

MolDraw how-to articles (part 2)

Guides and articles from the MolDraw blog.

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

See Where a Molecule Is Electron-Rich: Electrostatic Potential (MEP) Plugin

<https://www.moldraw.com/blog/mep-plugin-electrostatic-potential-map.html>

Colour a 3D surface by approximate electrostatic potential and read the partial charge of every atom. A practical guide to the free MolDraw MEP plugin.

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

Short answer: Install **Electrostatic Potential (MEP)** from Settings > Plugins, draw a molecule and open the **MEP** tab. You get the Gasteiger partial charge of every heavy atom. Press **Show in 3D** to colour a surface around the 3D model: red is electron-rich, blue is electron-poor. It is an approximate map for comparing regions, not a quantum calculation.

Why look at charge, not just structure?

A skeletal formula hides where the electrons are. Yet charge distribution explains a lot of chemistry: why water is polar, where a hydrogen bond forms, and which carbon a nucleophile attacks.

Textbooks show this with colourful electrostatic potential maps. These usually come from quantum-chemistry software, which takes time to set up and run. The MEP plugin gives you a quick, approximate version of the same picture for any molecule you draw.

What an MEP map shows

The **molecular electrostatic potential** (MEP) at a point is the energy a small positive test charge would feel there, from all the nuclei and electrons of the molecule. A map shows this value on a surface around the molecule, using colour:

- **Red** means a negative potential. The region is electron-rich and attracts positive charges, protons and electrophiles. Lone pairs on oxygen and nitrogen are typical red spots.
- **Blue** means a positive potential. The region is electron-poor and attracts negative charges and lone pairs. Hydrogens on O-H and N-H groups are typical blue spots.
- **Pale colours** in between are close to neutral, for example most C-H regions.

How MolDraw approximates it

The plugin calculates **Gasteiger (Gasteiger-Marsili) partial charges**. This method shares charge between bonded atoms according to their electronegativity, step by step, until it

settles. It uses only the atoms and bonds, so it is fast and runs in your browser. The charges then colour a solvent-accessible surface around the 3D model.

This is a qualitative picture. It ranks which atoms are more negative or more positive. It does not give potential energies you can quote.

What the plugin shows

MEP for chloramphenicol. The oxygen atoms are the most negative and sit at the top of the charge table.

Colour scale	Red for electron-rich (–) to blue for electron-poor (+).
Charge table	Atom number, element and Gasteiger charge for every heavy atom, most negative first.
Show in 3D	Paints the charge-coloured surface on the 3D model.
Opacity	Makes the surface more or less see-through, so you can see the ball-and-stick model inside.
Refresh charges / Turn surface off	Recalculate after you edit the drawing, or go back to the plain 3D view.

How to install the MEP 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 Electrostatic Potential (MEP). An **MEP** tab appears in the analysis panel.

How to make and read an MEP map

1. Draw a molecule, or load one by name with the PubChem search box.
2. Open the **MEP** tab. The charges are calculated straight away.
3. Read the top of the charge table. These are the most electron-rich atoms.
4. Press **Show in 3D**. The 3D view opens with the coloured surface.
5. Move the **Opacity** slider until you can see the atoms under the surface. Rotate the model and match each red or blue patch to an atom.
6. If you change the drawing, press **Refresh charges**. Press **Turn surface off** when you are done.

Ways to use it in class and in the lab

- **Polarity:** show water, methanol and a hydrocarbon one after another. Students see at once which molecules have strongly coloured regions.
- **Hydrogen bonding:** red oxygen and nitrogen atoms are likely acceptors; blue O–H and N–H hydrogens are likely donors. To show the lone pairs that make an atom an acceptor, [add lone pairs to one atom or the whole molecule](#).
- **Carbonyl reactivity:** draw acetone or an ester. The oxygen is negative and the carbonyl carbon is positive, which is where a nucleophile attacks.

- **Substituent effects:** compare phenol with aniline, or a molecule with and without a nitro group, to see how charge shifts.
- **Slides and handouts:** a coloured surface makes an abstract idea easy to see in a lecture. For a flat slide where heteroatoms must stand out from the back row, [show the 2D drawing as coloured balls and sticks](#).

Tips and honest limitations

- Compare atoms within one molecule, or across closely related molecules. Do not read the numbers as energies.
- Gasteiger charges depend on the bonds you draw, not on the 3D shape. Rotating a bond does not change them. They also depend on the protonation state you draw, so [find the major charged form at your pH with the pKa plugin](#) first.
- Atom-centred charges cannot show every feature of a real potential, such as the electron-rich face of an aromatic ring or the positive cap (σ -hole) on heavier halogens.
- For publication-quality maps, use a quantum-chemistry program. Use this plugin to build intuition and to make quick comparisons.

Building up to charge maps? Start with the [Lewis structure generator](#) and the [VSEPR geometry calculator](#).

Questions and answers

What do red and blue mean on an electrostatic potential map?

Red marks electron-rich regions with a negative potential, such as lone pairs on oxygen and nitrogen. Blue marks electron-poor regions with a positive potential, such as hydrogens on O-H and N-H groups. Pale colours in between are close to neutral.

Is the MolDraw MEP a quantum-chemical calculation?

No. It uses Gasteiger partial charges mapped onto a solvent-accessible surface. It is fast and good for comparing regions, but it is an approximation, not a quantum-chemical electrostatic potential.

Why are hydrogen atoms missing from the charge table?

The table lists heavy atoms only and sorts them with the most negative first, so the most electron-rich sites are at the top.

Do I need an account to use the MEP plugin?

Yes. The plugin is free, but you sign in with a free MolDraw account to install it and to compute charges.

Complete Guide to All MolDraw Free Chemistry Tools

<https://www.moldraw.com/blog/moldraw-all-free-chemistry-tools-guide.html>

Complete guide to every free MolDraw chemistry tool: structure converters, SMILES and InChI utilities, lab calculators, druglikeness tools, XYZ to SMILES, reaction drawer, periodic table, and more—with direct links.

This is the full linked directory of every free MolDraw chemistry tool—converters, calculators, drawing utilities, and teaching resources. Use it as a quick reference or share it on other sites with attribution to MolDraw.

Published: 24 Jun 2026 · Category: Tools · Publisher: Scidart Academy

Quick guide: how to use MolDraw tools

MolDraw is a free browser chemistry platform. You do not need to install software for most workflows.

1. **Draw or edit a structure** — open the [MolDraw editor](#) for 2D drawing, 3D viewing, SMILES export, and downloads.
2. **Browse all tools** — start at the [Tools Hub](#) or the [free chemistry tools directory](#).
3. **Pick the tool that matches your input** — SMILES, name, formula, XYZ coordinates, CAS number, MOL/SDF block, etc.
4. **Convert or calculate** — run the tool in the browser, then copy the result or download the file.
5. **Return to the editor** — many tools link back to MolDraw when you want to edit the structure further.

Best for: students, educators, lab teams, and researchers who need quick chemistry utilities without desktop software. **MolDraw editor** Draw, view 3D, export formats [Open editor](#) → **Tools Hub** Browse every tool category [Open hub](#) → **Tools directory** Indexed tool URLs [Open directory](#) → **Shorter tools guide** Grouped overview article [Read guide](#) →

Drawing and structure tools

Tool	What it does	Link
MolDraw editor	2D drawing, 3D viewing, name search, PNG/SVG/SDF/XYZ/PDB export	Open MolDraw editor
Chemical reaction drawer	Draw reactions with reactants, products, arrows, reagents, conditions	Open Chemical reaction drawer
SMILES to structure	Paste SMILES and visualize 2D structure	Open SMILES to structure
Structure to SMILES	Draw in 2D editor and get SMILES in real time	Open Structure to SMILES
SMILES to 3D structure	3D view plus PNG, SDF, XYZ, PDB, MOL, OBJ, X3D download	Open SMILES to 3D structure
XYZ / Gaussian to 2D	Convert XYZ, .gjf, or .com coordinates to inferred 2D structure	Open XYZ / Gaussian to 2D
XYZ to SMILES	Convert XYZ coordinates to SMILES with editable cleanup	Open XYZ to SMILES

Tool	What it does	Link
Name to structure	Resolve names to 2D structure, SMILES, formula, MW, PubChem CID	Open Name to structure
Formula to structure	Search formulas like C ₉ H ₈ O ₄ and compare PubChem candidates	Open Formula to structure
Lewis structure generator	Build Lewis dot structures from formula and charge	Open Lewis structure generator
Protein viewer	Load proteins by PDB ID or file; export formats	Open Protein viewer

SMILES, MOL, SDF, PDB, and file converters

Tool	What it does	Link
SMILES to MOL	Convert SMILES to MOL for editor/ELN workflows	Open SMILES to MOL
SMILES to SDF	Generate SDF from SMILES for datasets	Open SMILES to SDF
SMILES to MOL2	Convert SMILES to MOL2 for docking prep	Open SMILES to MOL2
SMILES to PDB	Convert SMILES to downloadable 3D PDB	Open SMILES to PDB
SMILES to PDBQT	Convert SMILES to PDBQT for docking	Open SMILES to PDBQT
MOL to SMILES	Convert MOL/SDF blocks to SMILES	Open MOL to SMILES
MOL2 to SMILES	Convert MOL2 ligand blocks to SMILES	Open MOL2 to SMILES
PDB to SMILES	Convert ligand PDB text to SMILES	Open PDB to SMILES
PDB to PDBQT	Transform PDB coordinates to PDBQT	Open PDB to PDBQT
SDF to InChI	Convert SDF/MOL blocks to InChI	Open SDF to InChI
SDF to InChIKey	Generate InChIKey from SDF/MOL blocks	Open SDF to InChIKey
MOL to InChI	Convert MOL/SDF to InChI	Open MOL to InChI
MOL to InChIKey	Convert MOL/SDF to InChIKey	Open MOL to InChIKey

InChI, InChIKey, IUPAC, CID, and CAS tools

Tool	What it does	Link
SMILES to InChI	Generate InChI from SMILES	Open SMILES to InChI
SMILES to InChIKey	Convert SMILES to InChIKey	Open SMILES to InChIKey
InChI to SMILES	Convert InChI back to SMILES	Open InChI to SMILES
InChIKey to SMILES	Resolve InChIKey to SMILES	Open InChIKey to SMILES
InChI to InChIKey	Convert full InChI to InChIKey	Open InChI to InChIKey
InChIKey to InChI	Resolve InChIKey to full InChI	Open InChIKey to InChI
IUPAC to SMILES	Convert systematic names to SMILES	Open IUPAC to SMILES
SMILES to IUPAC	Generate IUPAC names from SMILES	Open SMILES to IUPAC

Tool	What it does	Link
CID to SMILES	Resolve PubChem CIDs to SMILES	Open CID to SMILES
CAS to SMILES	Convert CAS numbers to SMILES with metadata	Open CAS to SMILES
CAS to structure	Look up CAS and show 2D structure with SMILES and CID	Open CAS to structure

Formula, mass, and spectroscopy tools

Tool	What it does	Link
Formula and mass tools	Hub page for formula and mass utilities	Open Formula and mass tools
Molecular weight calculator	MW, molar mass, element breakdown, percent composition	Open Molecular weight calculator
SMILES to molecular formula	Convert SMILES to molecular formula	Open SMILES to molecular formula
SMILES to molecular weight	Calculate MW from SMILES with metadata	Open SMILES to molecular weight
Exact mass calculator	Monoisotopic exact mass from formula	Open Exact mass calculator
Mass spectrum predictor	Predict isotope pattern and molecular ion region	Open Mass spectrum predictor
Grams to moles calculator	Convert grams ↔ moles using molar mass	Open Grams to moles calculator

Lab, stoichiometry, and solution calculators

Tool	What it does	Link
Molarity calculator	Molarity from mass, MW, and volume	Open Molarity calculator
Molality calculator	Molality from solute amount and solvent mass	Open Molality calculator
Dilution calculator	$C_1V_1 = C_2V_2$ for stock and solvent volumes	Open Dilution calculator
Solution prep calculator	Solute mass for target molarity and final volume	Open Solution prep calculator
Chemical equation balancer	Balance equations with presets and guidance	Open Chemical equation balancer
Limiting reagent calculator	Limiting reactant, excess, leftover, theoretical yield	Open Limiting reagent calculator
Percent yield calculator	Percent yield, actual yield, or theoretical yield	Open Percent yield calculator
pH calculator	pH, pOH, strong acid/base, buffer, and pKa helpers	Open pH calculator

