

Embed and developer tools

MolDraw Docs · LabCanvas · 4 pages · moldraw.com/docs/

MolScript

Short answer: MolScript is a short text language for reaction schemes and curly arrow mechanisms. Open Templates in the left rail and pick the MolScript tab. Write species as SMILES and one move line per arrow, then click Draw on canvas. MolDraw draws the scheme and checks every arrow.

You write a few lines of text. MolDraw draws the structures, plus signs, reaction arrows, conditions, lone pairs, charges and curly arrows. The result is normal canvas content. You can edit it, export it or save it as chemfig. The AI chat also writes MolScript when you ask it for a mechanism.

For a long tutorial, read MolScript: a text language for mechanisms. For finished examples, see the MolScript gallery.

Draw your first script

- 1 Open the editor and click **Templates** in the left rail.
- 2 Click the **MolScript** tab.
- 3 Pick a script from **Example...**, or type your own.
- 4 Read the list under the editor. **No problems: the arrows give the products drawn** means it is ready.
- 5 Click **Draw on canvas**, or press **Ctrl** + **Enter**.

The scheme is placed beside your drawing as one undo step. On a phone, the editor opens as a bottom sheet.

A complete example

This is the SN2 script from the examples list:

```
title: SN2 of bromomethane
[OH-:1] "hydroxide" + [CH3:2][Br:3] "bromomethane" ->[SN2][acetone] C0 "methanol" + [Br-]
move :1 -> 1..2
move 2-3 -> 3
```

- `title:` puts a heading above the scheme.
- Species are SMILES. `:1` , `:2` , `:3` are atom map numbers on the atoms the arrows touch.
- `"hydroxide"` is a label drawn under the species.
- `->[SN2][acetone]` is a reaction arrow with text above and below it.
- `move :1 -> 1..2` is a curly arrow from the lone pair on atom 1 to a new bond between 1 and 2.
- `move 2-3 -> 3` moves the 2 to 3 bond onto atom 3.

Scheme operators

Write	Draws
<code>+</code>	Plus between co-reactants or co-products
<code>-></code>	Reaction arrow
<code><-></code>	Resonance arrow
<code><=></code>	Equilibrium arrow
<code>=></code>	Retrosynthesis arrow

Put spaces around operators. A line that starts with an operator continues the scheme, so a multi-step mechanism reads one step per line.

Curly arrow ends

End	Meaning
<code>:n</code>	Lone pair on atom n
<code>n</code>	Atom n (a radical's arrow starts at its dot)
<code>n-m</code>	The existing bond between n and m
<code>n..m</code>	A bond being formed between n and m
<code>hn</code>	A hydrogen on atom n

Use `->` in a move for a two-electron arrow and `~>` for a one-electron fish-hook. This example from the gallery splits bromine with light:

```
[Br:1][Br:2] ->[hv] [Br] + [Br]
move 1-2 ~> 1; 1-2 ~> 2
```

`push` writes a resonance chain once. `push :3 > 1 > 2` is the same as `move :3 -> 3-1; 1-2 -> 2:`

```
C[C:1](=[0:2])[0-:3] <-> CC([0-])=O
push :3 > 1 > 2
```

Options and directives

- **Species options** go in braces after a species. Examples: `{ts}` for a transition state bracket, `{highlight=2/3-4:blue}`, `{ox=1:II}` for an oxidation state, `{flip}`.
- **Names:** `let enolate = [CH2-:1]C(C)=O "enolate"`, then use `$enolate`.
- **Abbreviations:** `[Ph]`, `[Me]`, `[tBu]`, `[Boc]`, `[R1]`, `[Ar]` and others.
- **Directives:** `title:`, `per-row:` (2 to 8, default 4) and `layout:` (`row`, `grid`, `cycle` or `branch`). Also `number: species`, `check:` (`warn`, `strict` or `off`) and `#` for a comment.

Electron checking

MolDraw replays every arrow on the electrons. The structures it gets must match the products you wrote. Problems show under the editor with a line number, for example *C (map 2) has no lone pair*. Click a problem to jump to its line. It also reports an atom over its octet and an arrow from an atom with no electrons left. Stereocentres are followed too, so a missed SN2 inversion is reported. **Draw on canvas** stays off while there are errors.

Editor help

- Words, options and map numbers are suggested as you type. Press **Tab** to take the first suggestion.
- **Language guide** opens the full tutorial.
- Bad lines are marked in the editor.

More examples

The gallery shows the same mechanisms that are in the **Example...** list. For curly arrow drawing by hand, see curved arrow mechanisms. For arrow pushing theory, read the curly arrows guide.

