



Schrödinger

Open-Source 2D Sketcher

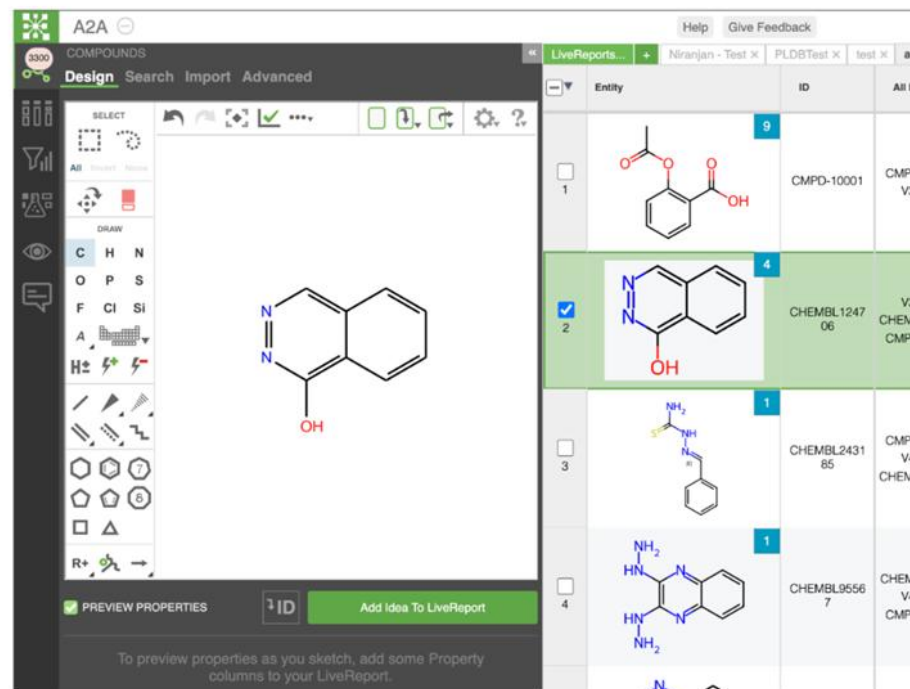
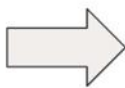
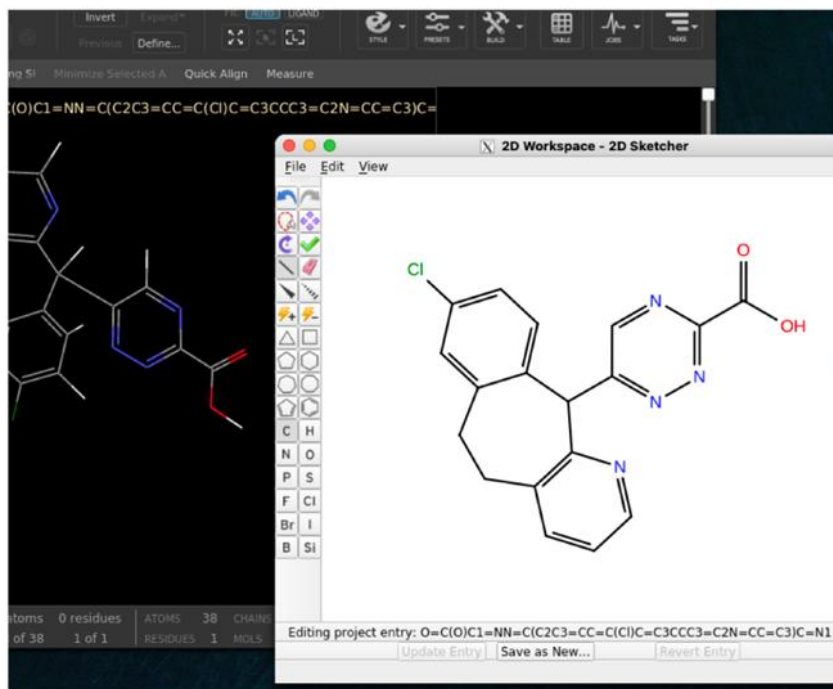
Chris Von Bargaen

RDKit UGM 2025

Back in 2022...

