



**Schrödinger**

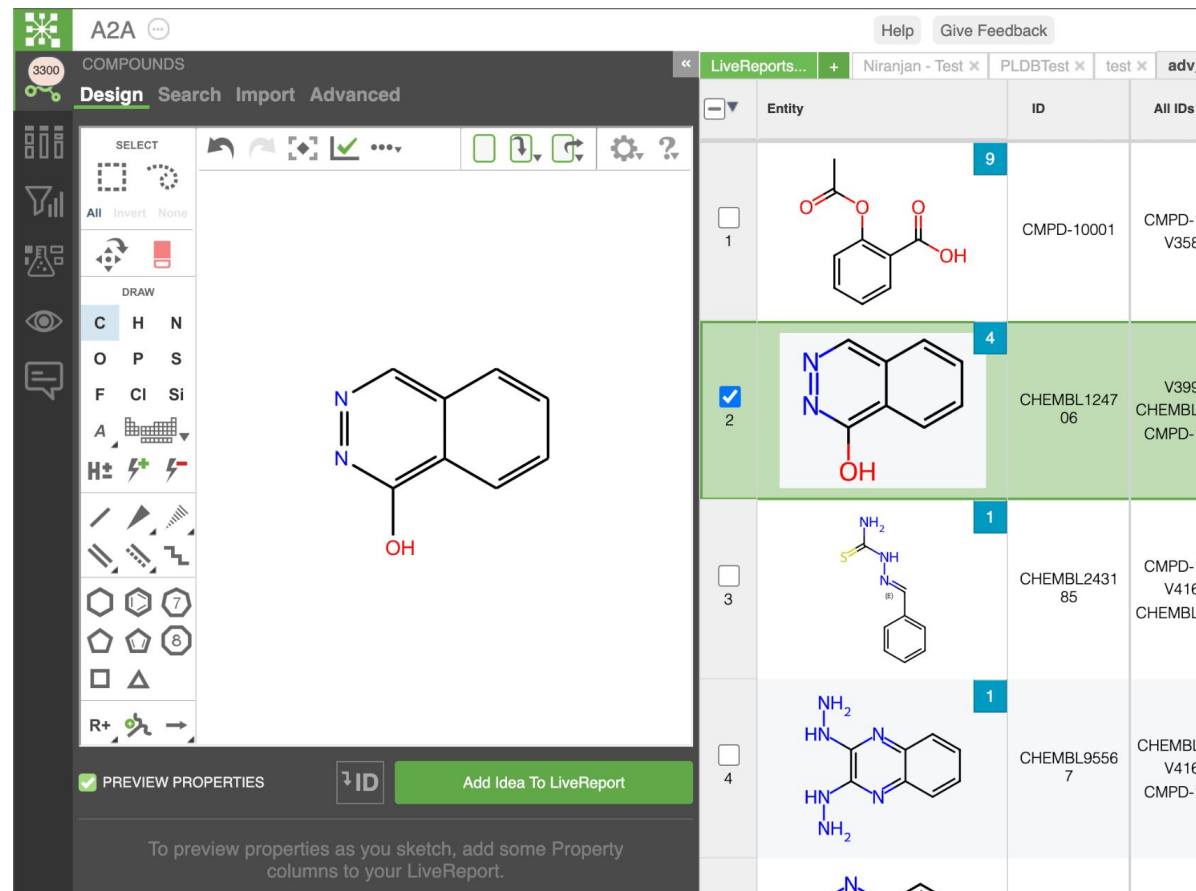
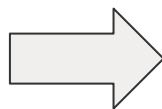
