.
8. Export with **Export PNG** or **Export CSV**.

What the viewer does

Plot	Auto, Stick or Profile style, Zoom, Pan, + and –, Reset view and Zoom to ion. A Labels slider sets how many peaks are labelled.
Display	Base peak = 100%, Isotope overlay, Mirror (theory below) and Neutral losses can each be turned on or off.
Calculator	Formula, SMILES or one-letter peptide. Gives monoisotopic mass, average (molar) mass, exact m/z of the chosen ion and most abundant m/z.
Ions	Positive and negative adducts, including $[M+H]^+$, $[M+Na]^+$, $[M+K]^+$, $[M+NH_4]^+$, $[M+2H]^{2+}$, $[2M+H]^+$, $[M-H]^-$, $[M+Cl]^-$ and $[M+HCOO]^-$.
Pattern	Auto resolution, Unit (nominal), High (0.01 Da) or Fine structure. A halogen check notes Cl and Br patterns.
Checks	ppm and mDa error, a common adducts table with found peaks, and neutral loss labels between main peaks.
Export	PNG of the plot and CSV of the data. Profile data also gets a centroid list.

Ways to use it in class and in the lab

- **Teaching halogen patterns:** load **Chlorobenzene EI** and **Dibromobenzene EI**. Students see the 3:1 and 1:2:1 clusters next to the theory.
- **Characterisation data:** check the found and calculated m/z for a new compound before you write it up. The tool treats an error within 5 ppm as a good match for high-resolution data.
- **Peptides:** load **Peptide ESI**, enter the sequence in one-letter code and pick $[M+2H]^{2+}$ or $[M+3H]^{3+}$ to match charge states.
- **Fragment reading:** use the neutral loss labels to discuss which groups break off in EI. To compare with an expected pattern, [predict an EI mass spectrum from your drawing](#) with the Spectroscopy plugin, and treat it as a rough estimate.

Tips and limits

- Enter the neutral formula and let the Ion menu add or remove atoms. Do not enter the ion formula yourself.
- For mzML and mzXML, only the first spectrum is shown. Export the scan you need if it is not the first.
- At unit resolution, different losses can share a nominal mass. CO and C₂H₄ both give a gap of 28, so both may be listed.
- The SMILES reader covers common organic SMILES. If one fails, enter the formula instead.
- A good isotope match supports a formula but does not prove a structure. Use NMR and IR as well.

New to mass spectra? Our guide on [how to read a mass spectrum](#) explains molecular ions, fragments and isotope peaks.

Questions and answers

Can I use the viewer without a spectrum file?

Yes. Type a formula, SMILES or peptide in the calculator box and pick an ion. You get the monoisotopic mass, average mass, exact m/z and the isotope pattern without opening any data.

Why is the molecular ion small or missing in my EI spectrum?

Electron ionisation at 70 eV leaves the ion with a lot of excess energy, so many molecular ions break up before they reach the detector. Alcohols and branched compounds are common examples. A softer method such as ESI or CI usually shows the intact molecule.

Why is the tallest peak in my cluster not the monoisotopic ion?

Every carbon has about a 1.1% chance of being ^{13}C . In large molecules such as peptides, the ions that hold one or more ^{13}C atoms can outnumber the all- ^{12}C ion. The calculator shows both the exact m/z and the most abundant m/z .

Why does the tool say a ppm error is not meaningful?

Your file has unit-resolution masses, such as a typical EI spectrum from a quadrupole. The m/z values are whole numbers or close to it, so a ppm error tells you nothing. Use high-resolution data for ppm checks.