Questions and answers

What is MolScript?

MolScript is a text language for reaction schemes and curly arrow mechanisms. You write SMILES and move lines, and MolDraw draws and checks the scheme.

Where is the MolScript editor in MolDraw?

Click Templates in the left rail and open the MolScript tab.

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

Use ~> instead of → in a move line, for example move 1-2 ~> 1.

Why does MolScript say an atom has no lone pair?

The arrow starts at a lone pair the atom does not have after earlier arrows. Check the map number or start the arrow at a bond.

Can I export a MolScript scheme to LaTeX?

Yes. The drawn scheme is normal canvas content, so you can export it as chemfig code like any drawing.

Source: <https://www.moldraw.com/docs/developers/molscript-language-for-reactions-and-mechanisms/>

Embed MolDraw and demos

Short answer: To put the editor on your page, paste an iframe that points to <https://www.moldraw.com/embed>. Set its height to about 640 pixels. To show a step by step demo, use an iframe to <https://www.moldraw.com/demos/embed.html?demo=<id>>, or the `<moldraw-demo>` tag on moldraw.com pages.

You do not host anything. The frame loads MolDraw from moldraw.com and your page stays yours. The embed article has a live preview and a **Copy embed code** button.

Embed the editor

- 1 Copy the snippet below.
- 2 Paste it into the HTML of your page, or into an HTML block in your course or blog tool.
- 3 Change `height` to fit your layout.
- 4 Open the page and draw a bond to test it.

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

Size the frame

Use	Height
Short page or quick sketch	About 480
Default, toolbar and a small structure	640
Reaction schemes	About 800

Keep `width="100%"` so the editor fills the column. On a phone, a tall frame means more scrolling.

What readers get

- The full drawing tools, canvas and 3D panel.
- A slim bar at the top with **Edit in MolDraw**. It opens the full editor in a new tab and leaves your page open.
- No account needed to draw or download from the frame.
- **Sign in** inside the frame opens moldraw.com in a new tab.

NOTE

Only `/embed` may be framed on other sites. Other MolDraw pages refuse to load in a cross site frame.

Embed an interactive demo

A demo shows a MolDraw task on a light copy of the editor. A cursor moves to each control and a caption explains the step. A demo is about 10 KB and stays sharp at any size. Browse them in the demo gallery.

On another site

```
<iframe src="https://www.moldraw.com/demos/embed.html?demo=turn-on-grid"
  title="MolDraw demo: Turn on the canvas grid" loading="eager"
  style="width:100%;max-width:980px;height:640px;border:0"></iframe>
```

Query	Values	Default
<code>demo</code>	The demo id, as in the gallery	<code>turn-on-grid</code>
<code>theme</code>	<code>light</code> , <code>dark</code> or <code>auto</code>	<code>auto</code> , which follows the reader's system theme
<code>autoplay</code>	<code>false</code> to wait for a click	Plays
<code>loop</code>	<code>false</code> to stop at the end	Loops

The frame reports its height to your page with a `moldraw-demo:height` message. Listen for it and set the iframe height to avoid a scroll bar.

On a moldraw.com page

```
<script src="/demos/player.js" defer></script>
<moldraw-demo src="/demos/turn-on-grid.json"></moldraw-demo>
```

The tag takes `src` , `autoplay="false"` , `loop="false"` and `theme="light"` , `"dark"` or `"auto"` .

Controls

- `Left` and `Right` move between steps. `Space` plays or pauses.
- **Try it yourself** swaps the copy for the real editor and runs a guided tour of the same steps. It runs in a sandbox, so the reader's own settings and designs are not changed.

Write your own demo

A demo is one JSON file with a title, a starting state and a list of steps. The authoring guide lists every target, action and state key. The grid article shows a demo inside a blog post.

Common problems

Symptom	Fix
The frame is blank	Your site or course tool blocks iframes. Use an HTML or embed block that allows them, or link to MolDraw instead.
The editor is cramped	Raise <code>height</code> . Readers can also click Edit in MolDraw .
The demo frame has a scroll bar	Listen for <code>moldraw-demo:height</code> and set the iframe height.

To open the editor with a structure already drawn, use a link instead of a frame. See URL parameters and deep links.

Questions and answers

How do I embed a molecule editor on my website?

Paste an iframe with src set to <https://www.moldraw.com/embed> and a height of about 640 pixels. Readers can draw right on your page.

Do readers need a MolDraw account to use the embed?

