Peter Eckmann

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Google Scholar
GitHub
Website

Research Interest

Machine learning for drug discovery

Education

Undergraduate, University of California San Diego *(Sept. 2021 - June 2025)*

B.S. Computer Science
3.952 GPA

High school student, University City High School, San Diego *(Sept. 2017 - June 2021)*

4.86 GPA

Honors and Awards

Finalist, Outstanding Undergraduate Researcher Award, North American colleges and universities, Computing Research Association *(Dec. 2023)*
NSF Research Experiences for Undergraduates Award *(June - Sept. 2022, June - Sept. 2023)*
Regents Scholarship, UC San Diego *(2021 - 2025)*
Salutatorian, University City High School *(2021)*
Finalist, National Merit Scholarship Corporation *(2021)*
Broadcom MASTERS Top National 300, Science Fair project *(2017)*

Research Experience

Undergraduate researcher, Dr. Rose Yu Lab, UC San Diego *(Sept. 2021 - Present)*

Involved in a collaboration between Dr. Rose Yu (Department of Computer Science and Engineering) and Dr. Michael Gilson (Skaggs School of Pharmacy and Pharmaceutical Sciences) to develop machine learning methods for drug discovery. Especially focused on generative modeling for small-molecule drug discovery, few-shot compound activity prediction, and multi-fidelity learning.

Undergraduate researcher, FAIR Data Informatics Lab, UC San Diego *(Sept. 2019 - Present)*

Following a high school internship, worked mainly under Dr. Anita Bandrowski to develop computational tools that ensure biomedical research reproducibility. Among other projects, developed a machine learning-based technique to match different versions of scientific articles.

Undergraduate researcher, NSF Research Experiences for Undergraduates, UC San Diego *(June 2022 - Sept. 2022, June 2023 - Sept. 2023)*

Researched and developed few-shot learning techniques for scoring candidate compounds in drug discovery (2022), and applied multi-fidelity learning to drug design (2023).

Visiting researcher, Charité and Berlin Institute of Health, Berlin, Germany *(June 2022 - Sept. 2022)*

Developed institutional tools that track scientific reporting standards for researchers in the Charité.

Relevant Technical Skills

- Proficiency in **Python**, **PyTorch**, **RDKit**, and other scientific Python tools (NumPy, SciPy, pandas)
- Proficiency in Unix-related tools and working in high-performance computing clusters
- Experience with **networkx** and **PyTorch Geometric**
- Very familiar with docking using **AutoDock** and **DOCK6**, and related preparatory steps using **Chimera** and **OpenBabel**
- Experience with running molecular dynamics simulations using the **AMBER suite**

Conference Publications

Eckmann P, Wu D, Heinzelmann G, Gilson M, Yu R (2024). MF-LAL: Drug Compound Generation Using Multi-Fidelity Latent Space Active Learning. *AIDrugX* and *Machine Learning in Structural Biology* workshops at the *Conference on Neural Information Processing Systems* (2024, December 15). Available at https://arxiv.org/abs/2410.11226

Eckmann P, Sun K, Zhao B, Feng M, Gilson M, Yu R (2022). LIMO: Latent Inceptionism for Targeted Molecule Generation. *Proceedings of the 39th International Conference on Machine Learning (ICML)*, in *Proceedings of Machine Learning Research* 162:5777-5792 (2022, June 17-23) [Spotlight]. https://proceedings.mlr.press/v162/eckmann22a.html, Code: https://github.com/Rose-STL-Lab/LIMO, Website: https://www.limo-aimd.com/

Patents

Yu R, **Eckmann P**, Sun K, Zhao B, Feng M, Gilson M (2023). Computational architecture to generate representations of molecules having targeted properties. United States patent pending US20240005179A1. June 16, 2023. https://patents.google.com/patent/US20240005179A1/en

Journal Publications

Eckmann P, Anderson J, Yu R, Gilson M (2024). Ligand-Based Compound Activity Prediction via Few-Shot Learning. *Journal of Chemical Information and Modeling*, 64 (14), 5492-5499.