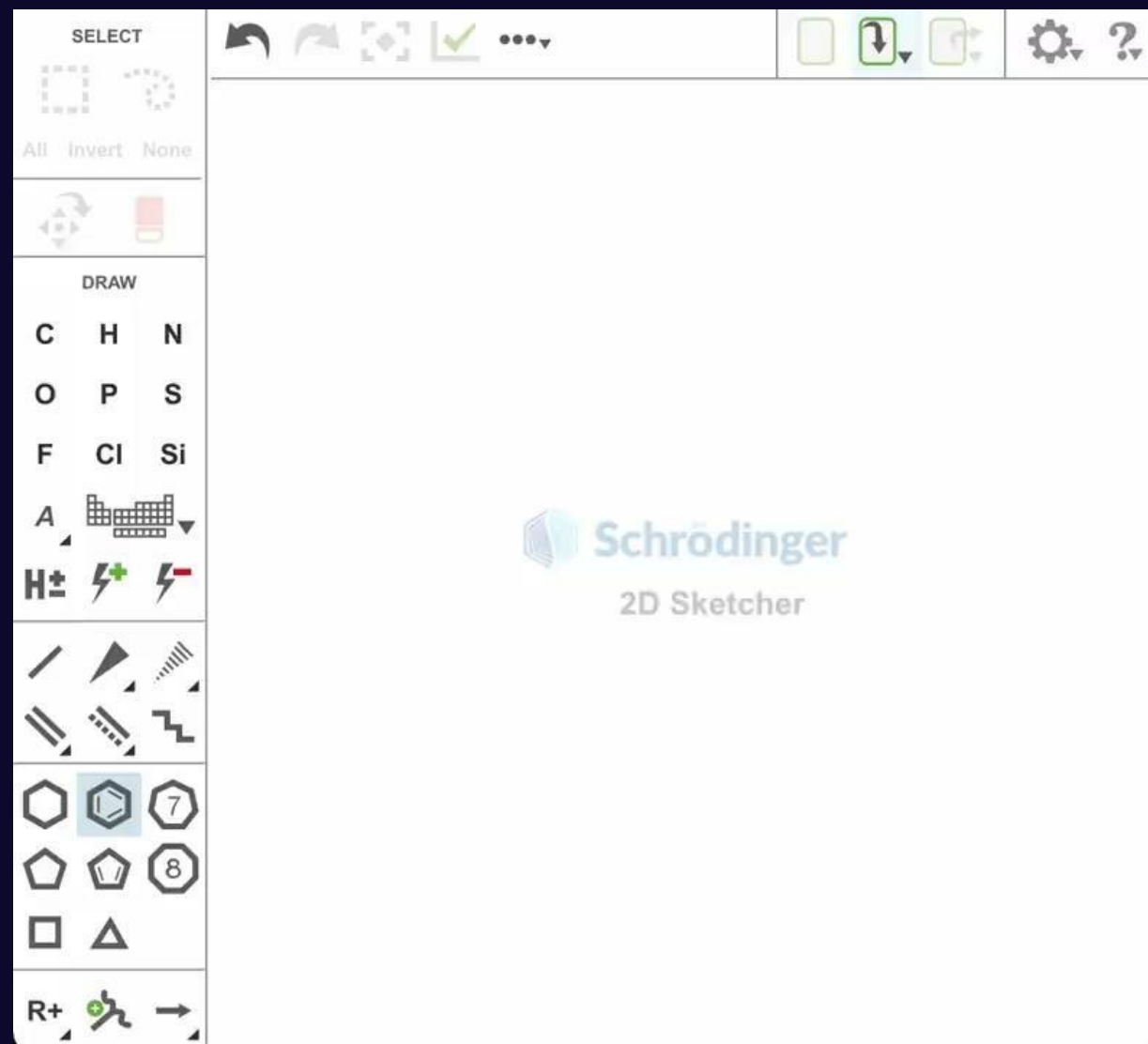
The Need

Need for a browser compatible sketcher using RDKit as its chemistry engine



2D Sketcher Features

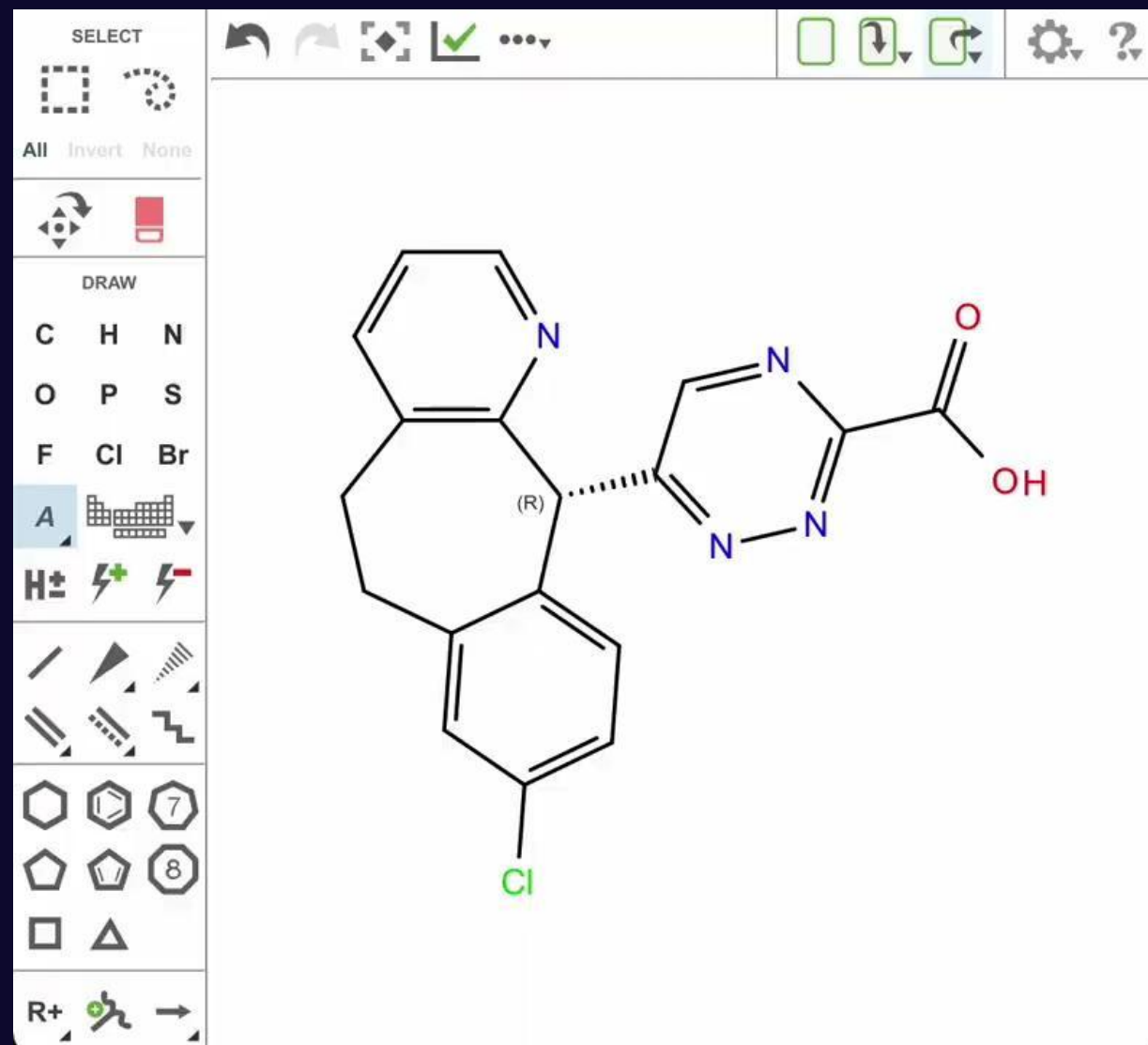
- Flexible drawing tools for atoms, bonds, rings, and query features
- Intuitive and efficient UX/UI
 - sensible hotkeys
 - 3-button mouse support
 - rich context menus
- Able to generate static images with highlighting and annotations
- Used across the Schrödinger platform to provide a consistent experience



