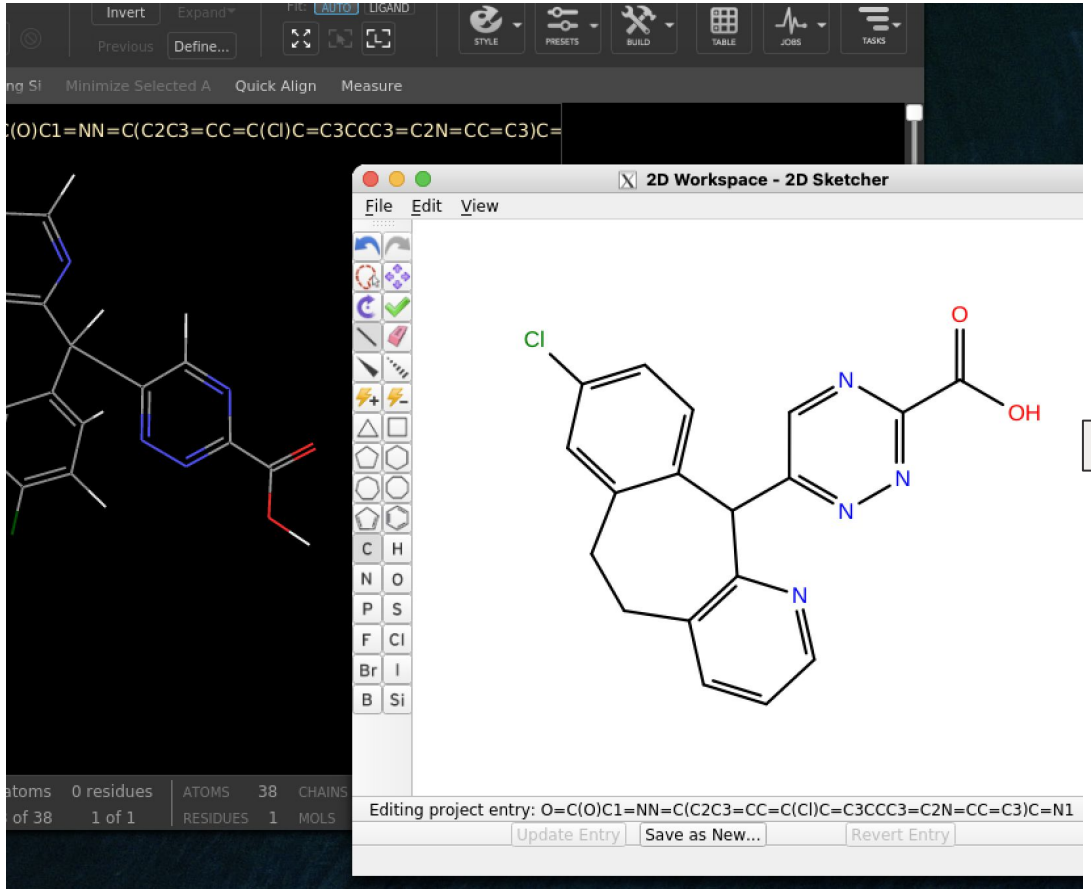
Building a Cross-Compiled 2D Sketcher

