

LEXIN CHEN

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Computational Scientist | Machine Learning for Drug Discovery

Skills

Comp Chem Structure-Based Drug Design (Glide, Maestro), Molecular Docking, Protein-Ligand Modeling, RDKit, Molecular Visualization (PyMOL), HTS/DEL, Virtual Screening, CADD, Activity Cliff Handling

AI/ML Scikit-learn, QSAR/QSPR Modeling, Property Prediction, Molecular Representation Learning, PyTorch.

Technology Python, Bash, Docker, HPC, Git, AWS, Schrödinger Suite, HPC and CI/CD for Scientific Workflows.

Education

Ph.D. in Chemistry Gainesville, FL
University of Florida Aug 2025

B.S. in Biochemistry Stony Brook, NY
Stony Brook University May 2021

Experiences

Revolution Medicines Remote
Scientist I, Computational Chemistry Dec 2025 - Present

- Developed a scalable workflow for **macrocycle bioactive conformation prediction**, achieving **<1Å** RMSD agreement with crystal structure.
- Benchmarked machine learning and physics-based methods, demonstrating improved accuracy and **3x** faster sampling for macrocycle conformational analysis.

University of Florida Gainesville, FL
Graduate Research Assistant | Advisor: Ramón Miranda-Quintana Oct 2022 - Aug 2025

- Developed DELight, an end-to-end ML** pipeline to predict protein-ligand interactions from complex DNA-Encoded Library (DEL) screen data.
- Developed chemical similarity and search tools (MDANCE) for billion-scale molecular comparison with **25x speedup**, enabling efficient data curation and benchmarking for deep learning models on HPC clusters.
- Co-developed a billion-scale clustering algorithm** (BitBirch) to model and navigate massive chemical spaces, facilitating pattern discovery and feature analysis for AI-driven hit identification.

Schrodinger New York, NY
Software Developer Intern May 2024 - Aug 2024

- Developed algorithms for a structure-based prediction tool (Glide), improving model reliability by 15%** and gaining production-level experience in evaluating and deploying AI-adjacent models for drug discovery.
- Applied molecular docking (Glide) to drug discovery problems, requiring proficient handling of diverse chemical structures and an understanding of preprocessing requirements.
- Drove product adoption by collaborating cross-functionally to integrate new features into the commercial Schrödinger platform, translating user feedback into actionable product improvements.

Selected Projects

DELight: ML Cheminformatics Framework for DEL

[Code](#) | [Docs](#) | [Article](#) Oct 2022 - Present

- Architected an **end-to-end ML pipeline** to predict protein-ligand interactions from complex biological screen data.
- Engaged with computational chemists** to define needs and drove adoption of the framework by creating clear documentation and case studies demonstrating impact on hit identification.
- Solved **extreme class imbalance** challenges through bias-aware learning, enhancing prediction of rare high-value compounds relevant to hit identification

Publication Summary

15 peer-reviewed publications (7 first-author) in high-impact journals (e.g., *J. Chem. Theory Comput.*, *J. Chem. Inf. Model.*), focusing on **machine learning for molecular property prediction** and the development of scalable AI algorithms for chemical and biological data.

Selected Honors

Lindau Nobel Young Scientist • Pfizer Emergent Leader • CCG Excellence Award • Penny J. Gilmer Grant