The RDKit Engine

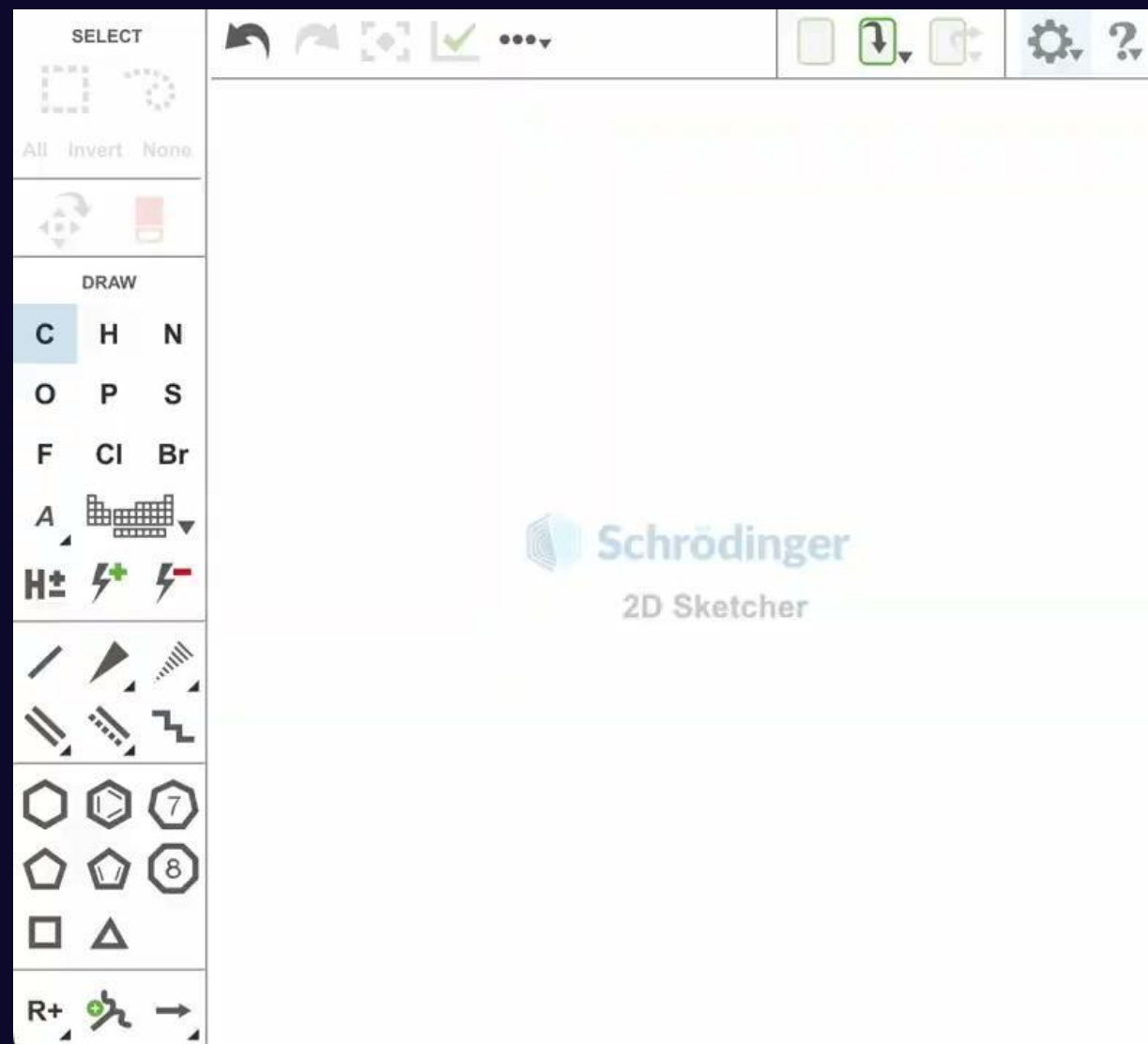
Utilizes an **RWMol as the underlying model**, which in addition to general molecular editing uses the RDKit for:

- chemical file format support
- stereochemistry perception
- 2D coordinate generation/manipulation
- hydrogen addition/removal
- atomic-level properties
- valence errors
- building query molecules
- S-Group data
- creating reactions
- coloring schemes
- ...and more...



Build Details

- Written using C++20
- Compiled with CMake
- Builds on all **major OS platforms**
- Build instructions using emscripten to cross-compile into **WebAssembly**
- Dependencies:
 - [RDKit](#)
 - [Qt](#)
 - boost, eigen, fmt, sqlite, zlib, zstd



Open Access

[schrodinger.com/2dsketcher](https://www.schrodinger.com/2dsketcher)

The screenshot shows the Schrödinger 2D Sketcher web application. The browser address bar displays <https://www.schrodinger.com/2dsketcher>. The top navigation bar includes the Schrödinger logo, links for Company, Platform, Life Science, Materials Science, Pipeline, Investors, a search icon, My Account, and a CONTACT US button. Below this is a secondary navigation bar with Overview, Products, Support, and Download. The main interface features a left-hand toolbar with 'SELECT' and 'DRAW' sections. The 'DRAW' section includes buttons for elements C, H, N, O, P, S, F, Cl, Si, a ring size selector (A), and a charge selector (H±). The central workspace is a large white area with the Schrödinger 2D Sketcher logo. A text box is overlaid on the workspace, stating: 'All logic is browser/client side. Once the sketcher is loaded in the browser, no information is sent back to Schrödinger.' At the bottom of the page, a disclaimer reads: 'The Schrödinger Sketcher does not collect or retain any structural information or the referring URL. Moreover, use of this sketcher has no implication regarding ownership of intellectual property.' A user icon is visible in the bottom right corner.

