# Super-Glue: Interactive Web Tool to Facilitate Chemistry <> ML Collaboration

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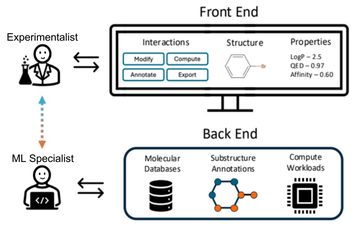
EXPEDITION MEDICINES

## Overview

### Background and Motivation




Machine learning (ML) is transforming Medicinal Chemistry enabling rapid pharmaceutical development. However, it lacks the intuition honed by expert chemists through decades of knowledge acquisition. Super-Glue aims to "glue" together expert knowledge with ML, enhancing model performance, fostering cross-domain trust, and integrating AI into existing drug discovery pipelines.

**Overall Goal:** To create an interactive web tool to facilitate the collaboration of expert medicinal chemistry knowledge with ML in a scalable and data-driven manner.

### Objectives: Aggregated User Stories (from over 20)

- **Experimentalist** exploring drug discovery with limited coding experience, seeking a user-friendly interface to **visualize** molecules, **highlight** key functional groups, and leverage AI for **property prediction** based on existing data.
- **ML specialist** proficient in predictive modeling but new to cheminformatics, seeking a curated, **annotated molecular dataset** in a **structured format** that integrates seamlessly with **Python workflows**.

## Technologies Used

### Frontend

- Ketcher[1] – a web-based chemical structure editor that is open-source and free to use
- React
- Vite
- Ant Design
- 3Dmol.js[2] – enables 3-D molecular modeling

### Backend

- Flask – web framework that is simple and easy to learn and offers high flexibility
- RDKit[3] – open-source toolkit for cheminformatics
- Unittest
- ADMET_ai[4] – Python package that provides fast and accurate ADMET predictions

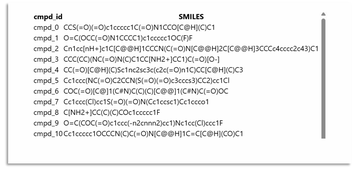
## Design Flow

### Home Page

- Login, **upload** a .csv file, and view previously uploaded files.

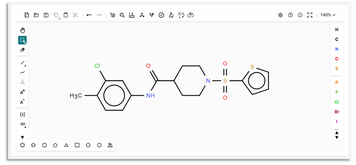

### Summary Page

- After uploading, **preview** the dataset in a tabular view.
- Toggle to view **all saved highlights** across all molecules.



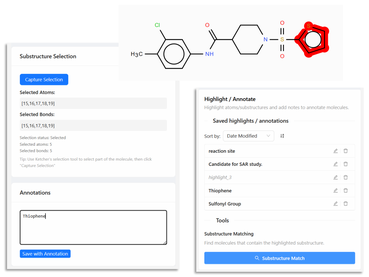

### Molecular Visualization

- Molecules are rendered with **Ketcher**, enabling real-time interaction with structures directly in the browser.



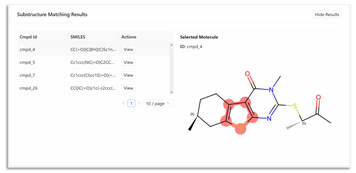
### Annotation + Highlighting

- **Highlight atoms or substructures, add annotations** for reactions or key features.
- Saved highlights are listed in a table for easy review.



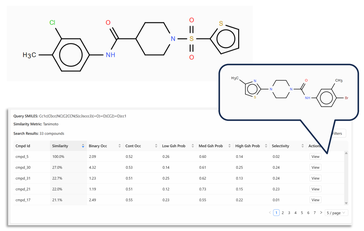

### Substructure Matching

- Search for molecules with **matching substructures** using saved highlights.
- Results include a table with **highlighted regions** for quick pattern recognition.




### Similarity Search

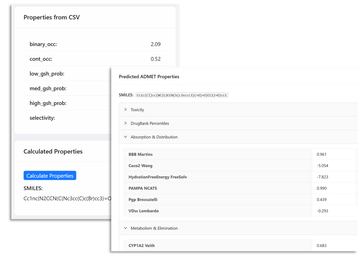
- Identify **structurally similar compounds** using various similarity **metrics.**
- Adjust **thresholds** and view ranked results with similarity scores.



## Design Flow

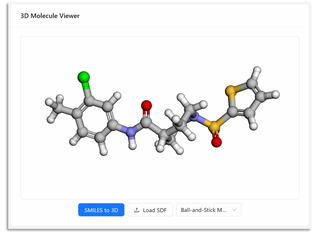
### Property Computations

- Calculate simple properties like **logP** with **RDKit**.
- Run drug-likeness predictions using **ADMET_ai**.




### 3-D Modeling

- Visualize molecules in an **interactive 3D viewer** – rotate, zoom, explore.
- Upload **SDF Files** for accurate geometries, or auto-generate from SMILES.




## Conclusion

### Main Takeaways

- Super-Glue allows users to upload their molecular data, annotate their findings, find similar molecules, and predict complex properties crucial drug development,
- Super-Glue is a platform that combines AI with human intuition, by fostering trust, enabling collaboration, and optimizing drug discovery

### Future Work

- Containerization for cloud deployment
- We plan to expand similarity search to larger databases like PubChem for greater accuracy and utility
- Finetuning of ADMET using client specific data for generative AI

### References

1. Ketcher: Web-based chemical structure editor. https://github.com/epam/ketcher/releases/tag/v3.2.0, doi: https://doi.org/10.1186/1758-2946-3-S1-P3.
2. Nicholas Rego and David Koes, "3Dmol.js: molecular visualization with WebGL", Bioinformatics, 31(8): 1322-1324, 2015, doi: https://doi.org/10.1093/bioinformatics/btu829.
3. RDKit: Open-source cheminformatics. https://www.rdkit.org, doi: https://doi.org/10.5281/zenodo.591637.
4. ADMET-AI: a machine learning ADMET platform for evaluation of large-scale chemical libraries. https://github.com/swansonk14/admet_ai, doi: https://doi.org/10.1093/bioinformatics/btae416

https://github.com/SuperGlue2025/SuperGlue2025

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