No. They can draw and download in the frame without an account. Edit in MolDraw opens the full editor in a new tab.

Why is the embedded MolDraw frame blank?

Your platform probably blocks iframes. Use an HTML or embed block that allows them, or link to [moldraw.com](https://www.moldraw.com).

How do I make the demo iframe fit its content?

Listen for the `moldraw-demo:height` message from the frame and set the iframe height to the value it sends.

Source: <https://www.moldraw.com/docs/developers/how-to-embed-moldraw-and-interactive-demos/>

URL parameters and deep links

Short answer: Add a query to the MolDraw address to open the editor with a structure drawn, for example [https://www.moldraw.com/?smiles=CCN\(CC\)CC](https://www.moldraw.com/?smiles=CCN(CC)CC). Other parameters load a reaction, a molfile, an InChI or a template. Some start a guided tour, a tutorial video or sign in.

Deep links let you share a structure, a reaction or a lesson in one click. The structure parameters work on the editor address, <https://www.moldraw.com/>.

Make a structure link

- 1 Copy the SMILES of your structure. Use **Copy SMILES** in the editor. See copy and paste SMILES.
- 2 URL encode it. Characters like `#`, `=` and `+` must be encoded (`%23` , `%3D` , `%2B`).
- 3 Add it after <https://www.moldraw.com/?smiles=>.
- 4 Open the link. The editor starts with that structure on an empty canvas.

The link does not replace the reader's saved designs. Their last design stays in **My designs**.

Structure parameters

Parameter	Value	Example
<code>smiles</code>	A SMILES string	/?smiles=CC(C)Cc1ccc(cc1)C(C)C(=O)=O
<code>reaction</code>	Reaction SMILES with <code>>></code> between reactants and products	/?reaction=C%3D0.C%5BMg%5DBr%3E%3ECCO
<code>mol</code>	A molfile (also read as <code>molfile</code> or <code>sdf</code>)	Use the hash for long files
<code>cdxml</code>	ChemDraw CDXML text	
<code>inchi</code>	An InChI string	/?inchi=InChI%3D1S%2FCH4%2Fh1H4
<code>template</code>	The id of a Templates panel scheme	/?template=claisen-condensation

Each structure parameter also works after `#` instead of `?` , for example

<https://www.moldraw.com/#mol=...>. The part after `#` is never sent to the server, so use it for long molfiles. If a link has several structure parameters, `reaction` wins, then `mol` , `cdxml` , `inchi` and `smiles` .

A reaction link draws the reactants, an arrow and the products. A template link draws the named reaction or mechanism as an editable scheme. If the id is unknown you see *Template "..."* was not found. The named reaction pages use template links for their **Open full mechanism in MolDraw** buttons.

Learning and help parameters

Parameter	Value	What it does
<code>tour</code>	A demo id, for example <code>turn-on-grid</code>	Runs a guided tour in the real editor. It rings each control and waits for the reader.
<code>tutorial</code>	An 11 character YouTube video id	Opens a floating tutorial video over the editor. Drag it, collapse it or close it.
<code>t</code>	Seconds, used with <code>tutorial</code>	Starts the video at that time.

Demo ids come from the demo gallery. See [embed MolDraw](#) and [demos](#).

Account parameters

Parameter	What it does
<code>signin=1</code>	Opens the sign in window
<code>signup=1</code>	Opens the create account window
<code>pro=waitlist</code>	Opens the Founding Lifetime License offer

See [sign in](#) and [create a free account](#).

Page addresses

Address	Opens
<code>/</code>	The editor in English
<code>/de/</code> , <code>/es/</code> , <code>/fr/</code> , <code>/ja/</code> , <code>/zh/</code> and others	The editor in that language
<code>/my</code>	My designs
<code>/embed</code>	The editor for an iframe on your own site

A language the reader picked in the app wins over the address. See [change the language](#).

Links from AI agents

When an AI agent works in MolDraw through the MCP connector, it can return an **open in MolDraw** link. That link carries a share token and opens the agent's structure in the editor. These links expire with the agent's working structure.

Tips

- Test a link in a private window. You then see what a new visitor sees.
- Put structure links in slides, worksheets and chat messages. Readers get an editable structure, not a picture.
- To make a SMILES from a name first, use the name to structure tool or the SMILES notation guide.

Common problems

Symptom	Fix
The link opens an empty canvas	The SMILES was not encoded. Encode <code>#</code> , <code>+</code> and <code>=</code> .
Only part of a molfile arrives	The address was too long for the server. Put the molfile after <code>#</code> instead of <code>?</code> .
The structure looks wrong	Check the SMILES in Paste SMILES first.