Ayoubi R, Ryan J, Biddle MS, Alshafie W, Fotouhi M, Bolivar SG, Moleon VR, **Eckmann P,** Worrall D, McDowell I, Southern K, Reintsch W, Durcan TM, Brown C, Bandrowski A, Virk H,

Edwards AM, McPherson P, Laflamme C (2023). Scaling of an antibody validation procedure enables quantification of antibody performance in major research applications. *eLife*, 12:RP91645.

Eckmann P, Bandrowski A (2023). PreprintMatch: a tool for preprint publication detection applied to analyze global inequities in scientific publishing. *PLoS ONE* 18(3): e0281659.

Bandrowski A, Pairish M, **Eckmann P**, Grethe J, Martone ME (2023). The Antibody Registry: ten years of registering antibodies. *Nucleic Acids Research*, 51(D1), D358-D367.

Schulz R, Barnett A, Bernard R, Brown NJ, Byrne JA, **Eckmann P**, Gazda MA, Kilicoglu H, Prager EM, Salholz-Hillel M, Ter Riet G, Vines T, Vorland CJ, Zhuang H, Bandrowski A, Weissgerber TL (2022). Is the future of peer review automated? *BMC Research Notes*, *15*(1), 1-5.

Menke, J, **Eckmann P**, Ozyurt IB, Roelandse M, Anderson N, Grethe J, Bandrowski A (2022). Establishing Institutional Scores With the Rigor and Transparency Index: Large-scale Analysis of Scientific Reporting Quality. *Journal of Medical Internet Research*, *24*(6), e37324.

Weissgerber T, Riedel N, Kilicoglu H, Labbé C, **Eckmann P**, Ter Riet G, Byrne J, Cabanac G, Capes-Davis A, Favier B, Saladi S, Grabitz P, Bannach-Brown A, Schulz R, McCann S, Bernard R, Bandrowski A (2021). Automated screening of COVID-19 preprints: can we help authors to improve transparency and reproducibility? *Nature Medicine* 27:6-7, 2021.

Preprints

Thumuluri V, **Eckmann P,** Gilson M, Yu R (2024). Technical report: Improving the properties of molecules generated by LIMO. *arXiv*:2407.14968 [cs.LG].

Eckmann P, Wu D, Heinzelmann G, Gilson M, Yu R (2024). MFBind: a Multi-Fidelity Approach for Evaluating Drug Compounds in Practical Generative Modeling. *arXiv*:2402.10387v1 [q-bio.BM].

Invited Talks

Learning on Graphs and Geometry (LoGG) Reading Group, Valence Labs *(Mar. 2024)*. MFBind: a Multi-Fidelity Approach for Evaluating Drug Compounds in Practical Generative Modeling. Link: https://portal.valencelabs.com/events/post/mfbind-a-multi-fidelity-approach-for-evaluating-drug-compounds-in-5GhXYNdjBuYTwrW

Conference Abstracts

Eckmann P, Bandrowski A. PreprintMatch: a new tool to match manuscripts across multiple similarity metrics. *International Neuroinformatics Coordinating Facility Assembly*, held virtually (2021, April 19-29) [Poster presentation]. https://neuroinformatics.incf.org/node/264

Eckmann P, Riedel N, Kilicoglu H, Labbé C, Ter Riet G, Byrne J, Cabanac G, Capes-Davis A, Favier B, Saladi S, Grabitz P, Bannach-Brown A, Schulz R, McCann S, Bernard R, Weissgerber T, Bandrowski A. Automated screening of COVID-19 preprints: can we help authors to improve transparency and reproducibility? *Annual Meeting, Association for Interdisciplinary Meta-Research and Open Science (AIMOS)*, held virtually (2020, December 3-4) [Poster presentation]. https://osf.io/ep9qh/

Eckmann P, Riedel N, Kilicoglu H, Labbé C, Ter Riet G, Byrne J, Cabanac G, Capes-Davis A, Favier B, Saladi S, Grabitz P, Bannach-Brown A, Schulz R, McCann S, Bernard R, Weissgerber T, Bandrowski A. Automated screening of COVID-19 preprints: can we help authors to improve transparency and reproducibility? *Research Reproducibility 2020*, held virtually (2020, December 2-3) [Oral presentation]. https://pwd.aa.ufl.edu/researchre-pro/wp-content/uploads/sites/8/2020/11/Paper_3-3_Eckmann_Peter.pdf

Review Activity

Reviewer, *International Conference on Learning Representations* 2025