SELECT

All Invert None

DRAW

C H N

O P S

F Cl Si

A

H±

7

8

R+

The Schrödinger Sketcher does not collect or retain any structural information or the referring URL. Moreover, use of this sketcher has no implication regarding ownership of intellectual

Open Source

- Open source codebase
- C++ source with CMake
- GitHub-hosted runners
 - MacOS app
 - Windows app
 - Ubuntu app
 - WebAssembly (Wasm)
 - debug/valgrind build
- BSD 3-Clause license



github.com/schrodinger/sketcher

schrodinger / sketcher

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KevKeating SKETCH-2491: fixing delayed fitToScreen calls (#52) ✓58b2ae1 · 4 days ago1,034 Commits

.github	SKETCH-2518. Disable memtest for now	5 days ago
build	SKETCH-2184: Enabling WASM builds (#15)	6 months ago
data	SHARED-11512: update monomer DB (#47)	5 days ago
external	Fix macos-latest runner; skip failing test_select_options_...	5 days ago
include/schrodinger	SHARED-11610: Combine any type of mol into rdmols (#45)	5 days ago
src	SKETCH-2491: fixing delayed fitToScreen calls (#52)	4 days ago
test	SKETCH-2491: fixing delayed fitToScreen calls (#52)	4 days ago
wasm	SKETCH-2184: Enabling WASM builds (#15)	6 months ago
.clang-format	SKETCH-2205. Add Boost::json as a dependency (#9)	last year
.gitignore	SKETCH-2452 add ellipse selection	5 days ago
CMakeLists.txt	SKETCH-2507. Disable WASM tests (#34)	last month
LICENSE	Add BSD 3-Clause License	last year
README.md	Update README.md dependencies link	3 months ago
premake	SKETCH-2033. Update target dependencies; fix local Sch...	2 months ago

READMEBSD-3-Clause license

Schrödinger 2D Sketcher

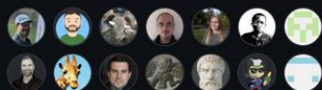
Sketcher Build and Test passing



AboutSchrödinger 2D Sketcherwww.schrodinger.com/2dsketcherReadmeBSD-3-Clause licenseActivityCustom properties5 stars3 watching1 forkReport repository

ReleasesNo releases publishedCreate a new release

PackagesNo packages publishedPublish your first package

Contributors41
+ 27 contributors

LanguagesC++ 98.1%Yacc 0.6%CMake 0.4%Python 0.3%HTML 0.2%Lex 0.2%Other 0.2%

Downloadable Artifacts

Summary

Jobs

✓ build (macos-latest, app)

✓ build (ubuntu-latest, app)

✓ build (windows-latest, app)

✓ build (ubuntu-latest, wasm)

Run details

Usage

Workflow file

build (ubuntu-latest, app) summary

✓ All tests passed

62 tests passed

[Job summary generated at run-time](#)

build (windows-latest, app) summary

✓ All tests passed

62 tests passed

[Job summary generated at run-time](#)

Annotations

1 notice

















ⓘ build (windows-latest, app)

The windows-latest label will migrate from Windows Server 2022 to Windows Server 2025 b...

[Show more](#)