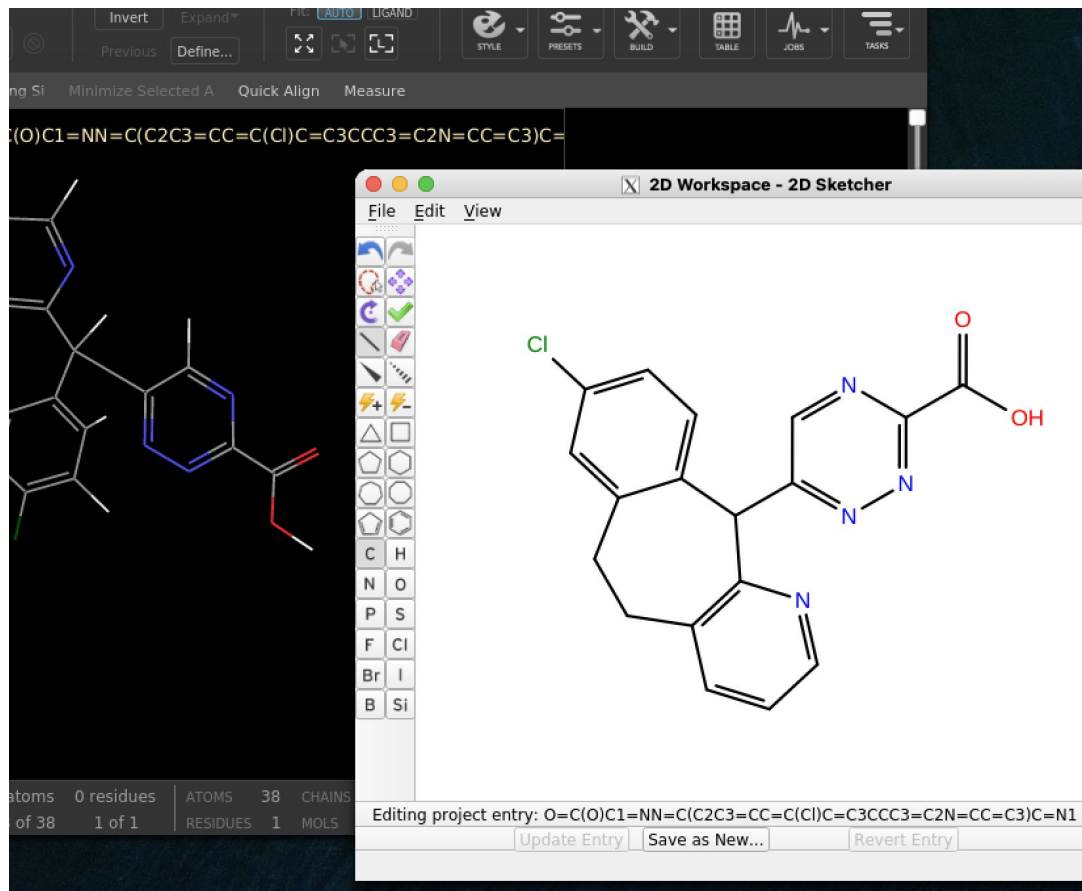
# **Building a Cross-Compiled 2D Sketcher**

