

Import, export and sharing

MolDraw Docs · LabCanvas · 3 pages · moldraw.com/docs/

Copy and paste SMILES

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

- 1 Select a molecule, or nothing for the whole canvas.
- 2 Click **Copy SMILES** in the editor row.
- 3 To draw from text, click **Paste SMILES** and paste the string.

More copy formats

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

TIP

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

To learn SMILES, read the SMILES notation guide.

Questions and answers

How do I get the SMILES of my drawing?

Can I paste a MOL file?

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

Download and file formats

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

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

Which format to pick

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

Save the whole canvas

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

Questions and answers

What format should I use for a journal figure?

Can I export to ChemDraw?

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

Search PubChem

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

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

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

Questions and answers

Can I search by CAS number?

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