Artifacts

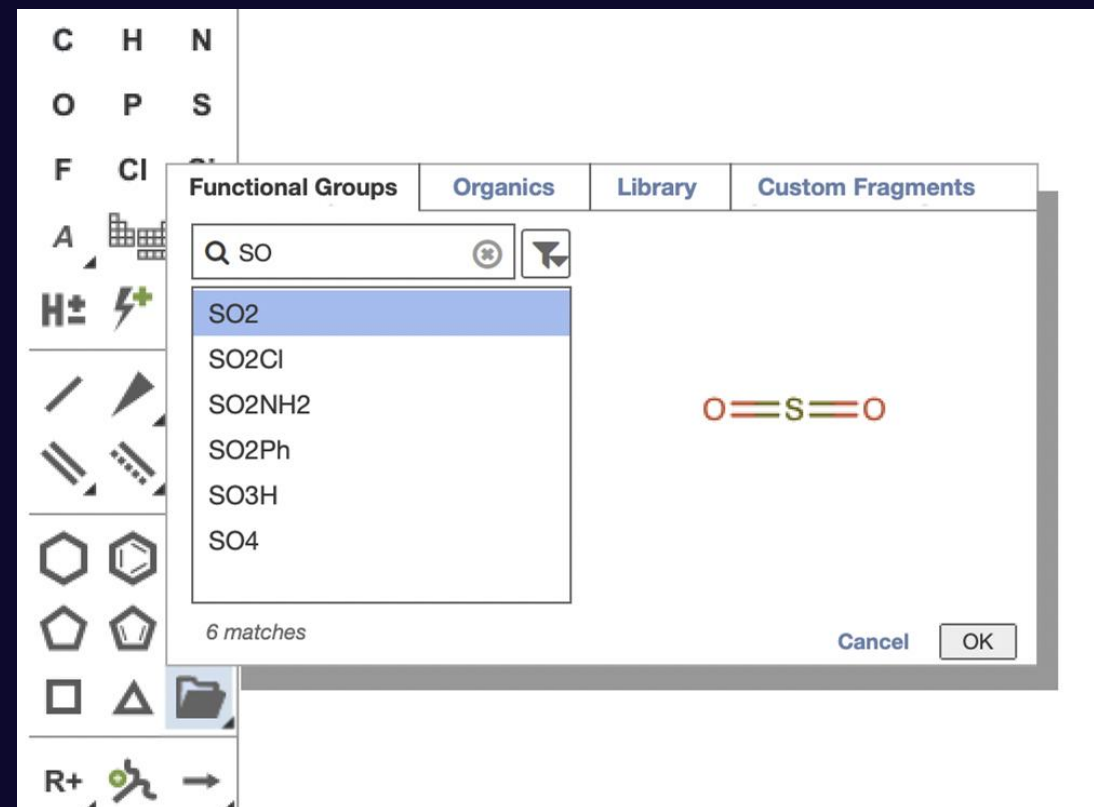
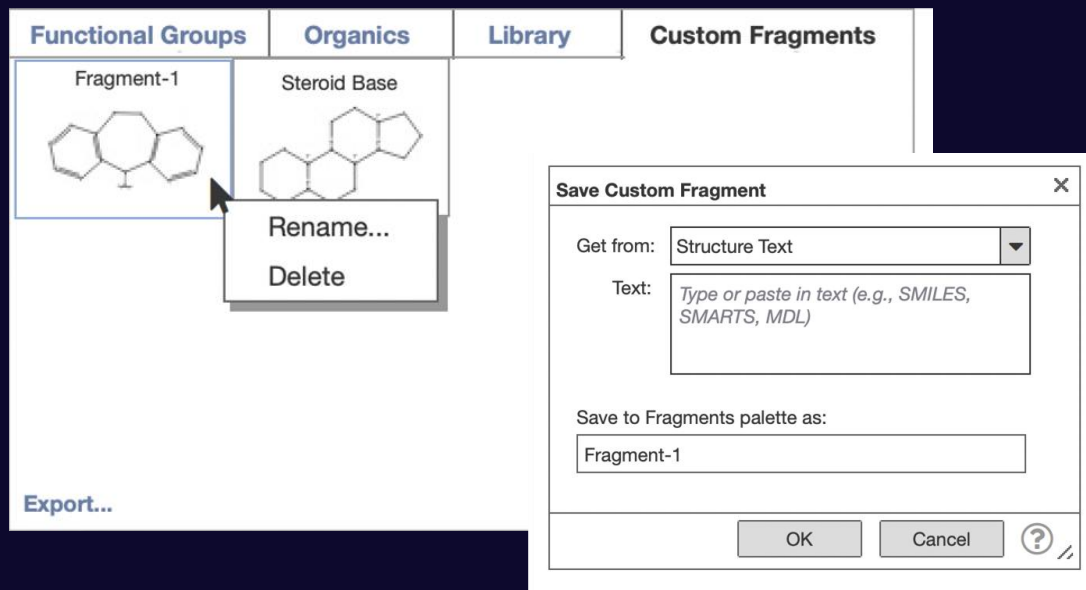
Produced during runtime

Name	Size	Digest			
 sketcher-macos-latest-app	11.9 MB	sha256:c961a043ae...			
 sketcher-ubuntu-latest-app	16.8 MB	sha256:6730e589c8...			
 sketcher-wasm.tar.gz	8.45 MB	sha256:68e6173115...			
 sketcher-windows-latest-app.exe	19.7 MB	sha256:ded402d4c3...			