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# The Need

Need for a browser compatible sketcher using RDKit as it's chemistry engine



# A WebAssembly Sketcher

Use emscripten to cross-compile sketcher  
C++ executable into WASM

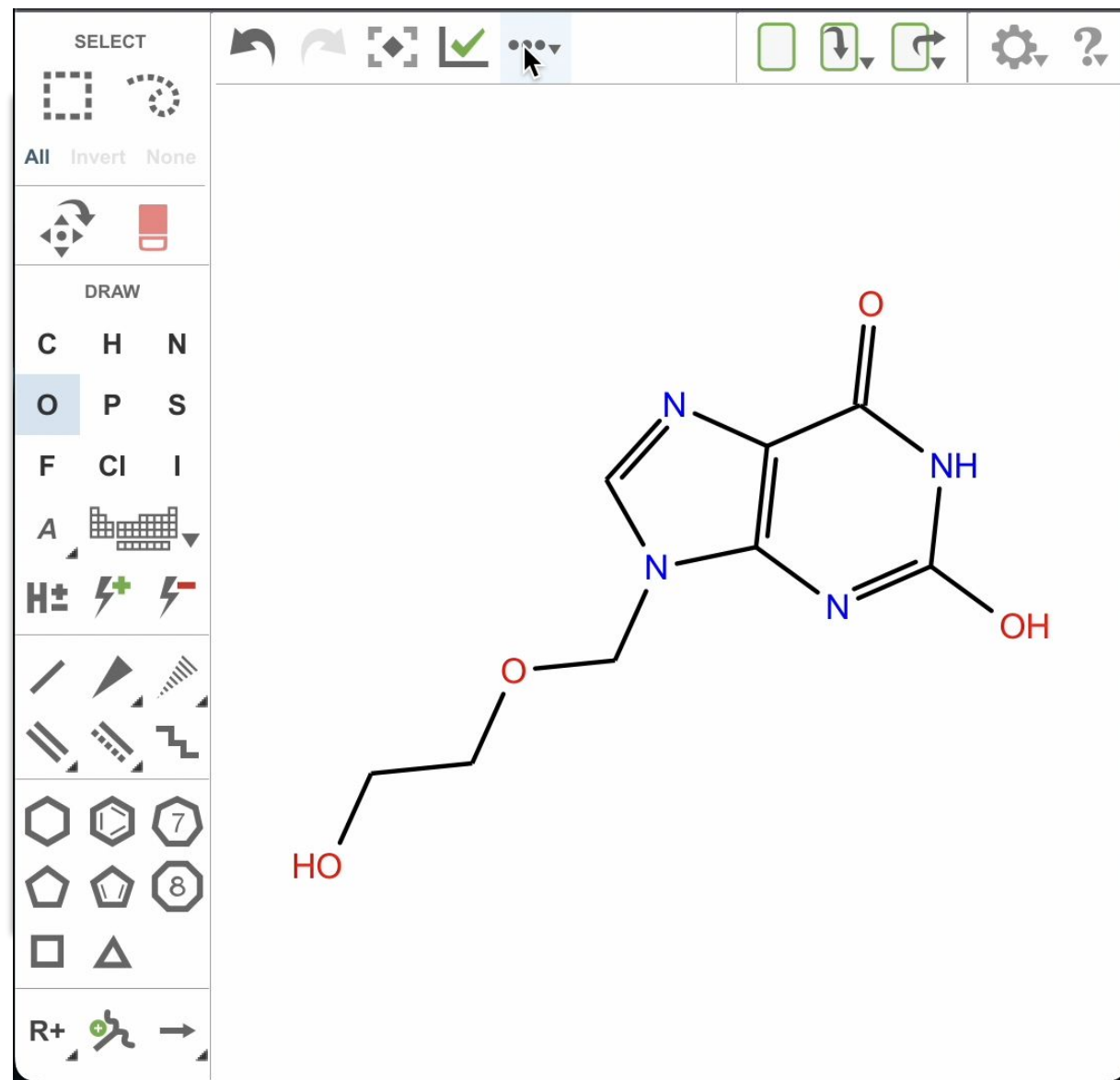
Dependencies:

- RDKit
- Qt6
- coordgenlibs
- zlib, boost

Overhaul of the UI

Comparable tools to other sketchers

Consistency across Schrodinger platform



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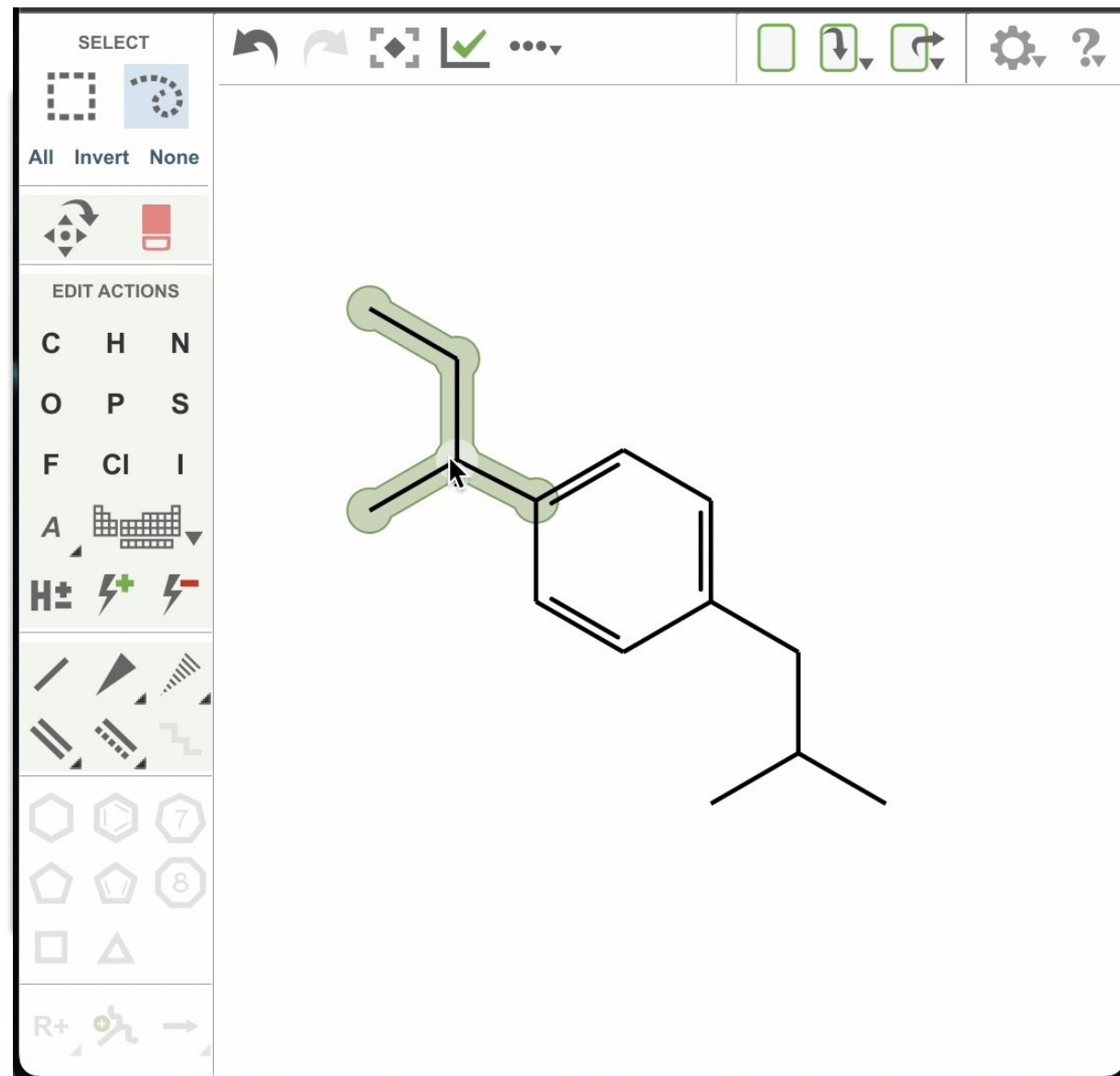
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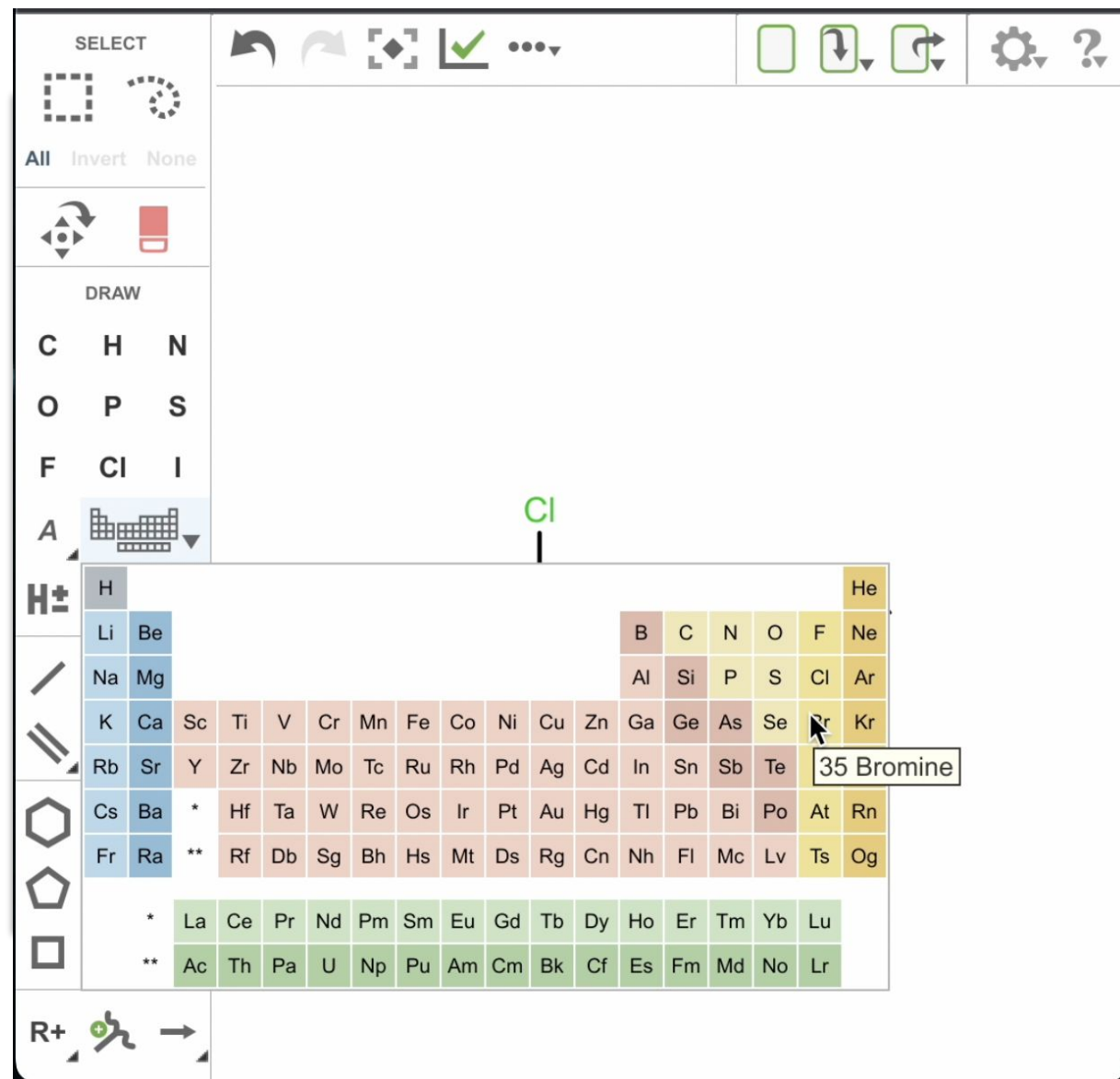