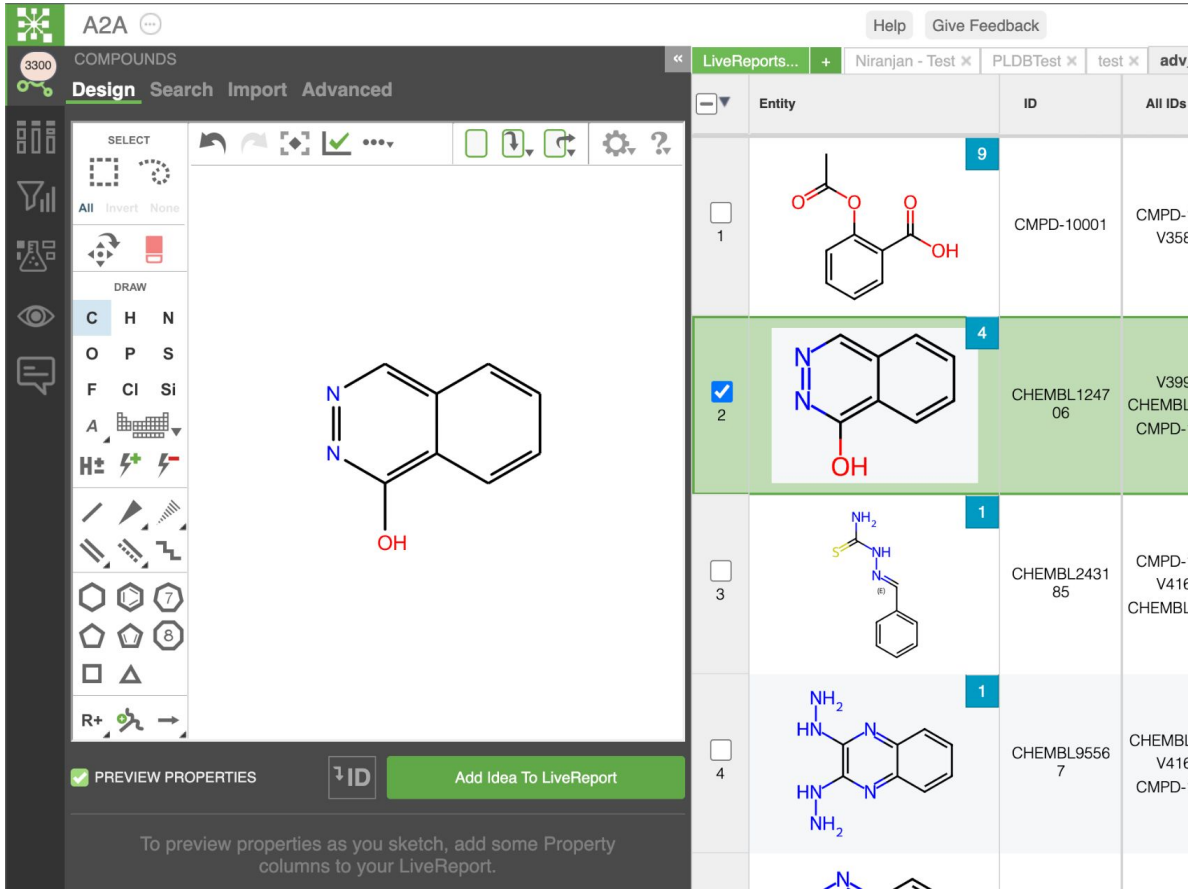
Chris Von Bargen

RDKit UGM 2022
October 2022