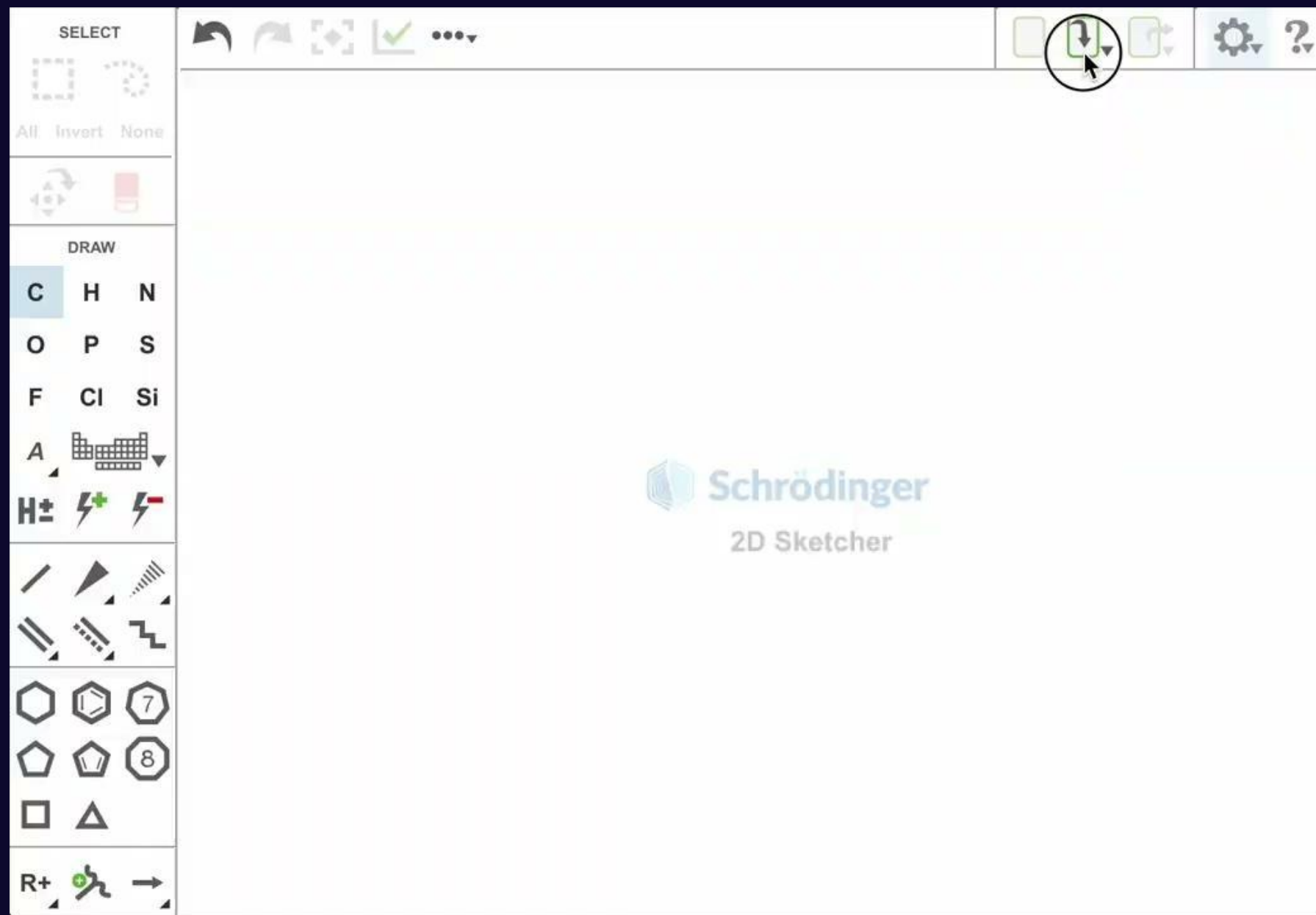
Requested Features

- Fragment/Template library support
- Add/edit arbitrary S-Group data
- Polymer/SRU/Copolymer support
- Support for link nodes
- Developer mode to interrogate atom indices