Tool	What it does	Link
pKa calculator	pKa from pH, pH from pKa, Henderson-Hasselbalch	Open pKa calculator

Druglikeness and medicinal chemistry tools

Tool	What it does	Link
Lipinski rule calculator	Rule of Five: MW, LogP, HBD, HBA from SMILES or name	Open Lipinski rule calculator
Druglikeness calculator	Lipinski + Veber-style druglikeness score	Open Druglikeness calculator
LogP calculator	PubChem XLogP from SMILES or compound name	Open LogP calculator
TPSA calculator	Topological polar surface area from SMILES or name	Open TPSA calculator

Teaching and reference tools

Tool	What it does	Link
Interactive periodic table	Search all 118 elements with configuration, phase, and mass	Open Interactive periodic table
TLC diagram tool	Draw TLC plates with lanes, spots, Rf labels, and export	Open TLC diagram tool
MolDraw course	Interactive chemistry course	Open MolDraw course
Molecule reference pages	Caffeine, aspirin, ibuprofen, glucose, and more	Open Molecule reference pages
Reaction guide pages	Aldol, Wittig, Grignard, Suzuki, Heck, Diels-Alder, and more	Open Reaction guide pages

Suggested workflows

Student or classroom

- Draw structures: [MolDraw editor](#)
- Balance equations: [Chemical equation balancer](#)
- Lab math: [Molarity](#), [Dilution](#), [Percent yield](#)
- TLC reports: [TLC diagram tool](#)
- Periodic table: [Interactive periodic table](#)

Research or cheminformatics

- Identifier cleanup: [SMILES ↔ InChI ↔ InChIKey](#) converters
- Registry lookup: [CAS to structure](#), [CID to SMILES](#)
- Docking prep: [SMILES to PDBQT](#), [PDB to PDBQT](#)
- Early ADME triage: [Lipinski](#), [LogP](#), [TPSA](#)

Computational chemistry

- Coordinates back to 2D: [XYZ / Gaussian to 2D structure](#)
- Coordinates to SMILES: [XYZ to SMILES](#)
- 3D export: [SMILES to 3D structure](#)

FAQ

Are MolDraw tools free?

Yes. The browser tools and calculators listed here are free to use at moldraw.com.

Do I need an account?

No account is required for most tools. The main editor and calculators work in the browser. Some community features need sign-in.

What is the fastest way to find a tool?

Use the [Tools Hub](#) or search this guide by input type ([SMILES](#), name, formula, XYZ, CAS, etc.).

Can I republish this list on another site?

Yes, with attribution to MolDraw by Scidart Academy.

Molecule Structures and Properties

<https://www.moldraw.com/blog/molecules/>

MolDraw molecule pages with 2D structures, 3D viewers, SMILES, InChIKey, molecular formula, molecular weight, exact mass, computed properties, downloads, FAQs, and conversion links.

Stimulant

Caffeine

Caffeine structure, 3D viewer, SMILES, InChIKey, [exact mass](#), computed properties, downloads, FAQ, and methylxanthine class information.

C₈H₁₀N₄O₂ 194.19 g/mol LogP -0.1 [Open page](#)

Aspirin Structure, Formula, Molecular Weight, SMILES & 3D Viewer

<https://www.moldraw.com/blog/molecules/aspirin.html>

Aspirin structure, formula, molecular weight, exact mass, SMILES, InChIKey, 2D image, 3D viewer, computed properties, downloads, conversion links, synonyms, functional groups, and

[FAQ.](#)

Molecule reference

Aspirin, also called acetylsalicylic acid, is a salicylate NSAID and antiplatelet agent. This page gives the aspirin structure, identifiers, properties, class, and a direct MolDraw editor link.

Published: 6 Jun 2026 · Data identifiers cross-checkable with PubChem CID 2244

Structure

Aspirin contains a benzene ring bearing a carboxylic acid and an acetylated phenolic oxygen. It is a common classroom example for ester [functional groups](#) and aromatic carboxylic acids.

[Draw or edit aspirin in MolDraw](#)

3D Viewer

Loading aspirin 3D conformer...

The 3D preview loads a [PubChem](#) 3D conformer for visualization and quick inspection.

Properties and Use

- Common name: Aspirin
- IUPAC name: 2-acetyloxybenzoic acid
- Class: salicylate nonsteroidal anti-inflammatory drug
- Typical chemistry context: ester hydrolysis, aromatic substitution patterns, acid derivatives, and medicinal chemistry examples.

Computed properties

LogP (XLogP)	1.2	TPSA	63.6 Å ²
H-bond donors	1	H-bond acceptors	4
Rotatable bonds	3	Heavy atoms	13

Synonyms and functional groups

Synonyms

Acetylsalicylic acid
2-Acetoxybenzoic acid
2-(Acetyloxy)benzoic acid
O-Acetylsalicylic acid
Acylpyrin

Functional groups present

Aromatic ring
Carboxylic acid
Ester
Aryl carboxylate scaffold

Downloads

[PNG](#) [SVG](#) [SDF](#) [PDB](#) [MOL](#) [PDBQT](#)

Convert this molecule

[SMILES](#) → [MOL](#) [SMILES](#) → [PDB](#) [SMILES](#) → [PDBQT](#) [SMILES](#) → [InChI](#) [SMILES](#) → [Formula](#) [SMILES](#) → [Weight](#)

Safety and handling

Educational note only: aspirin is a biologically active compound. Use the relevant SDS and institutional procedures for storage, handling, and disposal. This page is not medical advice or an SDS replacement.

Related molecule structures

Ibuprofen Another NSAID with a carboxylic acid group **Paracetamol** Analgesic with phenol and amide groups **Caffeine** Bioactive heterocycle for comparison [All molecule pages](#)

FAQ

What is the formula of aspirin?

Aspirin has the molecular formula C₉H₈O₄.

What is aspirin's molecular weight?

The [molecular weight](#) is 180.16 g/mol and the exact mass is 180.04225873 Da.

Which functional groups are in aspirin?

Aspirin contains an aromatic ring, a carboxylic acid, and an ester.

See it in 3D: [interactive aspirin molecule model](#) (ball-and-stick, space-filling, shape and bond angles) · [all 3D molecule models](#)

Caffeine Structure, Formula, Molecular Weight, SMILES & 3D Viewer

<https://www.moldraw.com/blog/molecules/caffeine.html>

Caffeine structure, formula, molecular weight, exact mass, SMILES, InChIKey, 2D image, 3D viewer, computed properties, downloads, conversion links, synonyms, functional groups, and FAQ.

Molecule reference

Caffeine is a naturally occurring methylxanthine stimulant found in coffee, tea, cacao, and many beverages. This page provides the caffeine structure, identifiers, basic properties, drug class, and a direct MolDraw editor link.

Published: 6 Jun 2026 · Data identifiers cross-checkable with PubChem CID 2519

Structure

Caffeine contains a fused xanthine ring system with three N-methyl substituents and two carbonyl groups. The structure is commonly used in teaching heterocycles, methylxanthines, and bioactive small molecules.

[Draw or edit caffeine in MolDraw](#)

3D Viewer

Loading caffeine 3D conformer...

The 3D preview loads a [PubChem](#) 3D conformer for visualization. It is useful for orientation and teaching, not a substitute for computational optimization.

Properties and Use

- Common name: Caffeine
- IUPAC name: 1,3,7-trimethylpurine-2,6-dione
- Class: methylxanthine stimulant
- Typical chemistry context: heterocyclic compounds, natural products, pharmacology examples, and structure drawing practice.

Computed properties

LogP (XLogP)	-0.1	TPSA	58.4 Å ²
H-bond donors	0	H-bond acceptors	3
Rotatable bonds	0	Heavy atoms	14

Synonyms and functional groups

Synonyms

Guaranine1,3,7-TrimethylxanthineMethyltheobromineTheineCafeina

Functional groups present

Methylxanthine heterocycleLactam carbonylsTertiary ring nitrogensN-methyl groups

Downloads

[PNG](#) [SVG](#) [SDF](#) [PDB](#) [MOL](#) [PDBQT](#)

Convert this molecule

[SMILES](#) → [MOL](#) [SMILES](#) → [PDB](#) [SMILES](#) → [PDBQT](#) [SMILES](#) → [InChI](#) [SMILES](#) → [Formula](#) [SMILES](#) → [Weight](#)

Safety and handling

Educational note only: caffeine is biologically active and should be handled according to the relevant safety data sheet, institutional procedures, and local regulations. This page is not medical advice or an SDS replacement.

Related molecule structures

Aspirin Drug-like aromatic acid and ester example **Paracetamol** Analgesic with phenol and amide groups **Glucose** Hydroxyl-rich biological small molecule All molecule pages

FAQ

What is the formula of caffeine?

Caffeine has the molecular formula C₈H₁₀N₄O₂.

What is the molecular weight of caffeine?

The **molecular weight** is 194.19 g/mol and the monoisotopic exact mass is 194.08037557 Da.

Can I open caffeine in MolDraw?

Yes. Use the editor button on this page to open caffeine from its **SMILES** string in the MolDraw editor.

See it in 3D: [interactive caffeine molecule model](#) (ball-and-stick, space-filling, shape and bond angles) · [all 3D molecule models](#)

Glucose Structure, Formula, Molecular Weight, SMILES & 3D Viewer

<https://www.moldraw.com/blog/molecules/glucose.html>

Glucose structure, formula, molecular weight, exact mass, SMILES, InChIKey, 2D image, 3D viewer, computed properties, downloads, conversion links, synonyms, functional groups, and FAQ.

Molecule reference

Glucose is a monosaccharide carbohydrate and a central biological energy source. This page includes the glucose structure, 3D viewer, **SMILES**, InChI, molecular properties, class, and MolDraw editor link.

Published: 6 Jun 2026 · Data identifiers cross-checkable with PubChem CID 5793

Structure

Glucose is commonly drawn in cyclic pyranose form for carbohydrate chemistry. It is useful for discussing stereochemistry, hydroxyl-rich molecules, hydrogen bonding, and biological small molecule structures.

[Draw or edit glucose in MolDraw](#)

3D Viewer

Loading glucose 3D conformer...

The 3D preview loads a [PubChem](#) 3D conformer. Carbohydrate stereochemistry should be checked carefully for publication or modeling use.

Properties and Use

- Common name: Glucose
- IUPAC context: aldohexose carbohydrate; commonly represented as D-glucopyranose in cyclic form
- Class: monosaccharide carbohydrate; reducing sugar
- Typical chemistry context: carbohydrate stereochemistry, cyclic hemiacetals, hydroxyl functional groups, and biomolecule drawing practice.

Computed properties

LogP (XLogP)	-2.6	TPSA	110 Å ²
H-bond donors	5	H-bond acceptors	6
Rotatable bonds	1	Heavy atoms	12

Synonyms and functional groups

Synonyms

D-Glucopyranose Blood sugar Grape sugar D-Glc Traubenzucker

Functional groups present

Hydroxyl groups Cyclic hemiacetal Pyranose ring ether Polyol carbohydrate

Downloads

[PNG](#) [SVG](#) [SDF](#) [PDB](#) [MOL](#) [PDBQT](#)

Convert this molecule

[SMILES](#) → [MOL](#) [SMILES](#) → [PDB](#) [SMILES](#) → [PDBQT](#) [SMILES](#) → [InChI](#) [SMILES](#) → [Formula](#) [SMILES](#) → [Weight](#)

Safety and handling

Educational note only: glucose is commonly used in teaching and biology contexts, but laboratory material should still be handled according to its SDS, institutional procedures, and local disposal rules. This page is not an SDS replacement.

Related molecule structures

[Caffeine](#) Contrasting heterocycle with fewer hydrogen-bond donors [Paracetamol](#) Phenol-containing small molecule for H-bond comparison [Aspirin](#) Aromatic acid and ester reference molecule [All molecule pages](#)

FAQ

What is the formula of glucose?

Glucose has the molecular formula C₆H₁₂O₆.

What is glucose's molecular weight?

The [molecular weight](#) is 180.16 g/mol and the exact mass is 180.06338810 Da.

Which functional groups are in glucose?

Glucose in cyclic glucopyranose form contains multiple hydroxyl groups, a cyclic hemiacetal, and an ether oxygen in the pyranose ring.