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

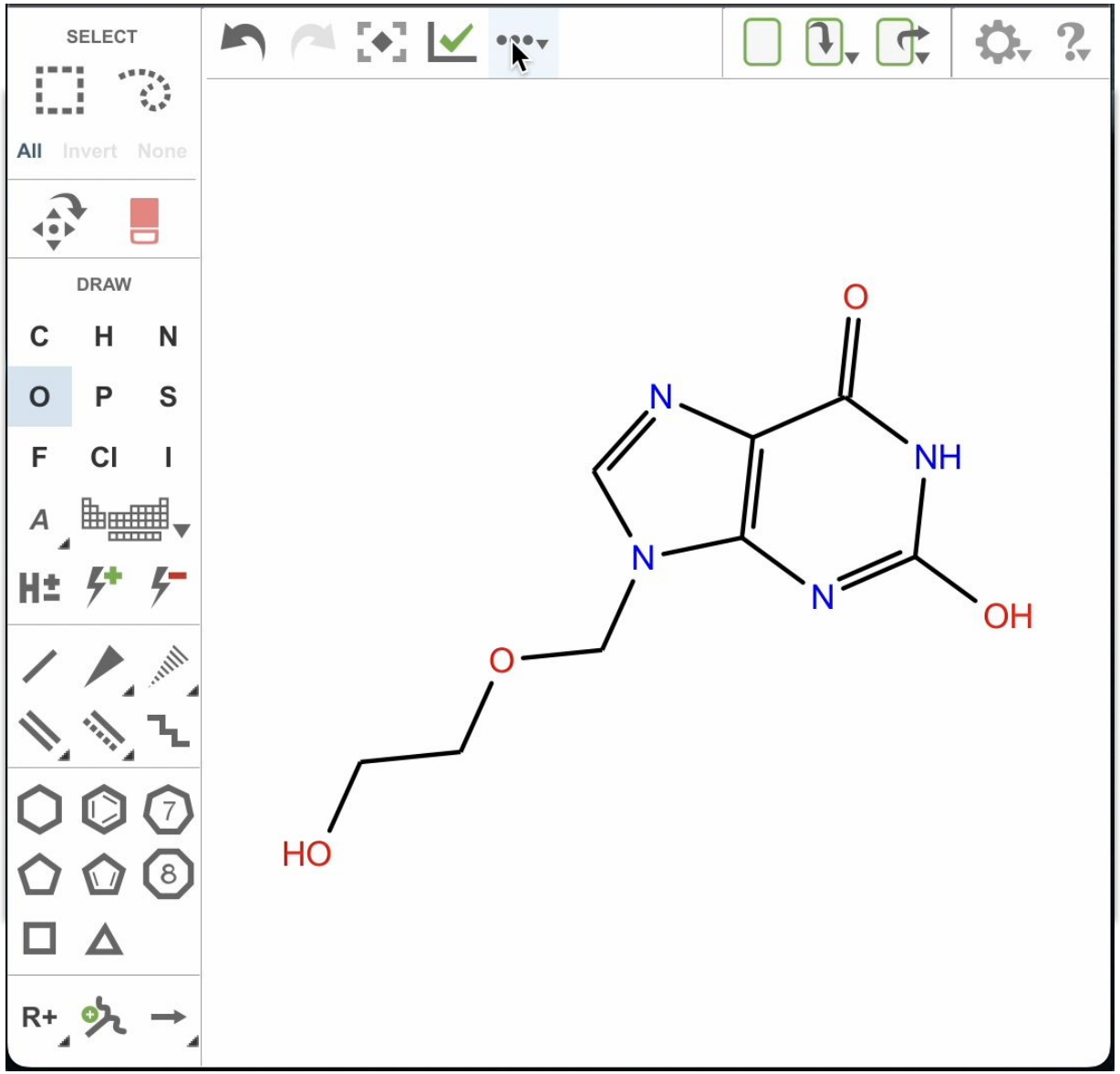
Dependencies:

- RDKit
- Qt6
- coordgenlibs
- zlib, boost

Overhaul of the UI

Comparable tools to other sketchers

Consistency across Schrodinger platform



A WebAssembly Sketcher

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

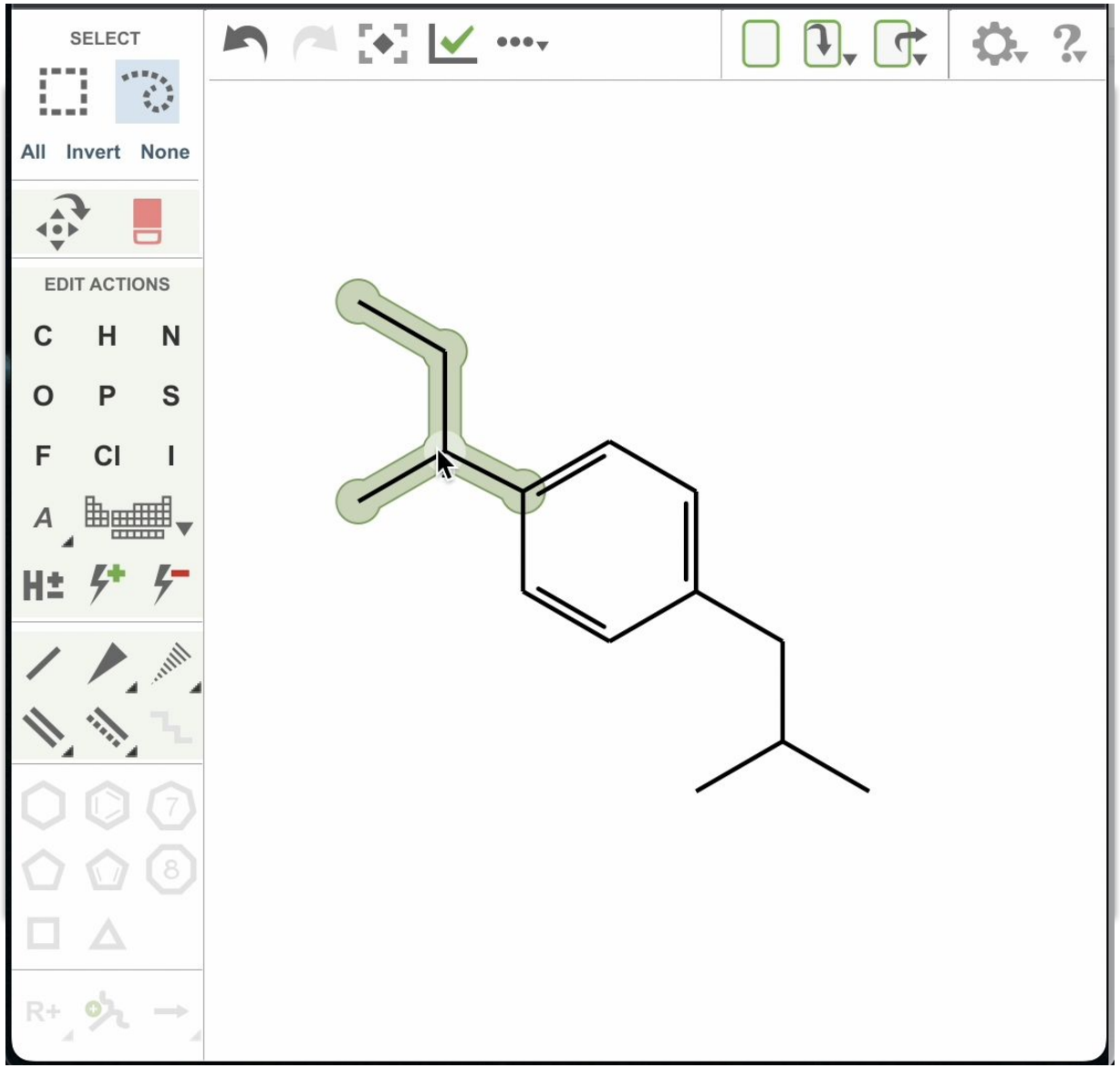
Dependencies:

- RDKit
- Qt6
- coordgenlibs
- zlib, boost

Overhaul of the UI

Comparable tools to other sketchers

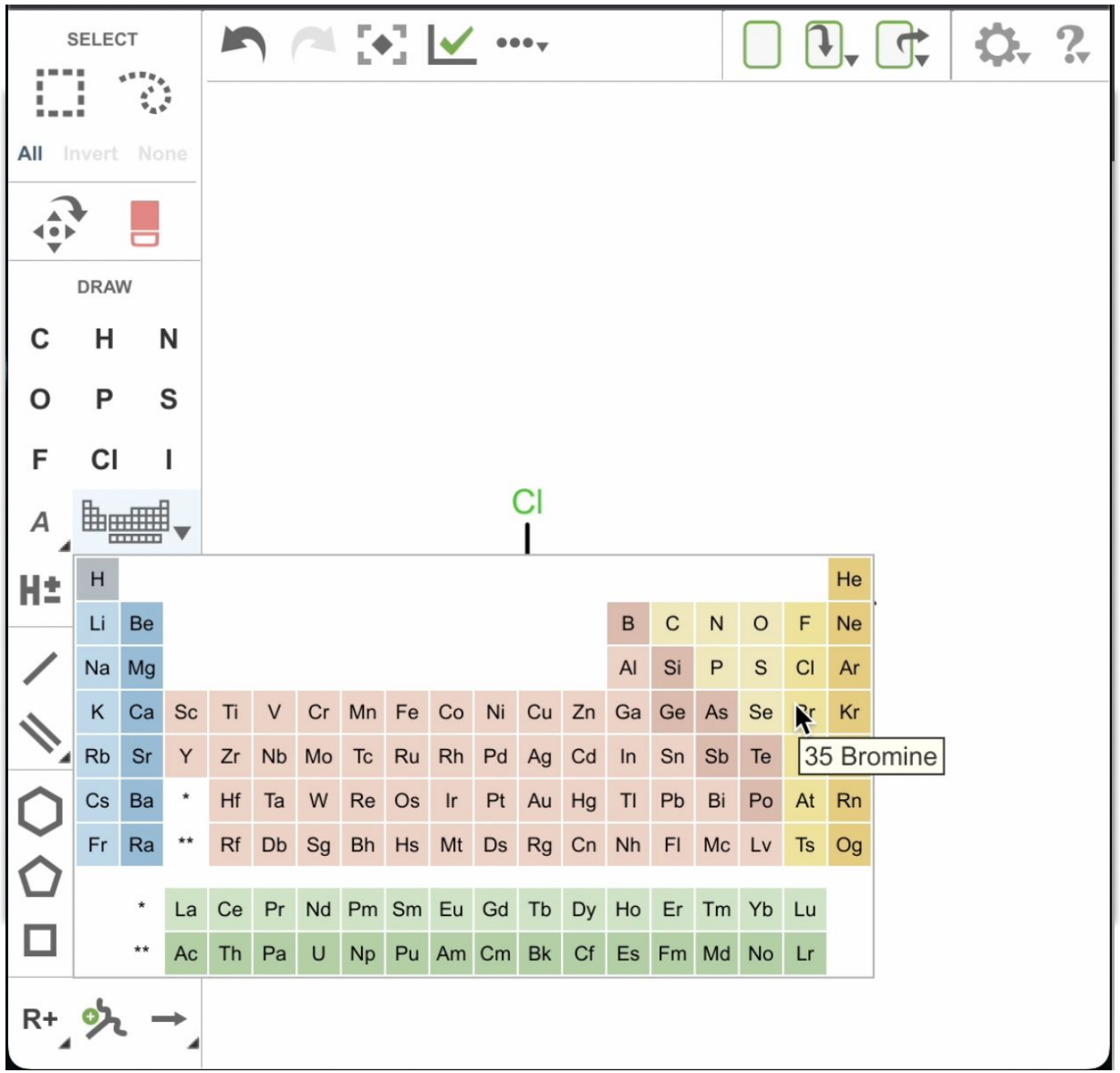
Consistency across Schrodinger platform



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