Questions and answers

How do I open MolDraw with a SMILES already drawn?

Add `?smiles=` and the URL encoded SMILES to `https://www.moldraw.com/`. The editor opens with that structure.

Can I link to a reaction in MolDraw?

Yes. Use `?reaction=` with a reaction SMILES such as `CC=O.N>>CC=N`, URL encoded. MolDraw draws reactants, arrow and products.

Does a SMILES link overwrite my saved drawing?

No. The link opens on an empty canvas. Your earlier designs stay in My designs.

How do I share a molfile in a link?

Put it after #mol= instead of ?mol=. The hash part is not sent to the server, so long files fit.

Source: <https://www.moldraw.com/docs/developers/moldraw-url-parameters-and-deep-links/>

Connect AI agents with MCP

Short answer: Add <https://mcp.moldraw.com/mcp> as a remote MCP server in your AI app. Sign in with your MolDraw account and click Approve. The agent can then search compounds, create and edit structures, export files and save designs to My designs.

MCP (Model Context Protocol) is a standard way for AI apps to use outside tools. MolDraw runs a hosted MCP server. An AI agent can use it to draw and edit structures with the same operations as the editor. This is separate from the AI chat inside MolDraw, which uses your own API key.

Connect your AI app

- 1 Open the connector or MCP settings of your AI app.
- 2 Add a remote server with the URL `https://mcp.moldraw.com/mcp`.
- 3 Your browser opens MolDraw. Sign in, or create a free account.
- 4 Read the page **Let ... use MolDraw**. It lists who is asking and what the app can do.
- 5 If asked, add your name and designation. Then click **Approve**.
- 6 Back in your AI app, ask it to draw a structure.

The same address works for every MCP client. You sign in on the MolDraw page, so your MolDraw password is never shared with the AI app. You can disconnect later from the app that asked for access.

What the agent can do

Tool	What it does
Search molecule	Finds a compound by name, CAS number or PubChem CID
Create structure	Starts a working structure from SMILES, a molfile or a name
Get molecule	Reads counts, SMILES, formula and atom ids, with an image preview
Modify structure	Adds groups, changes atoms or bonds, deletes atoms, adds fragments, swaps substructures
Convert structure	Converts between SMILES, molfile and 3D SDF
Export structure	Exports SVG, PNG, molfile, SMILES or 3D SDF

Tool	What it does
Save, list and open designs	Reads and writes your My designs
List editor tools and Editor action	Runs named editor operations: reaction schemes with plus signs and reagent arrows, text labels, alignment, library templates, glassware, orbitals, rings, colours, clean up and aromatize

Results include an image of the structure and an **open in MolDraw** link. Apps that support MCP Apps also show an inline MolDraw editor in the chat.

Example prompts

- *Draw caffeine.*
- *Change the methyl group at position 7 to ethyl.*
- *Give me the SMILES, then export SVG.*
- *Draw the Claisen condensation as a scheme with reagents on the arrow.*

Privacy and limits

- Structures the agent creates are working documents. They last 7 days unless you save them as a design.
- Saved designs go to your normal My designs library.
- Chat transcripts are not stored. The server only sees tool calls and structure data.
- Every working document is tied to your account.
- Each account can make up to 120 tool calls per minute.
- Tools that change a structure are marked apart from tools that only read.

Read the full MCP privacy and security notes.

Common problems

Symptom	Fix
The app cannot connect	Check the URL ends in <code>/mcp</code> . Your app must support remote MCP servers over HTTP.
The sign in page says the link is missing data	Start the connection again from your AI app. Do not open the consent page by hand.
The agent's link opens an old structure	Working documents expire after 7 days. Ask the agent to save a design.

Symptom	Fix
Calls fail after many quick edits	You hit the rate limit. Wait a minute.

For links the agent returns, see URL parameters and deep links. For text based mechanisms an agent can write, see MolScript.

Questions and answers

Does MolDraw have an MCP server?

Yes. Point any MCP client at <https://mcp.moldraw.com/mcp> and sign in with your MolDraw account.

Do I need a MolDraw account to use the MCP connector?

Yes. The connector signs in with your MolDraw account. A free account works.

Can the AI agent save drawings to My designs?

Yes. It can save, list and open your designs. Other working structures expire after 7 days.

Does the MCP connector need my AI API key?

No. Your AI app runs the model. MolDraw only provides the drawing tools.

Source: <https://www.moldraw.com/docs/developers/connect-ai-agents-to-moldraw-with-mcp/>