See it in 3D: [interactive glucose molecule model](#) (ball-and-stick, space-filling, shape and bond angles) · [all 3D molecule models](#)

Ibuprofen Structure, Formula, Molecular Weight, SMILES & 3D Viewer

<https://www.moldraw.com/blog/molecules/ibuprofen.html>

Ibuprofen structure, formula, molecular weight, exact mass, SMILES, InChIKey, 2D image, 3D viewer, computed properties, downloads, conversion links, synonyms, functional groups, and FAQ.

Molecule reference

Ibuprofen is a propionic acid derivative NSAID. This page provides the ibuprofen structure, 3D conformer preview, identifiers, core properties, drug class, and a direct MolDraw editor link.

Published: 6 Jun 2026 · Data identifiers cross-checkable with PubChem CID 3672

Structure

Ibuprofen contains an arylpropionic acid core with an isobutyl substituent on the aromatic ring. It is useful for teaching chirality, aromatic substituent effects, and medicinal chemistry structure-property relationships.

[Draw or edit ibuprofen in MolDraw](#)

3D Viewer

Loading ibuprofen 3D conformer...

The preview uses a [PubChem](#) 3D conformer. Stereochemistry and conformation should be verified for research-grade modeling.

Properties and Use

- Common name: Ibuprofen
- IUPAC name: 2-[4-(2-methylpropyl)phenyl]propanoic acid
- Class: propionic acid derivative NSAID
- Typical chemistry context: carboxylic acids, chiral centers, arylpropionic acid drugs, and conformer visualization.

Computed properties

LogP (XLogP)	3.5	TPSA	37.3 Å²
H-bond donors	1	H-bond acceptors	2
Rotatable bonds	4	Heavy atoms	15

Synonyms and functional groups

Synonyms

2-(4-Isobutylphenyl)propanoic acid Motrin Brufen Ibuprofen 15687-27-1

Functional groups present

Aromatic ring Carboxylic acid Alkyl aryl side chain Propionic acid stereocenter

Downloads

[PNG](#) [SVG](#) [SDF](#) [PDB](#) [MOL](#) [PDBQT](#)

Convert this molecule

[SMILES](#) → [MOL](#) [SMILES](#) → [PDB](#) [SMILES](#) → [PDBQT](#) [SMILES](#) → [InChI](#) [SMILES](#) → [Formula](#) [SMILES](#) → [Weight](#)

Safety and handling

Educational note only: ibuprofen is a biologically active compound. Follow the relevant SDS, institutional procedures, and local regulations for handling and disposal. This page is not medical advice or an SDS replacement.

Related molecule structures

[Aspirin](#) NSAID with aromatic acid and ester groups [Paracetamol](#) Analgesic with phenol and amide groups [Caffeine](#) Bioactive methylxanthine reference [All molecule pages](#)

FAQ

What is the formula of ibuprofen?

Ibuprofen has the molecular formula C₁₃H₁₈O₂.

What is ibuprofen's molecular weight?

The [molecular weight](#) is 206.28 g/mol and the exact mass is 206.130679813 Da.

Which functional groups are in ibuprofen?

Ibuprofen contains an aromatic ring, a carboxylic acid, and an alkyl aryl side chain with a propionic acid stereocenter.

Paracetamol Structure, Formula, Molecular Weight, SMILES & 3D Viewer

<https://www.moldraw.com/blog/molecules/paracetamol.html>

Paracetamol structure, formula, molecular weight, exact mass, SMILES, InChIKey, 2D image, 3D viewer, computed properties, downloads, conversion links, synonyms, functional groups, and FAQ.

Molecule reference

Paracetamol, also known as acetaminophen, is an analgesic and antipyretic compound. This page includes the paracetamol structure, 3D viewer, identifiers, properties, class, and MolDraw editor link.

Published: 6 Jun 2026 · Data identifiers cross-checkable with PubChem CID 1983

Structure

Paracetamol contains a para-substituted phenol and an acetanilide group. It is a compact example for discussing phenols, amides, aromatic substitution patterns, and medicinal chemistry identifiers.

[Draw or edit paracetamol in MolDraw](#)

3D Viewer

Loading paracetamol 3D conformer...

The 3D preview loads a [PubChem](#) 3D conformer for visual reference.

Properties and Use

- Common names: Paracetamol, acetaminophen
- IUPAC name: N-(4-hydroxyphenyl)acetamide
- Class: analgesic and antipyretic; anilide derivative
- Typical chemistry context: phenols, amides, hydrogen bonding, and simple drug-like small molecules.

Computed properties

LogP (XLogP)	0.5	TPSA	49.3 Å ²
H-bond donors	2	H-bond acceptors	2
Rotatable bonds	1	Heavy atoms	11

Synonyms and functional groups

Synonyms

Acetaminophen 4-Acetamidophenol N-(4-Hydroxyphenyl)acetamide APAP 4'-Hydroxyacetanilide

Functional groups present

Phenol Amide Aromatic ring Acetamide substituent

Downloads

[PNG](#) [SVG](#) [SDF](#) [PDB](#) [MOL](#) [PDBQT](#)

Convert this molecule

[SMILES](#) → [MOL](#) [SMILES](#) → [PDB](#) [SMILES](#) → [PDBQT](#) [SMILES](#) → [InChI](#) [SMILES](#) → [Formula](#) [SMILES](#) → [Weight](#)

Safety and handling

Educational note only: paracetamol/acetaminophen is biologically active. Use the relevant SDS, institutional procedures, and local regulations for handling and disposal. This page is not medical advice or an SDS replacement.

Related molecule structures

[Aspirin](#) Analgesic reference with aromatic acid and ester groups [Ibuprofen](#) NSAID with a hydrophobic arylpropionic acid scaffold [Caffeine](#) Bioactive small molecule with heterocycle nitrogens [All molecule pages](#)

FAQ

What is the formula of paracetamol?

Paracetamol, also called acetaminophen, has the molecular formula C₈H₉NO₂.

What is paracetamol's molecular weight?

The [molecular weight](#) is 151.16 g/mol and the exact mass is 151.063328530 Da.

Which functional groups are in paracetamol?

Paracetamol contains a phenol, an amide, and an aromatic ring.

Predict ¹H, ¹³C and 2D NMR from Your Drawing: NMR Analyser Plugin

<https://www.moldraw.com/blog/nmr-analyser-plugin-predict-nmr-spectra.html>

Predict ¹H, ¹³C, COSY, HSQC and HMBC spectra for the structure you draw and use them to assign real spectra. A practical guide to the free MolDraw NMR Analyser.

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

Short answer: Install **NMR Analyser** from Settings > Plugins, draw a structure, open the **NMR** tab, choose **¹H**, **¹³C**, **COSY**, **HSQC** or **HMBC** and press **Predict**. You get a simulated spectrum with lettered peaks, a signal table with shift, integral, multiplicity and coupling constant, and atom highlights on your drawing. Use it as a guide for assignment, not as a measured spectrum.

Why predict a spectrum before you assign one?

Assigning an NMR spectrum means matching each signal to atoms in a structure. With a real spectrum in front of you, the hard part is knowing where to start. A predicted spectrum gives you a first guess for every signal.

Prediction also helps you check a proposed structure. If the predicted and measured spectra disagree badly, the structure or the assignment needs a second look. Students can practise the same way: predict, compare, then explain each difference.

What each experiment tells you

- **¹H NMR:** the chemical shift shows the environment of each proton. The integral shows how many protons give the signal. The splitting pattern and coupling constant (J, in Hz) tell you about neighbouring protons.
- **¹³C NMR:** usually one signal for each set of equivalent carbons, spread over a much wider ppm range than ¹H. It is a quick way to count carbon environments.
- **COSY:** cross-peaks link protons that couple to each other, usually through two or three bonds. Use it to walk along a chain of CH groups.
- **HSQC:** links each proton to the carbon it sits on (one bond).
- **HMBC:** links protons to carbons two or three bonds away. It joins fragments across quaternary carbons and heteroatoms.

A common route is: read the ¹H spectrum, use HSQC to put each proton on its carbon, use COSY to build spin systems, then use HMBC to connect them. New to the basics? Read [how to read an NMR spectrum](#) first.

What the plugin shows

Predicted ¹H spectrum of chloramphenicol. Each signal has a letter, and the table lists its shift, integral, multiplicity and J.

1D spectra	¹ H and ¹³ C plots with lettered peaks. Turn on Labels to match letters to atoms on the structure.
Signals	Label, shift (ppm), integral, multiplicity and coupling (Hz) for each signal. Hover a row to highlight its atoms on the canvas.
2D spectra	COSY, HSQC and HMBC as contour plots.
Spectrometer	Presets from 60 to 800 MHz, or a custom value up to 1200 MHz.
History and Overlay	Every prediction is kept in History. Overlay several 1D predictions to compare them.
Download	PNG or SVG of the plot, or the spectrum data as CSV.

How to install the NMR Analyser

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 NMR Analyser. An **NMR** tab appears in the analysis panel.

How to predict and use a spectrum

1. Draw your structure, or paste a SMILES with **Paste SMILES**.
2. Open the **NMR** tab and choose an experiment: **1H**, **13C**, **COSY**, **HSQC** or **HMBC**.
3. Press **Predict**. A 1D spectrum takes a few seconds; a 2D spectrum can take longer.
4. Set **Spectrometer** to the field of your instrument, so the multiplets look like your real data.
5. Drag a box to zoom into a ppm range, scroll to scale peak height, and double-click to reset.
6. Turn on **Labels** and **Signals**. Hover a row to see which atoms it belongs to.
7. Use the download button to save the plot or the data.

Ways to use it in class and in the lab

- **Lab reports:** predict the spectrum of your product, then compare it with the one you measured. Explain any signal that moved. To prepare the measured file, [reference, integrate and pick peaks in the browser NMR viewer](#).
- **Isomer problems:** predict two candidate isomers, overlay their ¹H spectra and look for the signals that tell them apart.
- **Teaching splitting:** switch between 60 MHz and 600 MHz. The same J in Hz covers more ppm at low field, so multiplets look wider and overlap more. This explains why benchtop spectra look crowded.
- **2D practice:** predict HSQC and HMBC for a small molecule and let students connect the fragments themselves.
- **Worked examples:** export SVG plots for slides and handouts.

Tips and honest limitations

- Predictions come from nmrdB.org: the Spinus model for ¹H and nmrshiftdb2 data (HOSE codes) for ¹³C. They need an internet connection.
- The predictor has no solvent option. OH and NH shifts in particular change with solvent, concentration and temperature.
- Draw stereochemistry where it matters. Diastereotopic protons can give different predicted shifts.
- Replace R groups and attachment points (*) with real atoms. The predictor works best on neutral organic molecules, so remove metals and salts.
- A prediction is a hypothesis. Confirm assignments with your own data, especially 2D spectra.

No account handy? The free [structure to NMR tool](#) gives a quick prediction without signing in.

Questions and answers

How accurate is a predicted NMR spectrum?

For common organic molecules it is a useful guide, but it is not a measurement. Exchangeable OH and NH protons and unusual ring systems can differ more, and the predictor has no solvent option. Always confirm an assignment against your experimental spectrum.

Does the NMR Analyser need an account or internet?

Yes to both. You sign in with a free MolDraw account to predict, and each prediction comes from the online nmrd.org service. Predictions you already made stay in History on your device.

Which 2D NMR experiments can it predict?

COSY, HSQC and HMBC. They are drawn as contour plots, and you can highlight the correlated atoms on your drawing.

Can I export the predicted spectrum?

Yes. The download button saves the plot as PNG or SVG, or the spectrum data as CSV.

View, Integrate and Clean Up NMR Spectra in Your Browser

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

A practical guide to the free MolDraw NMR viewer: open JCAMP-DX, CSV or Bruker 1H and 13C spectra, pick peaks, integrate, reference to the solvent and spot common impurities.

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

Short answer: Open the free [MolDraw NMR viewer](#) and drop in a JCAMP-DX, CSV/TXT or Bruker 1H or 13C file. You can zoom, pick peaks, integrate, reference the shift scale to the solvent, find common solvent and grease peaks, and export a PNG, CSV or JCAMP-DX file. The file is read in your browser and is not uploaded.

Try the NMR viewer here

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

Why use a browser NMR viewer?

Most NMR data is processed in licensed software on the spectrometer PC. That is less handy when you want to check a spectrum at home or on a laptop without a licence.