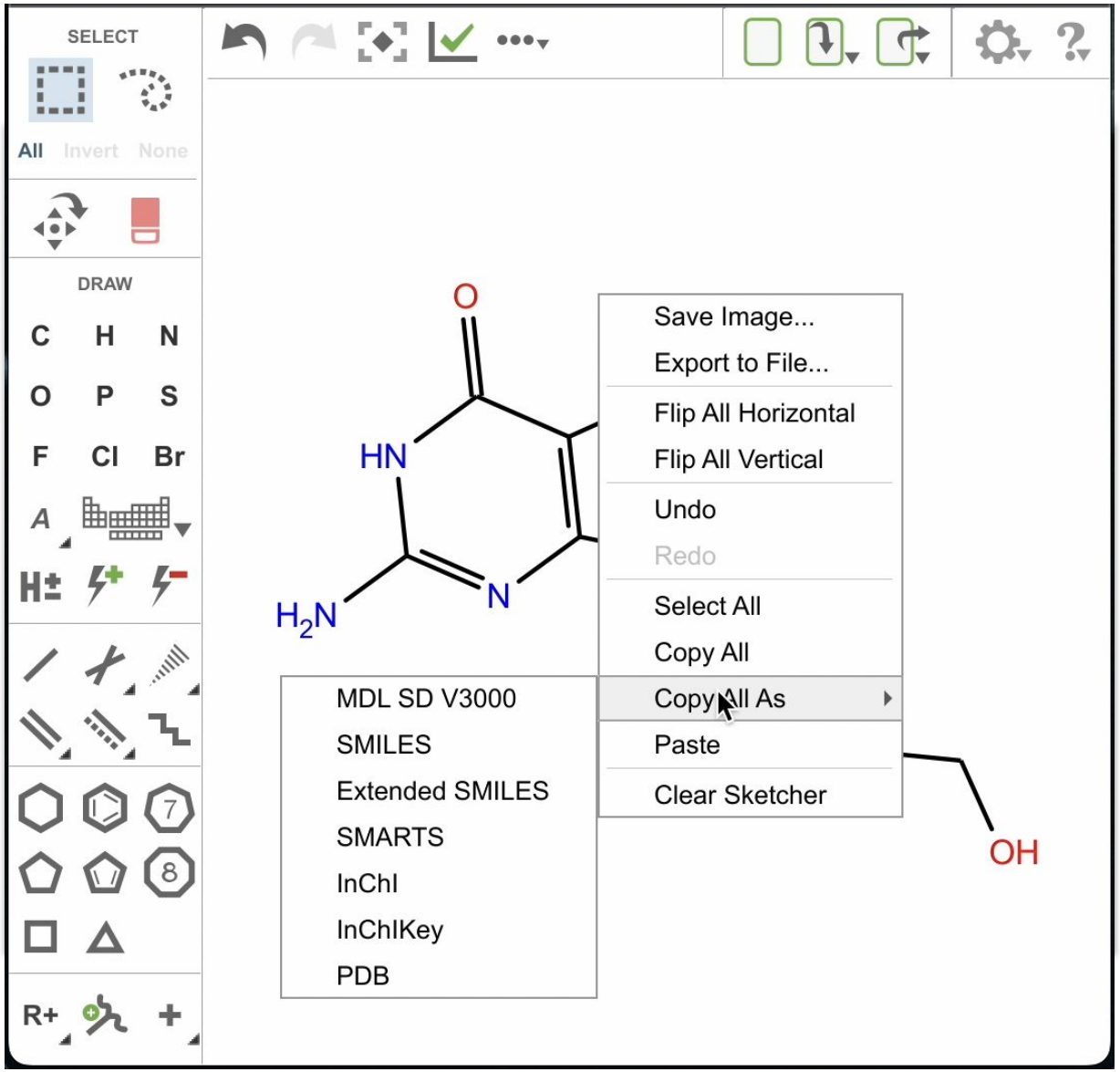
UI overall to address discoverability and consistency throughout:

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

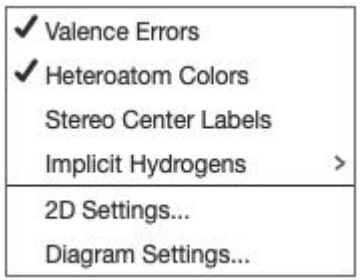
Continuous feedback from users within Schrodinger