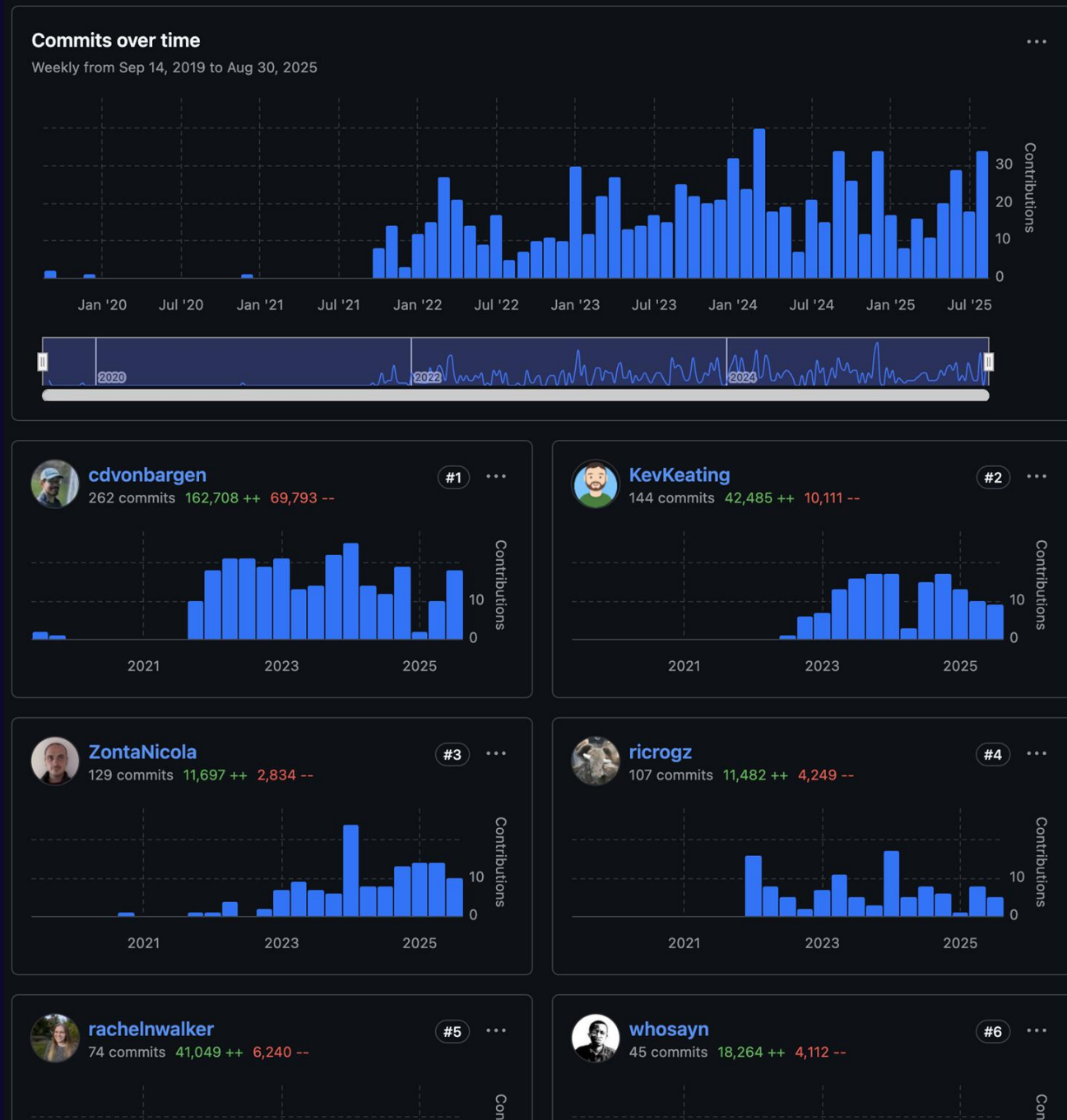
Monomer Sketcher

BETA Demo



Thanks

- Nicola Zonta
- Laura Beck
- Ricardo Rodriguez-Schmidt
- Ethan Alguire
- Kevin Keating
- Rachel Walker
- Hussein Faara
- Dan Nealschneider
- Juzer Zarif
- Sean Seekins
- Prachi Thakur



Community and Contributions

We are excited about opening the Schrödinger 2D Sketcher up to the community, looking for support and feedback!

- **Share Your Feedback:** open a [GitHub Discussion](#) to ask questions or suggest ideas
- **Report Bugs:** issues should be made through the [GitHub issue tracker](#)
- **Contribute Code:** please follow the standard [fork and pull model](#)
- GitHub: <https://github.com/schrodinger/sketcher>
- Open Access: <https://www.schrodinger.com/2dsketcher>

Thank You!