A browser viewer fills that gap. Open the exported file, read the shifts, check the integrals and see whether the "extra" peaks are just ethyl acetate or grease. Then save a clean figure for a lab report.

What a ¹H or ¹³C spectrum tells you

Chemical shift (δ , ppm) shows the electronic environment of a nucleus. Aromatic protons sit near 7–8 ppm, protons next to oxygen near 3.5–4.5 ppm and alkyl protons below about 2 ppm. Because ppm is a ratio, the same compound gives the same shifts on a 60 MHz or a 600 MHz magnet.

Splitting comes from coupling to nearby protons and is measured in Hz. A CH₂ next to a CH₃ shows as a quartet. The Hz width of a multiplet does not change with field, so it spans more ppm on a low-field benchtop magnet.

Integration is the area under a ¹H signal. It is proportional to the number of protons, so the ratios tell you, for example, that a signal is 2H and another is 3H. In routine ¹³C spectra the areas are not reliable.

Referencing fixes the zero of the scale. TMS is set to 0 ppm. Most people use the residual solvent peak instead, such as CHCl₃ at 7.26 ppm in CDCl₃ or DMSO-d₅ at 2.50 ppm in DMSO-d₆. A wrongly referenced scale can lead to a wrong assignment.

Which files it opens

JCAMP-DX	.jdx, .dx or .jcamp files, including compressed (ASDF) data. Most NMR software can export this format.
CSV or TXT	Two columns: ppm and intensity.
Bruker	Processed data: a zip of the experiment folder, or the 1r and procs files picked together.

If the file holds the spectrometer frequency, the viewer uses it. If not, set it under **Spectrometer**.

How to work through a spectrum

1. Press **Open spectrum file** or drop the file on the box. To practise first, press **Ethyl benzoate in CDCl₃**.
2. Set the field under **Spectrometer** with the 60 to 800 MHz buttons if your file did not include it. The peak table then gives correct Hz values.
3. Under **Reference (shift calibration)**, pick your solvent in the impurity box and press **Reference to solvent**. If you used TMS, press **TMS = 0 ppm**. To set any peak by hand, type it in **Peak at** and **should be**, then press **Apply**.
4. Zoom into each region. Use the **Threshold** slider or **Pick in view** to tidy the peak list.
5. Choose **Integrate** and drag across a signal you know, such as the CH₃ triplet. Type 3 in **First integral =**. Integrate the other signals and read their areas.
6. Press **Find impurities**. Compare the hits with your peaks before you remove anything.
7. Export with **Export PNG**, **Export CSV** or **Export JCAMP-DX**.

What the viewer does

View	Zoom, Pan, + and –, Y+ and Y– for peak height, and Reset view. Scroll and pinch also zoom.
Peaks	Automatic picking with a threshold, Pick peak to add by clicking, and a table of δ ppm, Hz and height.
Integrals	Drag to integrate. Areas are scaled to the first integral.
Referencing	Reference to solvent, TMS = 0 ppm, or click Reference and pick a peak.
Impurities	Matches peaks against the trace impurity tables of Fulmer et al. (2010) for 12 deuterated solvents. Lists likely and partial matches with their expected signals.
Clean figure	Remove, Remove all likely, Undo, Restore all, and Show original. The plot is marked Edited for display.
Export	PNG, CSV and JCAMP-DX of what is on screen.

Ways to use it in class and in the lab

- **Teaching labs:** give students a JCAMP-DX file of their product. They reference it, integrate it and report the shifts and proton counts with a figure.
- **Field strength demos:** load **Ethyl benzoate in CDCl₃** and then **Benchtop 80 MHz**. The same multiplets crowd together at low field.
- **Purity checks:** before you submit a compound, run Find impurities to name the small peaks from work-up solvents, water or grease.
- **Checking a prediction:** compare your peaks with a predicted spectrum from the [SMILES to NMR predictor](#). For 13C and 2D experiments, [predict COSY, HSQC and HMBC spectra with the NMR Analyser plugin](#).

Tips and limits

- Reference before you run Find impurities. The match uses a small ppm window, so an offset scale gives poor results.
- A match only means a peak sits where an impurity is expected. Check that all of its signals are present and that the multiplets look right.
- Impurity shifts move a little with concentration and temperature. Widen the $\pm$ ppm box with care, since more false hits appear.
- The viewer shows 1D spectra. It has no Fourier transform or phase correction, so process the FID first.
- If your browser cannot unzip a Bruker folder, unzip it and pick the 1r and procs files together.
- Removing peaks is a display edit. Keep the original file as your data.

New to NMR? Our guide on [how to read an NMR spectrum](#) covers shifts, splitting and integrals step by step.

Questions and answers

Can I open ^{13}C spectra as well as ^1H ?

Yes. The viewer reads the nucleus from the file. If the file does not say, it guesses from the ppm range. The impurity table has both ^1H and ^{13}C shifts.

Why do my ^{13}C integrals not match the number of carbons?

Routine ^{13}C spectra are recorded with proton decoupling. Carbons relax at different rates and get different NOE boosts, so quaternary carbons often look small. Only trust ^{13}C integrals from a spectrum run under quantitative conditions.

Can I process a raw FID in the viewer?

No. The viewer opens processed spectra: JCAMP-DX, two-column CSV or TXT, and Bruker processed data (the 1r and procs files). Do the Fourier transform and phasing in your spectrometer software first.

Should I hide impurity peaks before I put a spectrum in my thesis?

Keep the original spectrum as your data and report the impurities you found. A cleaned plot is only a display edit. The viewer labels it as edited, and you should say so in the caption if you use it.

See Which Form of a Molecule Exists at pH 7.4: pKa and Microspecies Plugin

<https://www.moldraw.com/blog/pka-plugin-protonation-states-microspecies.html>

Estimate pKa values, the major charged form and the share of each microspecies at any pH. A practical guide to the free MolDraw pKa and Microspecies plugin.

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

Short answer: Install **pKa & Microspecies** from Settings > Plugins, draw a molecule and open the **pKa** tab. Set the pH with the slider or a preset such as **Blood 7.4**. You see an estimated pKa for each acidic or basic group, the major charged form, the net charge, the isoelectric point and a chart of every microspecies from pH 0 to 14. Everything runs in your browser.

Why the protonation state matters

Most drug molecules carry acidic or basic groups. A carboxylic acid can lose a proton and become a carboxylate. An amine can gain a proton and become an ammonium ion. Which form you have depends on the pH of the solution and on the pKa of each group.

The pKa is the pH at which a group is half protonated and half deprotonated. Each pH unit away from the pKa shifts the ratio between the two forms by a factor of ten. This is the Henderson-Hasselbalch relationship that students meet in general chemistry.

A molecule with several ionizable groups can exist in several protonation states at the same time. Each of these states is a *microspecies*. The share of each one changes with pH. The form that dominates at blood pH (about 7.4) affects solubility, how easily the molecule crosses membranes and how it binds to a protein. It is also the form you usually want for docking or for a figure. The plugin gives you a quick estimate of all of this while you draw.

What the plugin shows

Cetirizine at pH 7.4. The chart covers pH 0 to 14, and the Sites table lets you type in a measured pKa.

Structure view	pKa sites labels each acidic or basic group with its estimate. Major at pH draws the main charged form.
Chart	The percentage of every microspecies from pH 0 to 14. Click the chart to jump to that pH.
pH controls	A slider, a number box and presets: Stomach 1.5, Skin 5.5, Blood 7.4 and pH 9.
Summary	Share of the major species, net charge at the chosen pH, isoelectric point and macro pKa values.
Tabs	Microspecies lists each form with its charge and percentage. Sites lists each group with its estimate and a box for your own value. About explains the method.

How to install the pKa 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 pKa & Microspecies. A **pKa** tab appears in the right panel.

You can also right-click a molecule on the canvas and choose **pKa & microspecies**.

How to find the major species at a given pH

1. Draw your molecule. If the canvas holds several molecules, select the one you want.
2. Open the **pKa** tab. With **Live** ticked, the plugin re-analyses whenever the drawing changes. Otherwise press **Analyse drawing**.
3. Set the pH with the slider, type a value, or press a preset such as **Blood 7.4**.
4. Read the summary: the major species, its share and the net charge.
5. Switch the structure view to **Major at pH** to see where the charges sit.
6. Open **Microspecies** to compare the other forms. Hover over one to highlight its curve on the chart.
7. Press **Insert major species** to add the charged form to the canvas, or **Replace drawing** to swap your structure for it.

Ways to use it in class and in the lab

- **Teaching acids and bases:** draw glycine. Textbook values are about 2.3 for the carboxylic acid and 9.6 for the amine, so the zwitterion should dominate at pH 7.4. Compare the plugin's estimates with those values and move the slider to show each form taking over.

- **Drug absorption:** press Stomach 1.5 and then Blood 7.4 to show how a weak acid or base changes charge along the body.
- **Docking and modelling prep:** insert the major species at pH 7.4 and export that form rather than the neutral drawing. To see where its charge sits, [colour the inserted form by electrostatic potential](#).
- **Quick calculations:** for buffer and ratio problems, pair the plugin with the [pKa calculator](#) and the [pH calculator](#).

Tips and limits

- Click a pKa label on the structure to jump to that group in the Sites table.
- If you have a measured pKa, type it in the **Your pKa** box. Leave the box empty to keep the estimate. Measured values beat estimates every time.
- A salt drawn with its counter-ion counts as two molecules. Select the drug part, or draw the neutral parent compound instead.
- If a molecule has no ionizable group between pH 0 and 14, the plugin tells you it stays neutral.

All values are estimates. The plugin finds each acidic or basic group, starts from a measured value for that type of group and adjusts it for nearby substituents with the Hammett and Taft equations. On a held-out test set of about 2,000 molecules the average error is 0.92 pKa units, and 71% of values fall within 1 unit. For common drugs the average error is about 0.45. Some ring systems, tautomers, amidines, enols and C-H acids can be off by 2 units or more. Use the results for teaching, quick checks and planning, not as a replacement for measurement.

Questions and answers

What is a microspecies?

A microspecies is one specific protonation state of a molecule, with each acidic or basic group either carrying its proton or not. A molecule with several ionizable groups can exist as several microspecies at once, and their shares change with pH.

How accurate are the pKa values?

They are estimates. On a held-out test set the average error is 0.92 pKa units, with 71% of values within 1 unit, and about 0.45 units for common drugs. Unusual ring systems and tautomeric heterocycles can be off by 2 units or more.

Does the plugin send my molecule to a server?

No. The calculation runs in your browser and uses no server and no AI model.

Can I use my own measured pKa values?

Yes. Open the Sites tab and type your value in the Your pKa box for that group. The chart, the summary and the major species update straight away.

View Protein Structures Online: PDB IDs, Chains and Sequences

<https://www.moldraw.com/blog/protein-structure-viewer-guide.html>

A practical guide to the free MolDraw Protein Viewer page: load a PDB entry by ID or file, style each chain, highlight residues from the sequence and export images or coordinates.

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

Short answer: Open the [Protein Viewer](#), type a four-character PDB ID and press **Load PDB ID**, or press **Upload PDB file**. Pick a **Default Chain Style**, then style each chain in the **Chains** list. Drag across the **Amino Acid Sequence** and right-click to restyle or hide that stretch. Save the view as PNG or JPG, or the coordinates as PDB, XYZ, OBJ or X3D.

Try the protein viewer here

The live viewer below is the same tool as the full page. It loads crambin (1CRN) when it opens.

Click to load the live viewer in this page, or [open the full protein viewer](#). Loading by PDB ID fetches the structure from the RCSB Protein Data Bank.

Why use a protein viewer in the browser?

A protein's function depends on its 3D shape. Desktop programs such as PyMOL or ChimeraX are powerful, but you need to install them and learn their commands. For a quick look, a class demonstration or a simple figure, a web page is often enough.

This page is the standalone web tool. MolDraw also has a [Protein viewer plugin](#) inside the editor. The plugin sits next to your drawing and adds more colour schemes, molecular surfaces and extra export formats. The standalone page is lighter and opens without the editor.

Protein structures in brief

The **Protein Data Bank (PDB)** is the public archive of experimentally determined structures of proteins, nucleic acids and their complexes. Most come from X-ray crystallography, NMR or cryo-electron microscopy. Each **entry** has a four-character ID, such as 1CRN for crambin or 4HHB for human deoxyhaemoglobin.