# RDKit Engine

The underlying model is an RWMol, which in addition to general molecular editing, uses RDKit for:

- stereochemistry perception
- coordinate generation
- hydrogen addition/removal
- valence errors
- serialization/deserialization support
- building query molecules
- coloring scheme



# Usability

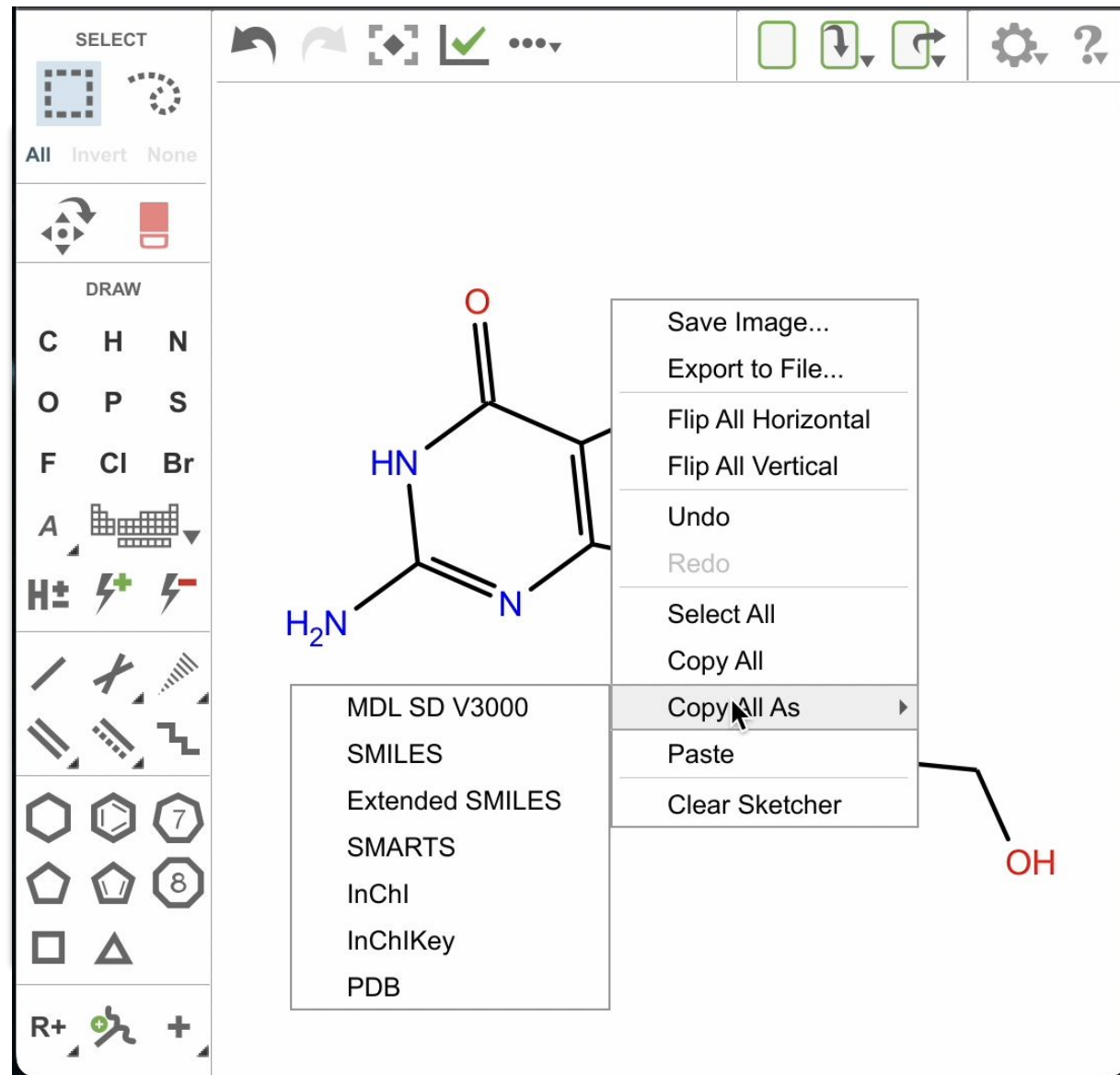
UI overall to address discoverability and consistency throughout:

- implicit mode indications
- sensible hotkeys
- 3-button mouse support
- rich context menus

Continuous feedback from users within Schrödinger

Short term: free public webpage

Long term: open source



# Future Improvements

The screenshot displays several key features of the Schrödinger software interface, highlighting planned future improvements:

- Valence and Heteroatom Settings:** A menu on the left includes checked options for "Valence Errors" and "Heteroatom Colors", along with "Stereo Center Labels", "Implicit Hydrogens", and links to "2D Settings..." and "Diagram Settings...".
- 2D Settings Dialog:** A dialog box titled "2D Settings" contains options for "Label all carbons" and "Color by molecule (overrides heteroatom color)", both currently unchecked. It also features sliders for "Atom font size" (set to 17.0) and "Bond line width" (set to 2.20), and a "Reset to Defaults" button.
- Functional Groups Search:** The "Functional Groups" tab is active, showing a search for "SO" with a list of 6 matches: SO2, SO2Cl, SO2NH2, SO2Ph, SO3H, and SO4. The SO2 entry is selected, and its structure (O=S=O) is displayed in the center.
- Organics Library:** The "Organics" tab shows a library of fragments. "Fragment-1" (a steroid-like structure) is selected, and a context menu offers "Rename..." and "Delete" options. An "Export..." button is visible at the bottom left.
- Save Custom Fragment Dialog:** A dialog box titled "Save Custom Fragment" allows users to save a fragment. It includes a "Get from:" dropdown (set to "Structure Text"), a "Text:" input field with a placeholder "Type or paste in text (e.g., SMILES, SMARTS, MDL)", and a "Save to Fragments palette as:" field (containing "Fragment-1").
- Arrow Selection Menu:** A small menu on the right lists arrow types: "Standard Arrow" (checked), "Double-Headed Arrow", "Equilibrium Arrow", and "Delete This Step".

- Sketching Beilstein generic queries
- Additional rendering options
- Additional format support: .xyz, .mae
- Additional reaction sketching tools
- Fragment library support



**Schrödinger**

**Thank you.**