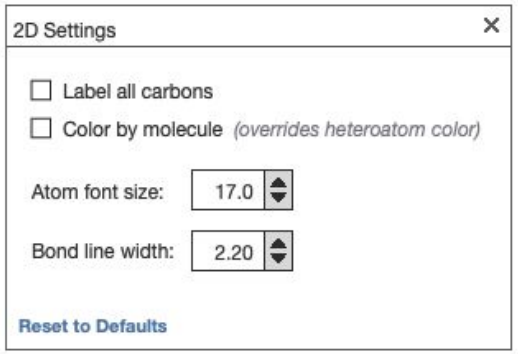
Short term: free public webpage

Long term: open source

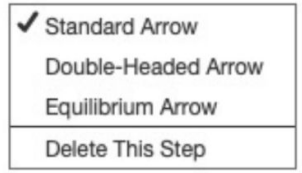


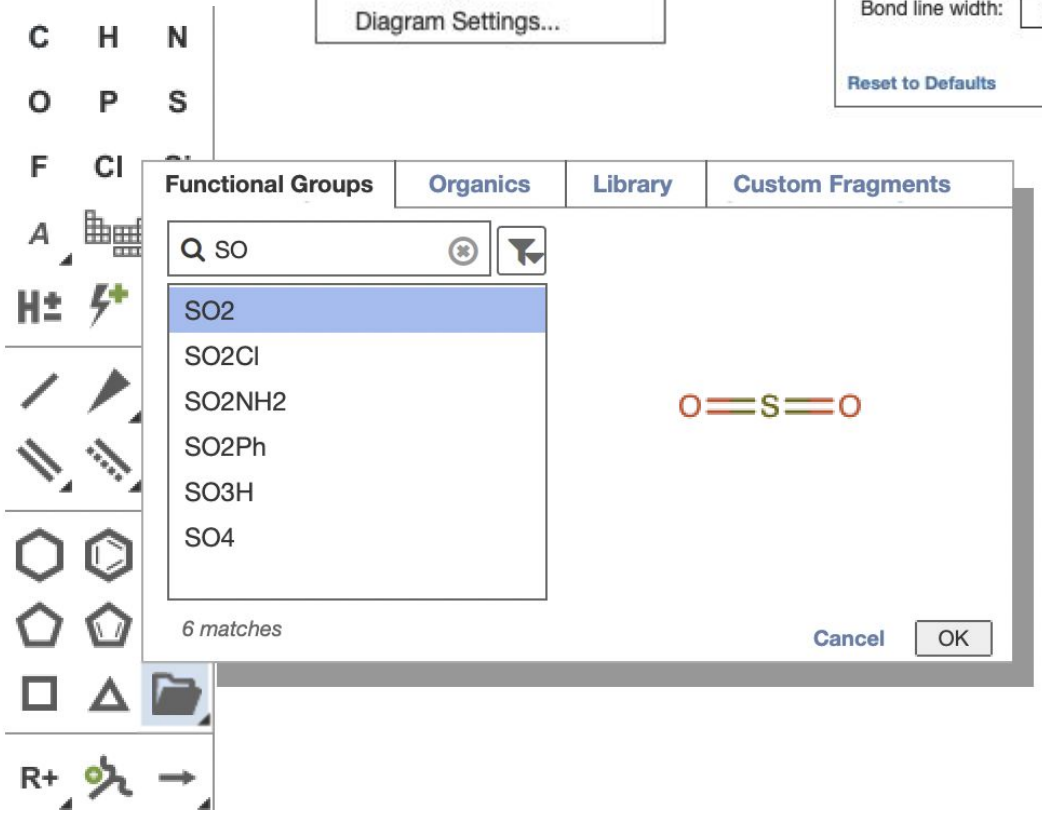
Future Improvements

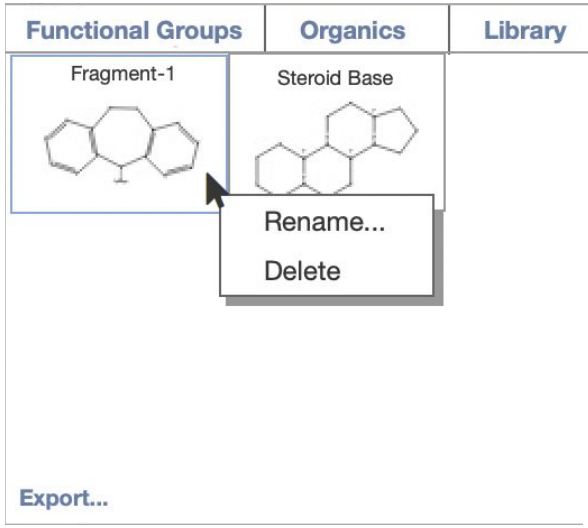


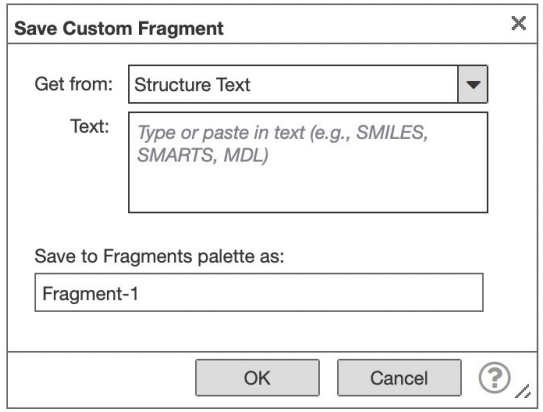


- Sketching Beilstein generic queries
- Additional rendering options
- Additional format support: .xyz, .mae
- Additional reaction sketching tools
- Fragment library support









Thank you.