An entry lists atom coordinates. Atoms belong to **residues**, the amino acids, which are numbered along each **chain**. Chains have letter IDs (A, B, C and so on). Haemoglobin, for example, has two α and two β chains. Ligands, ions and water are stored as separate hetero atoms. Parts of a chain that were not resolved in the experiment are simply missing from the model.

Each display style answers a different question. A **cartoon** traces the backbone and shows helices and β -strands, so you see the overall fold. **Sticks** show bonds between atoms, which you need for side chains and binding contacts. **Spheres** fill space and show packing. A

surface shows the outer shape and pockets; this page does not draw surfaces, but the in-editor plugin does.

Input and export formats

Load	A PDB ID, downloaded from RCSB in PDB format, or a .pdb file from your computer.
PNG and JPG	An image of the current view. JPG gets a white background.
PDB	The loaded file as it was read.
XYZ	The element and coordinates of every atom, including hetero atoms.
OBJ and X3D	Simple point-based models of the atom positions. They do not copy the cartoon or the styles on screen.

How to explore a structure step by step

1. Open the viewer. Crambin (1CRN) loads first, so you can try the controls straight away.
2. Type an ID in **PDB ID**, for example 4HHB, and press **Load PDB ID**. The status line lists the chains it found. To open your own file, press **Upload PDB file**.
3. Choose **Cartoon**, **Stick**, **Sphere** or **Line** in **Default Chain Style**. This sets every chain at once.
4. Drag in the 3D view to rotate the molecule, and scroll to zoom.
5. In **Chains**, each chain shows its residue count, a style menu, a colour picker and a **Hide** box. Press **Focus** to highlight that chain in orange sticks.
6. In **Amino Acid Sequence**, drag across residues in one chain. Right-click the selection to open **Selected Segment Style**, set **Style**, **Color** or **Hide segment**, and press **Apply**.
7. Use the download buttons to save your result. **Clear** empties the viewer.

What the viewer does

- **Per-chain styles:** give each chain its own style and colour, or hide it, to see how subunits pack.
- **Sequence view:** one-letter codes for each chain, linked to the 3D model.
- **Segment styles:** restyle, recolour or hide a selected stretch of residues. Each applied segment keeps its own style, so you can mark several sites.
- **Downloads:** PNG, JPG, PDB, XYZ, OBJ and X3D.

Ways to use it in class and in the lab

- **Teaching quaternary structure:** load 4HHB, give each chain a different colour and hide one or two chains to show how the subunits fit together.
- **Highlighting a site:** keep the protein as a cartoon and show a binding loop or a mutation site as coloured sticks.
- **Quick figures:** set up a view and download a PNG for a slide or a report.
- **Next steps:** turn a bound ligand into SMILES with [PDB to SMILES](#), work out a chain's mass with the [protein molecular weight calculator](#), or prepare a receptor with [PDB to](#)

Tips and limits

- Cartoon draws only the backbone trace of the chains, not ligands, ions or water. To see them, switch the chain to Stick, Sphere or Line.
- For large structures, Line is the lightest style.
- The sequence comes from the residues in the model. Unresolved residues do not appear, and residues the viewer does not recognise, such as nucleotides, show as X.
- A selection stays within one chain. Sequence selection uses drag and right-click, so a mouse is easiest.
- Loading by ID needs an internet connection.

Want surfaces, more colour schemes or GLB export? Use the [Protein viewer plugin](#) in the MolDraw editor.

Questions and answers

How is this page different from the Protein plugin in the MolDraw editor?

This page is a light, standalone viewer that opens without the editor. The Protein plugin sits next to your drawing in the editor and adds more colour schemes, molecular surfaces and extra export formats such as GLB and SDF.

Where do the structures come from?

When you press Load PDB ID, the page downloads the entry from the RCSB Protein Data Bank, so you need an internet connection. With Upload PDB file, the page reads the file in your browser.

Why can I not see the ligand or the water molecules?

Cartoon draws only the backbone trace of the chains. Set the chain to Stick, Sphere or Line in the Chains list to see ligands, ions and water as atoms.

Can I open mmCIF files?

No. The page reads the PDB format only. Most entries can be downloaded as a .pdb file from RCSB, but some very large structures are only offered as mmCIF. Those will not load here.

View PDB Protein Structures in 3D in Your Browser: Protein Viewer Plugin

<https://www.moldraw.com/blog/protein-viewer-plugin-pdb-3d.html>

Load any PDB entry by its four-character ID, show it as a cartoon or surface, style residues from the sequence and export images. A practical guide to the free MolDraw Protein viewer.

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

Short answer: Open the **Protein** tab next to Structure, type a four-character PDB ID such as 1HHO and press **Go**. The structure loads as a cartoon coloured by chain. Use **Display** and **Surface** to change the view, select residues in the sequence strip to style them, and use **Export** to save an image or a file. The viewer is on by default and needs no account.

Why look at a protein in 3D?

A protein's function depends on its shape. The amino-acid sequence folds into helices and sheets, and these pack into a three-dimensional structure with grooves and pockets. A small molecule drug usually works by fitting into one of those pockets. You cannot see any of that in a sequence or a 2D drawing.

The [Protein Data Bank](#) (PDB) is the public archive of experimentally determined structures of proteins, DNA and RNA. Each entry has a four-character ID, such as 1HHO for haemoglobin. The MolDraw Protein viewer loads these entries next to your drawing, so you can move from a ligand to its target without opening another program.

Different views answer different questions. A **cartoon** traces the backbone and shows secondary structure: helices as spirals and β -strands as arrows. **Sticks** show individual atoms, which you need for side chains and binding contacts. A **surface** shows the outer shape of the molecule, which makes pockets and grooves easy to see.

What the viewer offers

Haemoglobin (PDB 1HHO) as a cartoon with each chain in its own colour. The sequence strip sits below the viewer.

Load	Type a PDB ID and press Go to fetch it from RCSB, press Open for a local PDB file, or drop a file onto the viewer.
Display	Cartoon, Ribbon, Stick, Ball & stick, Sphere, Line or Cross. Colour by Chain, Amino acid, Shapely, Secondary structure, Hydrophobicity, B-factor or Spectrum, or pick your own colour. Set the opacity.
Surface	Show or hide a surface, choose SAS, SES, VDW or MS, and set its opacity.
Sequence strip	One-letter sequence for each chain. Select residues to give them their own style.
Export	GLB, PNG, JPG, PDB, SDF, XYZ, X3D and OBJ, with a Hi-res option.

How to get the Protein viewer

Need a quick look without opening the editor? The [standalone protein structure viewer](#) styles, colours and hides each chain on its own.

You do not need to install anything. The Protein viewer is on by default and works without an account. If you turned it off earlier:

1. Open the [MolDraw editor](#).
2. Click **Settings** (the gear), then **Plugins**.
3. Click **Install** next to Proteins. The **Protein** tab appears next to Structure.

How to load and style a protein

1. Click the **Protein** tab. A small example structure, crambin (1CRN), loads first.
2. Type a PDB ID in the **ID** box, for example 1HHO, and press **Go** or Enter.
3. Open **Display**. Keep Cartoon and choose **Secondary structure** to colour helices and strands differently, or choose **Chain** to tell the subunits apart.
4. Open **Surface**, press **Show** and lower the opacity so the cartoon stays visible underneath.
5. In the sequence strip, click one residue, drag across a range, or Ctrl/Cmd+click to add or remove a residue. In the style panel that opens, set **Style** to Stick and pick a colour.
6. Open **Export**, tick **Hi-res** if you need a large image, and choose PNG.

Ways to use it in class and in research

- **Teaching protein structure:** load 1HHO, colour by secondary structure and point out the helices. Then colour by chain to show that haemoglobin has four subunits.
- **Hydrophobic core:** colour by Hydrophobicity to show how nonpolar residues tend to sit inside the fold.
- **Drug targets:** load 6LU7, the SARS-CoV-2 main protease, add a surface and discuss where an inhibitor could bind.
- **Figures:** style a few key residues as sticks on a cartoon background and export a high-resolution image for a slide or report.
- **Next steps:** work out a chain's mass with the [protein molecular weight calculator](#), or prepare a receptor for docking with [PDB to PDBQT](#).

Tips and limits

- Good starting IDs: 1HHO (haemoglobin), 1BNA (B-DNA), 6LU7 (SARS-CoV-2 main protease) and 1GFL (green fluorescent protein).
- Each selection you style becomes its own region, so you can colour several sites differently. Use **Remove style** or **Clear selection** in the style panel to undo.
- B-factor colouring shows how much atom positions vary in the model. High values often mark flexible loops.
- To open a structure you saved earlier, drag the .pdb file from your computer onto the viewer.

Fetching by ID needs an internet connection, because the file comes from RCSB. The viewer needs WebGL; it shows a message if your browser cannot provide it. The sequence strip lists amino-acid residues only, so ligands, water and nucleic acids do not appear there. A PDB entry is an experimental model, and its quality depends on the method and resolution, which you can check on the entry's RCSB page.

Want to view a small molecule in 3D instead? See [how to view molecules in 3D](#).

Questions and answers

Do I need an account to view proteins?

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

Where do the structures come from?

When you type a PDB ID and press Go, the plugin downloads the entry from the RCSB Protein Data Bank. You can also open a PDB file from your computer.

How do I highlight an active site or a few residues?

Select the residues in the sequence strip below the viewer. A small style panel opens where you can switch them to sticks, change their colour or add a surface.

Which export formats are available?

The Export menu offers GLB, PNG, JPG, PDB, SDF, XYZ, X3D and OBJ. Tick Hi-res for a larger image.

Clean Up and Read Raman Spectra Online: Shift, Fluorescence and Spikes

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

A practical guide to the free MolDraw Raman viewer: convert nm to Raman shift, remove cosmic-ray spikes and fluorescence, smooth, pick peaks with likely bands and check D, G and 2D carbon bands.

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

Short answer: Open a JCAMP-DX, CSV/TXT or SPC file in the free [MolDraw Raman viewer](#), or press **Polystyrene**. If the x axis is in nm, pick your laser to get the Raman shift. Tick **Remove spikes**, smooth if needed and choose a baseline to take away fluorescence. Then read the peak table with likely bands and export a PNG or the cleaned CSV. Your files stay on your device.

Try the Raman viewer here

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

Why clean up Raman data before you read it?

Raw Raman spectra are rarely ready to read. Bands sit on a fluorescence hump, cosmic rays add spikes that look like peaks, and some instruments save the x axis in nm. Each fix is simple, but together they take time in a spreadsheet. The viewer puts them on one page, and you see each step on the plot before you trust a peak.

The science in brief

Raman shift. When laser light hits a sample, a tiny fraction scatters with less energy because it has excited a vibration. The Raman shift is that energy loss in cm^{-1} : $\text{shift} = 10^7 / \lambda_{\text{laser}} - 10^7 / \lambda_{\text{scattered}}$, with both wavelengths in nm. A band has the same shift with any laser.

Which bands are strong. A vibration is Raman active when it changes the polarisability of the molecule. Symmetric stretches, C=C and ring breathing are strong. Polar groups such as O-H, strong in IR, are often weak in Raman.

For those polar groups, [read the band positions in an IR spectrum](#). The two techniques fill each other's gaps.

In a molecule with a centre of symmetry, no vibration is both IR and Raman active. This is the rule of mutual exclusion. To check whether it applies, [find the molecule's point group with the Symmetry plugin](#).

Laser wavelength. Scattering is stronger at shorter wavelengths, so 532 nm gives more signal but often more fluorescence. Lasers at 785 or 1064 nm often reduce fluorescence at the cost of signal.

Fluorescence and spikes. Fluorescence adds a broad background that can be far stronger than the Raman bands. Cosmic rays hit the detector at random and give spikes one or two points wide.

Files you can open

- **JCAMP-DX** (.jdx, .dx). If the file records the laser wavelength, the viewer picks it up.
- **CSV or TXT** with two columns: Raman shift or wavelength in nm, then intensity.
- **SPC**, the Thermo/Galactic binary format (new format).

The viewer checks the units and headers to spot an nm axis. Pick several files to overlay them. To practise, [download the sample .jdx](#), a cyclohexane spectrum in nm from a 785 nm laser. All examples are simulated.

How to clean and read a spectrum, step by step

1. Press **Open Raman file(s)** or drop files on the box. Or press an example: **Polystyrene, Graphene vs graphite, Silicon, Cyclohexane** or **Sample .jdx (nm, 785 nm laser)**.
2. Under **Laser and x axis**, pick 532, 633, 785 or 1064 nm, or **Other** to type a value. If a file in nm was not detected, tick **File x axis is wavelength in nm**.
3. Under **Clean up**, tick **Remove spikes**. Raise the **threshold** if a real narrow band is touched.
4. Tick **Savitzky-Golay smooth** only for noisy data, with a small **window**.
5. Choose a **Baseline: Asymmetric least squares**, with its **Stiffness λ** slider and **p**, or **Polynomial** with an **Order**. With **Show before and baseline** ticked, check that the

red dashed line runs under the peaks.

6. Read **Peaks and likely bands**. Use the **Peak prominence** slider to show more or fewer peaks.
7. To compare files, tick **Normalise**. Then press **Export PNG** or **Export CSV**.

What the viewer does

x axis	Converts nm to Raman shift for 532, 633, 785, 1064 nm or a custom laser.
Spikes	Finds narrow points far above their neighbours and fills them in. The plot shows how many spikes were removed.
Smoothing	Savitzky-Golay, window 5 to 21 points, order 2 to 4.
Baseline	Asymmetric least squares or polynomial, shown as a red dashed line.
Peaks	Shift, height and FWHM for up to 25 peaks, each matched to a table of common Raman band ranges.
Carbon check	D, G and 2D positions, I_D/I_G , I_{2D}/I_G , 2D width and a note on layers and defects.
Export	PNG of the plot and CSV of the cleaned, visible spectra.

Ways to use it in class and in the lab

- **Polymer identification:** the Polystyrene example shows the strong ring breathing band near 1001 cm^{-1} and the aromatic C=C band near 1602 cm^{-1} after the fluorescence is removed.
- **Calibration checks:** crystalline silicon gives one sharp band at 520.7 cm^{-1} , and cyclohexane is a common shift standard. Compare your reference spectrum with the known values.
- **Graphene and carbon:** load Graphene vs graphite and compare the 2D band shape and D/G ratio. To see how much of the carbon is bonded to oxygen, [fit the C 1s region of an XPS spectrum](#).
- **Teaching Raman shift:** open the sample .jdx in nm and switch the laser to see how the conversion depends on it.

Tips and limits

- A baseline that follows the data too closely can eat broad bands. In ALS, a larger λ gives a stiffer line. In a polynomial, a lower order bends less.
- Smoothing lowers and widens sharp bands. Use the smallest window that works, and compare FWHM only between spectra treated the same way.
- Band assignments come from general ranges. The viewer uses organic groups when C-H stretch peaks are present, and carbon and inorganic bands when they are not. Confirm assignments with a reference.
- Band heights depend on the laser, optics and detector. Normalise to compare shapes, not absolute intensities.
- The CSV puts all visible spectra on the shift values of the first one, so other spectra are interpolated.

Questions and answers

Why does my Raman spectrum sit on a large sloping background?

That is usually fluorescence from the sample or from impurities. It is often much stronger than the Raman signal. A longer laser wavelength, such as 785 or 1064 nm, often reduces it. In the viewer, choose a baseline to subtract what remains.

Does the Raman shift depend on the laser wavelength?

No. The shift is the energy the light loses to a vibration, so a band sits at the same cm^{-1} with any laser. The absolute wavelength of the scattered light does change, which is why a file in nm needs the laser wavelength.

How can I tell a cosmic-ray spike from a real band?

A spike is one or two points wide and appears at a random place. If you record the spectrum again, it moves or disappears. A real band is wider and repeats in every acquisition.

Should I choose an ALS or a polynomial baseline?

Try asymmetric least squares first for curved fluorescence backgrounds. Use a polynomial for a smooth, gently bending background. In both cases, check that the red dashed line runs under the peaks and does not cut into broad bands.

Sketch a Molecule by Hand and Get a Clean Structure: Smart Draw Plugin

<https://www.moldraw.com/blog/smart-draw-plugin-sketch-to-structure.html>

Draw bonds, rings and atom labels with a stylus, finger or mouse, and Smart Draw turns them into a clean, editable structure. A practical guide to the free MolDraw plugin.

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Short answer: Install **Smart Draw** from Settings > Plugins and pick the **Smart Draw** tool in the left toolbar. Sketch bonds, rings and letters with a stylus, finger or mouse, then press **Convert** or **Enter**. MolDraw turns the strokes into a clean structure that you can edit and export like any other drawing. Recognition runs in your browser.

Why sketch instead of click?

Chemists learn to draw structures by hand. A skeletal formula is quick on paper: every corner and line end is a carbon, hydrogens on carbon are implied, and only heteroatoms get a letter. Most structure editors make you translate that habit into tool choices and clicks.

On a tablet or an interactive whiteboard, that translation is slow. You switch between the bond tool, the ring tool and the atom menu many times for one molecule. Smart Draw lets you draw the way you would on paper. It reads each stroke as a bond, a ring or a letter and builds the structure for you.

The result is not a picture of your handwriting. It is a normal MolDraw molecule with atoms and bonds, so you can clean it up, name it, copy its SMILES or analyse it with other plugins.

What Smart Draw recognises

A hand-drawn hexagon with one extra stroke becomes methylcyclohexane.

Straight stroke	A single bond.
Zigzag line	A chain, with one bond between each pair of corners.
Two parallel strokes	A double bond.
Closed shape	A ring with the same number of sides, from 3 to 8.
Circle inside a ring	Marks a five- or six-membered ring as aromatic.
Letters	Atom labels such as N, O, S or Cl. Letters written side by side, such as OH, are read together.
+ or –	A positive or negative charge on the nearest atom.

Strokes that end near an atom already on the canvas join that atom, so you can extend a structure you drew with the normal tools.

How to install Smart Draw

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 Smart Draw. The **Smart Draw** tool appears in the left toolbar.

How to sketch a structure

1. Select the **Smart Draw** tool in the left toolbar.
2. Draw a ring in one continuous stroke, for example a hexagon for cyclohexane. For fused rings or an exact benzene, [place ring templates with the ring tools](#) instead.
3. Add substituents as straight strokes from a ring corner. Draw a zigzag for a longer chain.
4. For a double bond, draw a second line of similar length close and parallel to the first.
5. Write a letter at the end of a bond to make it a heteroatom, for example O for an alcohol.
6. Check the preview. The Smart Draw bar shows what MolDraw reads, for example “3 bonds · N”, and nothing changes until you convert, so you can pause as often as you like. Use **Undo stroke** (Ctrl+Z) or **Clear** (Esc) to fix a mistake.
7. Press **Convert** or **Enter**. The strokes become a structure and MolDraw tidies the new part of the layout. If you prefer converting automatically, turn on **Auto** in the bar to convert after a 2.5 second pause.
8. Switch to the normal tools to add wedges, change bonds or fix anything that came out wrong.

Ways to use it in class and in the lab

- **Lecturing on a touch screen:** sketch a molecule live while you talk, then show its clean structure and name straight away.
- **Student practice:** students draw from memory, as they would in an exam, and get a real structure they can check.
- **Quick notes in the lab:** jot down a structure on a tablet with a stylus and copy its SMILES into your notebook.
- **Next steps:** check the formula with the [SMILES to formula tool](#), or learn the click-based way in [how to draw benzene, cyclohexane and fused rings](#).

Tips and limits

- Close each ring in one stroke and make the corners clear, so the number of sides is read correctly.
- Keep bonds reasonably straight and about the same length.
- Draw an aromatic ring as a hexagon with a circle inside it.
- On an iPad, use Apple Pencil and turn on the touch-screen options in Settings > Touch screen.

Smart Draw reads shapes, not chemistry. It does not draw wedge or hash bonds, so add stereochemistry with the normal bond tools afterwards. Neat handwriting matters for letters, and complex labels may need the normal atom tool. Always look at the result before you rely on it: a ring with an extra wobble or a misread letter changes the molecule.

Smart Draw works offline because recognition runs locally. Your sketch is not sent to a server.

Questions and answers

Does Smart Draw work offline?

Yes. Stroke recognition runs in your browser, and your sketch is not sent to a server.

Can I use it on a phone or tablet?

Yes. You can draw with a finger, a stylus or a mouse. A stylus gives the cleanest strokes.

What can Smart Draw recognise?

Single bonds, zigzag chains, double bonds drawn as two parallel lines, rings with 3 to 8 members, aromatic rings marked with a circle, connections to atoms already on the canvas, simple atom labels and plus or minus charges.

What happens if a stroke is not recognised?

The stroke stays on the canvas as grey ink. If nothing in the sketch can be read, MolDraw shows a short message. Delete the ink and draw it again, or use the normal tools.

Find a Molecule's Point Group and See Its Symmetry in 3D: Symmetry Plugin

<https://www.moldraw.com/blog/symmetry-plugin-point-groups-3d.html>

Draw a molecule and get its point group, every axis and mirror plane, animated symmetry operations and the character table. A practical guide to the free MolDraw Symmetry plugin.

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Short answer: Install **Symmetry and point groups** from Settings > Plugins, draw a molecule and open the **Symmetry** tab. Press **Analyse selection** or pick one of the examples. The plugin builds a 3D shape, names the point group, draws every axis and mirror plane, plays each operation and shows the character table.

Why symmetry matters in chemistry

Symmetry is hard to see on paper. A flat drawing hides the axes and planes that make two atoms equivalent. Yet symmetry decides a lot: whether a molecule can have a dipole moment, whether it can be chiral, which vibrations show up in IR or Raman spectra, and how orbitals are labelled.

A few terms help:

- A **symmetry operation** moves the molecule so that it looks exactly the same afterwards.
- A **symmetry element** is the axis, plane or point about which the operation happens.
- The main elements are the identity E , rotation axes C_n (turn by $360^\circ/n$), mirror planes σ , the centre of inversion i , and improper axes S_n (turn by $360^\circ/n$, then reflect through a plane at right angles to the axis).
- A **point group** is the full set of operations of a molecule. The number of operations is the group order.

Some familiar examples: water is C_{2v} , with one C_2 axis and two mirror planes (order 4). Ammonia is C_{3v} , with a C_3 axis and three vertical mirror planes (order 6). Benzene is D_{6h} (order 24), methane is T_d and carbon dioxide is $D_{\infty h}$.

Two quick rules show why this is useful. A molecule with any improper axis, including a mirror plane (S_1) or a centre of inversion (S_2), cannot be chiral. A molecule with a centre of inversion has no permanent dipole moment.

What the plugin shows

PCl_5 is D_{3h} , order 12: one C_3 axis, three C_2 axes, σ_h , three σ_v planes and an S_3 axis.

Badge	The point group (Schoenflies symbol) and its order. A summary line beside it describes the group in words.
Elements	Every axis, plane, centre and improper axis. Hover to highlight it in 3D; click to play it.

Operations	All operations grouped into classes. Click one to watch the atoms move onto equivalent atoms.
Character table	Irreducible representations with linear, rotational and quadratic functions, following Cotton and Harris and Bertolucci.
Projection	A view down the z axis that shows where the axes and planes lie.

How to install the Symmetry 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 Symmetry and point groups.

How to find a point group

1. Draw one molecule. If the canvas holds several, select the one you want.
2. Open the **Symmetry** tab. You can also use the Chemistry menu (**Symmetry and point groups** > **Open Symmetry**) or right-click the canvas and choose **Find symmetry (point group)**.
3. Press **Analyse selection**. MolDraw adds hydrogens, tries several conformers and minimises the 3D shape with MMFF94. Keep **Live** on to re-analyse when you edit the drawing.
4. Read the point group in the badge.
5. Open **Elements** and hover each entry to see it in 3D. Click it to play the operation.
6. Open **Character table** to link the group to spectroscopy and bonding.

No drawing at hand? The **Examples** list holds ready-made molecules sorted by point group, from bromochlorofluoromethane (C_1) to buckminsterfullerene (I_h).

Ways to use it in class and in the lab

- **Teaching the flowchart:** load water, ammonia and benzene in turn. Ask students to predict the group, then check the badge and the element list.
- **Showing operations live:** turn on **Numbers** and play a C_3 rotation or an S_4 operation. After each move the plugin says which atom landed where.
- **Spectroscopy courses:** use the character table to discuss which vibrations can be IR or Raman active. Then check a real sample: [open its Raman spectrum in the free Raman viewer](#) and compare the strong bands with its IR spectrum.
- **Checking a structure:** confirm whether a ligand or product is chiral or has a centre of inversion before you discuss its properties.

Tips and limits

- Use **Tight** tolerance for accurate structures and **Loose** for rough drawings. Normal sits in between.
- The 3D shape comes from a force-field conformer, not from your 2D layout. Flexible molecules may come out less symmetric than their textbook form. Compare with the

matching example, such as staggered (D_{3d}) and eclipsed (D_{3h}) ethane.

- Use the layer chips (**Axes, Planes, Centre, Sn axes, Numbers**) to keep busy groups readable.
- For C_{2v} molecules, the B_1 and B_2 labels depend on which plane is called xz. The plugin puts a planar molecule in the yz plane and says so.

Want to see the shape before the symmetry? The [VSEPR geometry calculator](#) predicts molecular shapes, and the [3D molecular model viewer](#) lets you rotate them.

Questions and answers

What is a point group?

A point group is the complete set of symmetry operations of a molecule. Every operation leaves at least one point fixed. Chemists name point groups with Schoenflies symbols such as C_{2v} , D_{3h} or T_d .

Is the Symmetry plugin free?

Yes. You need a free MolDraw account to install and use it.

Why does my molecule get a lower point group than the textbook?

MolDraw builds a 3D shape from your 2D drawing, and a flexible molecule may land in a less symmetric conformation. Try Loose tolerance, or compare with the matching built-in example.

Does it show character tables?

Yes, for the common point groups. The table lists the irreducible representations with their linear, rotational and quadratic functions. If a group has no stored table, the elements and operations are still shown.

Read TGA and DSC Curves Online: Mass Loss, Tg, Melting and ΔH

<https://www.moldraw.com/blog/tga-dsc-viewer-guide.html>

A practical guide to the free MolDraw TGA and DSC viewer: open instrument exports, find mass-loss steps with DTG, and read Tg, melting, crystallisation, ΔH and % crystallinity.

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Short answer: Open the [TGA and DSC viewer](#), press **Open TGA / DSC file(s)** or drop a CSV, TA Instruments, NETZSCH or METTLER text export onto the page. The viewer lists each TGA step with its onset, DTG peak, mass loss and the final residue. For DSC it finds the glass transition, melting and crystallisation, with ΔH and % crystallinity. Your files stay on your device.

Try the TGA and DSC viewer here

Press **CaC2O4·H2O (TGA + DSC)** in the live viewer to load a classic three-step example.

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

Why use a browser viewer for thermal analysis?

Thermal analysis software is often licensed to the computer next to the instrument, and exports from different makers disagree on units and on which way an endotherm points. The MolDraw viewer reads the common text exports, lets you set the sign convention, and measures steps and peaks the same way every time.

TGA and DSC in brief

Thermogravimetric analysis (TGA) records the mass of a sample as it heats. Each drop is a mass-loss step, such as loss of water or solvent, or decomposition. The mass left at the end is the residue, such as ash, filler or an oxide.

The **DTG** curve is the derivative of mass with temperature. It turns each step into a peak at the point of fastest loss. The **onset** temperature is usually found with tangents: the tangent at the steepest point meets the plateau before the step.

Calcium oxalate monohydrate is the textbook example. It loses water (12.3 % of the starting mass), then carbon monoxide (19.2 %), then carbon dioxide (30.1 %), and leaves calcium oxide.

Differential scanning calorimetry (DSC) measures the heat flow into a sample compared with a reference. The **glass transition (Tg)** is a step, caused by a change in heat capacity (Δc_p). **Melting** is an endothermic peak. **Crystallisation** on cooling is exothermic, as is **cold crystallisation** on heating a quenched polymer such as PET.

The area of a peak gives the enthalpy ΔH . For a semicrystalline polymer, **crystallinity** is $X_c = (\Delta H_m - |\Delta H_{cc}|) / (\Delta H_{100\%} \times w) \times 100$, where $\Delta H_{100\%}$ is the melting enthalpy of a fully crystalline polymer and w is the polymer weight fraction. Pure metals such as indium check the temperature and enthalpy calibration.

Files the viewer opens

CSV or TXT	Temperature or time, mass or mass %, and heat flow columns.
Instrument exports	TA Instruments Universal Analysis or TRIOS text exports, NETZSCH Proteus ASCII exports and METTLER STARe table exports.
Mass	Mass in mg is converted to % of the starting mass.
Segments	Heating and cooling ramps are split into segments. Isothermal holds are skipped.

How to analyse a run step by step

1. Press **Open TGA / DSC file(s)**, or drop files on the box. To explore first, press **Filled polymer TGA**, **PET DSC** or **Indium calibration**.
2. Choose **TGA**, **DSC** or **TGA + DSC**, then the **Segment**, for example the first heating ramp.
3. Open **Settings**. Check **Heating rate (K/min)**, **Sample mass (mg)** and **In the file, endothermic is**. Pick **Endo up** or **Exo up** under **Plot**.
4. Read the **TGA steps** table: onset, midpoint, DTG peak, endset, mass loss and residue.
5. Read the **DSC events** table. Press **x** to drop a false event. If a peak was missed, zoom to it and press **Integrate current view as a peak**.
6. Under **DSC crystallinity**, pick a **Polymer** or type **$\Delta H_{100\%}$ (J/g)**, and set **Polymer fraction w (%)** for filled samples.
7. Tick **Add to compare instead of replacing** to overlay more runs. Save with **Export PNG** or **Export CSV**.

What the viewer does

- **TGA steps:** the DTG curve on a second axis, shaded step ranges, and mass loss in % and in mg when the sample mass is known.
- **DSC events:** Tg with onset, midpoint, inflection, endset and Δc_p . Peaks with onset, peak, endset and ΔH , shaded above the baseline.
- **Baselines and smoothing:** choose a **Linear** or **Sigmoid** DSC baseline, and set **DTG smoothing ($^{\circ}\text{C}$)**.
- **Crystallinity presets:** $\Delta H_{100\%}$ values for twelve common polymers, including PE, PP, PET, PLA and nylon 6.
- **Calibration check:** when a melting onset is close to indium, tin, zinc or bismuth, the viewer compares the onset and ΔH with typical reference values.
- **Peaks with mass loss:** in runs with both mass and heat flow, DSC peaks that overlap a TGA step are labelled "with mass loss", which helps tell decomposition from melting.
- **Combined view and export:** TGA + DSC puts mass and heat flow on two axes. The CSV holds the processed curves and the results tables.

Ways to use it in class and in the lab

- **Hydrates and solvates:** compare the measured water loss with the value from the formula, using the [molar mass calculator](#).
- **Filler and ash content:** read the residue of a filled polymer run in air.
- **Polymer crystallinity:** load a PET heating run, find cold crystallisation and melting, and get X_c .
- **Batch comparison:** overlay runs and compare onsets and residues.

Tips and limits

- Check the endotherm sign first. A wrong sign swaps the melting and crystallisation labels.

- ΔH is the peak area divided by the heating rate, so a wrong rate gives a wrong ΔH .
- Onsets shift with heating rate, sample mass and gas. Compare only runs measured the same way.
- **Integrate current view as a peak** adds a peak, not a glass transition.
- With the X axis set to **Time**, the viewer shows raw curves without analysis marks.

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

Questions and answers

What is the difference between the TGA onset and the DTG peak?

The onset is where the step starts, from a tangent extrapolated back to the plateau. The DTG peak is where mass is lost fastest. On heating, the DTG peak lies above the onset, so state which one you report.

Why does my melting peak show up as exothermic?

The sign convention in the file was guessed the wrong way. Change In the file, endothermic is to the other option. Plot only sets whether endotherms point up or down on screen.

Can I get ΔH in J/g if my heat flow is in mW?

Yes. Type the sample mass in Sample mass (mg). The viewer then divides the heat flow by the mass and reports ΔH in J/g.

How do I check my DSC calibration with indium?

Open your indium run. When a melting onset lies close to that of indium, tin, zinc or bismuth, the viewer shows the onset and ΔH differences from typical values. Use your standard's certificate for the final check.

Make Ball-and-Stick Figures for Slides and Posters: Themes Plugin

<https://www.moldraw.com/blog/themes-plugin-ball-and-stick-style.html>

Switch any 2D structure in MolDraw to a coloured ball-and-stick look in two clicks, then export it as PNG or SVG. A practical guide to the free Themes plugin, with tips and limits.

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Short answer: Themes is installed by default. Draw a structure, click **Color & style** in the toolbar and set **Look** to **Ball and stick**. Every atom becomes a coloured sphere and every bond a stick. Export it with **Download** as PNG or SVG. Set Look back to **Default** for a normal skeletal structure.

Why use a ball-and-stick style in 2D?

Skeletal formulas are the standard language of organic chemistry. They are compact and precise, but they assume the reader knows the rules: carbons sit at the corners and most hydrogens are not drawn. Beginners often miss atoms that are only implied.

A ball-and-stick picture shows each drawn atom as a sphere. Colour tells you the element at a glance, so oxygen, nitrogen and halogen atoms stand out. Double and triple bonds appear as two or three parallel sticks. This style matches the colour code that many model kits and 3D viewers use, so students can link the page to the model in their hands.

It works best where people look from a distance or need to spot heteroatoms quickly: lecture slides, posters, worksheets and introductory handouts. For journal figures and exam answers, skeletal structures are still the right choice.

What the plugin changes

Chloramphenicol in the Ball and stick look. Callout 1 is the Color & style button, callout 2 the Look menu.

Atoms	Shaded spheres in CPK colours. Sphere size follows the element's covalent radius, so chlorine looks larger than oxygen.
Bonds	Sticks: one for a single bond, two for a double or aromatic bond, three for a triple bond.
Scope	This design only, or every open design with Apply to all .
Export	PNG and SVG downloads keep the look.

How to install the Themes plugin

You do not need to. Themes is on by default and works without an account. If you removed it, open **Settings** (the gear), then **Plugins**, and add Themes back from the list.

How to make a ball-and-stick figure

1. Draw or load a structure. You can paste a SMILES or search a molecule by name.
2. Click **Color & style** in the toolbar.
3. Under **Theme**, set **Look** to **Ball and stick**.
4. Turn on **Apply to all** if every open design should use the same look. Turn it off to style only this design.
5. Adjust colours if you like. Ring fill, opacity and colour overrides in the same panel still work.
6. Click **Download** and choose PNG or SVG.

Ways to use it in class and beyond

- **Lecture slides:** coloured spheres stay readable from the back of a room, where thin skeletal lines can fade.
- **Introducing skeletal formulas:** show the same molecule in both looks side by side. Ask students to find each carbon in the skeletal version.

- **Posters and handouts:** export an SVG so the figure stays sharp at any print size.
- **Spotting functional groups:** red oxygen and blue nitrogen spheres make alcohols, carbonyls and amines easy to point out.

Tips and limits

- Only atoms you draw become spheres. To show hydrogens as white balls, draw them as explicit H atoms.
- The look leaves out atom labels, lone pairs, implicit hydrogens and R/S labels. Formal charges still show.
- Wedge and hash bonds are drawn as plain sticks. If stereochemistry matters, use the Default look.
- The picture is flat and keeps your 2D layout and angles. For a rotatable model, open the [3D molecular model viewer](#).
- Switch back to **Default** for journal-style skeletal structures.

Need ready-made molecules to style? Browse the [molecule library](#), or read our guide on [turning on the grid](#) to line up your figures.

Questions and answers

Is the ball-and-stick theme a 3D model?

No. It is a 2D drawing style with shaded spheres, laid out exactly like your drawing. Use the 3D viewer when you need a model you can rotate.

Do I need an account to use the Themes plugin?

No. Themes is installed by default and works without an account.

Which colours does it use?

Standard CPK colours: carbon grey, hydrogen white, oxygen red, nitrogen blue, sulfur yellow, chlorine green and bromine dark red.

Does the style change my structure or its SMILES?

No. A theme changes only how the structure is drawn. The atoms, bonds and chemistry stay the same, and you can switch back to Default at any time.

Read a UV-Vis Spectrum Online: λ_{max} , Beer-Lambert, Colour and Tauc Band Gap

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

A practical guide to the free MolDraw UV-Vis viewer: open JCAMP-DX or CSV spectra, find λ_{max} , get ϵ or concentration from $A = \epsilon cl$, read the sample colour and fit a Tauc band gap.

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

Short answer: Open a JCAMP-DX or CSV/TXT file in the free [MolDraw UV-Vis viewer](#), or press an example such as **β -Carotene**. The viewer lists the λ_{max} peaks, works out ϵ or concentration from $A = \epsilon cl$, names the colour the sample shows, overlays a series and fits a Tauc plot for a band gap. It runs in your browser, and your files stay on your device.

Try the UV-Vis viewer here

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

Why use a browser viewer for UV-Vis data?

UV-Vis is one of the quickest measurements in a lab. The slow part comes after: you have a file and need λ_{max} , a molar absorptivity, a figure or a band gap. In a spreadsheet that means converting units, finding maxima by eye and building plots by hand. The viewer does these steps on one page, with nothing to install.

The science in brief

λ_{max} . Molecules absorb UV and visible light when an electron moves to a higher orbital, as in $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ transitions. λ_{max} is the wavelength where a band absorbs most. Longer conjugation moves it to longer wavelengths. β -carotene, with eleven conjugated C=C bonds, absorbs in the blue part of the visible range.

To get a rough idea of where a compound should absorb before you measure it, [predict UV-Vis bands from a drawn structure](#) with the Spectroscopy plugin.

Beer-Lambert law. Absorbance is $A = \epsilon cl$, where ϵ is the molar absorptivity ($\text{L mol}^{-1} \text{cm}^{-1}$), c the concentration (mol/L) and l the path length (cm). Also, $A = -\log_{10} T$. The law holds best for dilute solutions.

Colour. A sample looks the colour complementary to the light it absorbs. A band in the blue makes a solution look yellow. A band in the green, as in permanganate, makes it look purple.

Tauc plot. For a semiconductor, plot $(\alpha h\nu)^2$ against photon energy $h\nu$ for a direct allowed transition, or $(\alpha h\nu)^{1/2}$ for an indirect allowed one. Extend the straight part of the absorption edge to zero. The crossing point estimates the optical band gap, E_g .

Files you can open

- **JCAMP-DX** (.jdx, .dx). The viewer reads the x and y units from the file.
- **CSV or TXT** with two columns. The x column can be in nm, μm , cm^{-1} or eV. The y column can be absorbance or transmittance. Without headers, the viewer guesses from the numbers.

Pick several files at once to overlay them. To practise, use the simulated examples or [download the sample .jdx](#).

How to analyse a spectrum, step by step

1. Press **Open UV-Vis file(s)** or drop files on the box. You can also press an example: **β -Carotene**, **KMnO₄**, **Dye series (5 conc.)**, **ZnO band gap** or **Sample .jdx file**.
2. Choose **Absorbance** or **%T** for the y axis, and **nm**, **eV** or **cm⁻¹** for the x axis.
3. Read the **λ_{max} peaks** table. It gives each peak in nm, eV and cm⁻¹ with its absorbance and colour. Move the **Peak prominence** slider if a shoulder is missing or small bumps show up.
4. In the **Beer-Lambert** box, enter **Path l (cm)** and a **Concentration** in mol/L, mmol/L or $\mu\text{mol/L}$ to get ϵ and log ϵ . Or enter ϵ to get the concentration. Tap a table row or the plot to use another wavelength. **Use λ_{max} again** switches back.
5. For a band gap, open **Tauc plot and band gap**, choose the **Transition**, and press **Auto fit** or type your own **Fit from (eV)** and **to** values.
6. Press **Export PNG**, **Export CSV** or **Tauc PNG**.

What the viewer does

Peaks	Up to eight maxima for the selected spectrum, largest first.
Beer-Lambert	ϵ and log ϵ from a concentration, or concentration from ϵ , at λ_{max} or a wavelength you tap. A warning appears above $A = 1.5$.
Colour	The colour of the strongest visible band (380 to 780 nm), from a standard colour wheel.
Overlay	Several spectra in different colours, each with a show box, and an option to normalise each to its maximum.
Tauc plot	Direct or indirect, automatic or manual fit range, Eg in eV and nm, and R^2 .
Export	PNG of the spectrum or Tauc plot, and CSV of the visible spectra in the current units.

Ways to use it in class and in the lab

- **Conjugation and colour:** load β -Carotene, then add KMnO₄ with **Add to the plot instead of replacing**. Compare where each absorbs and why one looks yellow and the other purple.
- **Checking Beer-Lambert:** load the dye series. Select each spectrum by its name and enter its concentration. If the law holds, ϵ should come out about the same each time.
- **Unknown concentration:** enter ϵ from a calibration or the literature to get c.
- **Semiconductor films:** use the ZnO example to learn the Tauc method, then open your own film spectrum. For an organic semiconductor, compare that optical gap with the electrochemical gap from [HOMO and LUMO estimates in the cyclic voltammetry viewer](#).
- **Lab reports:** export a PNG for the figure and a CSV for the data.

Tips and limits

- Record a solvent blank on the spectrometer. The viewer does not subtract one.
- A weak shoulder on a large band may not appear as a peak.

- The Tauc plot uses absorbance in place of the absorption coefficient α . This is fine for finding where the line meets zero. For powders measured by diffuse reflectance, convert to the Kubelka-Munk function before you open the file.
- Check the shaded fit range and R^2 before you report Eg. Another range can give another answer.
- The colour is a guide. Real colour also depends on band width, concentration and the light source.
- The CSV puts all visible spectra on the x values of the first one, so spectra with different grids are interpolated.

Questions and answers

What absorbance range gives reliable Beer-Lambert results?

Aim for absorbances between about 0.1 and 1. Above 1.5 very little light reaches the detector, stray light matters and the line bends, so the viewer shows a warning. Dilute the sample or use a shorter cell.

Why does a sample that absorbs blue light look yellow?

We see the light that is not absorbed. If a band removes blue light from white light, the rest looks yellow, the complementary colour on the colour wheel.

Should I use a direct or an indirect Tauc plot?

Use the transition type known for your material. ZnO, for example, has a direct gap and silicon an indirect one. If the type is not known, say which plot you used when you report the band gap.

Can I use the viewer with unpublished data?

Yes. The page reads and draws your files in the browser, so the files stay on your device.

XPS Peak Fitting in Your Browser: Charge Correction, Shirley and Atomic %

<https://www.moldraw.com/blog/xps-viewer-peak-fitting-guide.html>

A practical guide to the free MolDraw XPS viewer: open VAMAS, CasaXPS or CSV data, charge correct to C 1s, subtract a Shirley background, fit peaks and doublets, and get atomic %.

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

Short answer: Open a VAMAS (.vms), CasaXPS text or CSV file in the free [MolDraw XPS viewer](#), or press **C 1s (polymer)**. Press **Set from C 1s** to charge correct, keep the Shirley background, then press **Auto peaks** or **C 1s template** and **Fit**. Read the atomic % and export a PNG or a CSV with the fit table. Your files stay on your device.

Try the XPS viewer here

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

Why fit XPS data in a browser?

XPS data often arrives as a VAMAS or text file from a shared facility. To read it, you correct for charging, remove the background, fit components and turn areas into composition. Full packages do this well, but they are not always at hand. The viewer covers the core steps on one page, for a first look, for teaching or for checking a fit someone sent you.

The science in brief

Binding energy. X-rays eject electrons from core levels. The spectrometer measures their kinetic energy, and $BE = h\nu - KE$, with the work function handled by the calibration. Al K α gives $h\nu = 1486.6$ eV and Mg K α 1253.6 eV. Only electrons from the top few nanometres escape, so XPS sees the surface.

Chemical shift. Bonds to more electronegative atoms move a core level to higher binding energy. In C 1s, C-C/C-H sits lowest, then C-O, C=O and O-C=O.

Charge correction. Insulators charge up and every peak shifts by the same amount. A common fix is to set the C-C/C-H peak of adventitious carbon to 284.8 eV, the viewer's default. Some labs use 285.0 eV. This is a convention with known limits, so state the value you used.

Shirley background. Electrons that lose energy on the way out raise the signal on the high binding energy side of each peak. The Shirley background models this step.

Spin-orbit doublets. p, d and f levels split into two peaks with a fixed area ratio: 1:2 for p, 2:3 for d and 3:4 for f. The split depends on the element, for example about 13.6 eV for Fe 2p in the viewer's table.

Atomic %. Divide each element's peak area by its sensitivity factor, then normalise the results to 100%.

Files you can open

- **VAMAS** (.vms), the ISO 14976 exchange format, with regular scans.
- **CasaXPS text exports** with K.E. or B.E. columns.
- **CSV, TXT, DAT or TSV** with an energy column and an intensity column.

Open one file at a time. Each region in a file gets its own button above the plot. To practise, [download the sample .vms](#), which holds a survey, C 1s and O 1s. All examples are simulated.

How to fit a region, step by step

1. Press **Open XPS file** or drop a file. Or press an example: **C 1s (polymer)**, **Si 2p (Si / SiO₂)**, **Fe 2p doublet**, **Survey scan** or **Sample .vms**.

2. If your data is in kinetic energy, set **Energy axis** to Kinetic energy and choose the **Source**.
3. Press **Set from C 1s**, or type a **Charge shift (eV)**. The reference starts at 284.8 eV and can be changed.
4. Pick a region, check the **Core level** (for example C 1s) and choose a **Background**. Zoom in and press **Fit window = current view**, or use **Whole region**.
5. Press **Auto peaks**, or choose **Add peak** and tap the plot, or press **C 1s template**. Then press **Fit**.
6. Edit label, BE, FWHM, %L or doublet type in the table, lock values, or drag peaks in **Move peak** mode. Press **Fit** again.
7. Check the envelope and the residual line under the spectrum. Then press **Export PNG** or **Export CSV**.

What the viewer does

Background	Shirley, linear or none, over a fit window you choose.
Peak shape	Gaussian-Lorentzian product, GL(m).
Fitting	Auto or manual peaks, a C 1s template, locks, Same FWHM for all peaks and Fit %L too . Reports the RMS residual and, where it can, a reduced χ^2 .
Doublets	p, d or f doublets with a split from a built-in table that you can edit.
Assignments	A suggested chemical state for each peak.
Atomic %	From two or more fitted regions, with sensitivity factors you can edit.
Survey	Element list with lines, confidence and a rough atomic %. Auger regions are shaded.
Export	PNG of the plot. CSV with the data, background, components, envelope, fit table and atomic %.

Ways to use it in class and in the lab

- **Polymer surface treatment:** fit C 1s before and after plasma treatment. Larger C-O, C=O and O-C=O components point to surface oxidation. XPS sees only the top few nanometres. For the bulk polymer, [find its melting point and crystallinity in the TGA and DSC viewer](#).
- **Native oxide on silicon:** the Si 2p example shows Si as a narrow doublet and SiO₂ as a broader peak at higher binding energy.
- **Unknown surfaces:** open a survey to see which elements are present.
- **Composition:** fit C 1s and O 1s in the sample .vms and read the O/C ratio from the atomic % box.

Tips and limits

- Give every component a chemical reason. Extra peaks always lower the residual, but that does not make them real.
- Metals often need an asymmetric line shape, which the viewer does not model. Transition metal 2p spectra can also show satellites and multiplet splitting, so a simple doublet fit is an approximation.

- The built-in sensitivity factors are approximate Al K α values relative to C 1s = 1. Enter factors from your instrument library for real numbers.
- Literature binding energies spread by a few tenths of an eV. Check suggested assignments against a reference.

Questions and answers

Why are all my peaks about 1 eV higher than expected?

An insulating sample charges up as electrons leave it, and every peak moves to higher binding energy by the same amount. Press Set from C 1s to move the C-C / C-H peak to the reference energy, or type the shift yourself.

How many components should I fit to a C 1s peak?

Only as many as the chemistry supports. Start from the bonds you expect in the sample, keep the widths similar, and add a peak only when the residual shows a clear, repeatable shape that a known chemical state explains.

Why use a Shirley background instead of a linear one?

Electrons that lose energy on the way out raise the signal on the high binding energy side of a peak. A Shirley background follows that step. A straight line can work for small peaks on a flat background.

Can I get atomic % from a survey scan alone?

Only roughly. The viewer gives a rough atomic % in the survey table. For better numbers, fit narrow scans of each element and use sensitivity factors from your own instrument.