Peter Eckmann

peckmann@ucsd.edu
Google Scholar, GitHub, Website

RESEARCH INTEREST: Machine learning for drug discovery

EDUCATION

Undergraduate, University of California San Diego, La Jolla, CA **2021-2025**
B.S. Computer Science
3.952 GPA

High school student, **University City High School, San Diego, CA** **2017-2021**
4.86 GPA

HONORS AND AWARDS

Finalist, Outstanding Undergraduate Researcher Award **Dec 2023**
Computing Research Association, Washington, D.C.
Award given to top 24 undergraduate students from all North American colleges and universities engaged in computing research.

NSF Research Experiences for Undergraduates award **June-Sept 2022, 2023**
Conducted summer research on machine learning in Dr. Rose Yu's Lab at UC San Diego.

Regents Scholarship, University of California San Diego **2021-2025**
Merit scholarship recognizing top ~1% of incoming undergraduates with exceptional academic achievements.

Salutatorian, **University City High School, San Diego** **2021**

Finalist, National Merit Scholarship Corporation **2021**

RESEARCH EXPERIENCE

Visiting researcher, Dr. Teresa Head-Gordon Lab **June - Aug 2024**
University of California, Berkeley, CA

Applied my previously developed machine learning approach to an NIH-funded drug discovery project to find inhibitors for a key protein of SARS-CoV-2.

Visiting researcher, QUEST Center for Responsible Research, Berlin Institute of Health at Charité **June 2022 - Sept 2022**
Berlin, Germany

Developed computational tools that track scientific reporting standards. Advisors: Dr. Tracey Weissgerber and Dr. Anita Bandrowski.

Undergraduate researcher, Dr. Rose Yu Lab **Sept 2021 - Present**
University of California San Diego, La Jolla, CA

Conducted research to develop machine learning methods for drug discovery in collaboration with computational chemist Dr. Michael K. Gilson. Led multiple projects, leading to first-author publications in top conferences and journals. Focused on generative modeling for small-molecule drug discovery, few-shot prediction, and multi-fidelity learning.

Undergraduate researcher, FAIR Data Informatics Lab **Sept 2019 - Present**
University of California San Diego, La Jolla, CA

Following a high school internship, researched computational tools to ensure biomedical research reproducibility, leading to a first-author and five co-authored publications. Among other projects, developed a machine learning technique to match different versions of scientific articles by semantic similarity. Advisor: Dr. Anita Bandrowski.

CONFERENCE PUBLICATIONS

Eckmann P, Wu D, Heinzelmann G, Gilson MK, Yu R (2024). MF-LAL: Drug Compound Generation Using Multi-Fidelity Latent Space Active Learning. In *AIDrugX* and *Machine Learning in Structural Biology* workshops at the *Conference on Neural Information Processing Systems (NeurIPS)* (2024, December 15). DOI: 10.48550/arXiv.2410.11226

Eckmann P, Sun K, Zhao B, Feng M, Gilson MK, Yu R (2022). LIMO: Latent Inceptionism for Targeted Molecule Generation. In *39th International Conference on Machine Learning (ICML)* (2022, June 17-23). DOI: 10.48550/arXiv.2206.09010 [Website]

JOURNAL PUBLICATIONS

Eckmann P, Anderson J, Yu R, Gilson MK (2024). Ligand-Based Compound Activity Prediction via Few-Shot Learning. *J. Chem. Inf. Model.* 64:5492–5499. DOI: 0.1021/acs.jcim.4c00485

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. DOI: 10.7554/eLife.91645

Eckmann P, Bandrowski A (2023). PreprintMatch: a tool for preprint publication detection applied to analyze global inequities in scientific publishing. *PLOS ONE* 18:e0281659. DOI: 10.1371/journal.pone.0281659

Bandrowski A, Pairish M, **Eckmann P**, Grethe J, Martone ME (2023). The Antibody Registry: ten years of registering antibodies. *Nucleic Acids Res.* 51:D358-D367. DOI: 10.1093/nar/gkac927

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 Res. Notes 15*:203. DOI: 10.1186/s13104-022-06080-6

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. *J. Med. Internet Res.* 24:e37324. DOI: 10.2196/37324

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? *Nat. Med.* 27:6-7. DOI: 10.1038/s41591-020-01203-7

PREPRINTS

Thumuluri V, **Eckmann P,** Gilson MK, Yu R (2024). Technical report: Improving the properties of molecules generated by LIMO. *arXiv*:2407.14968 [cs.LG]. DOI: 10.48550/arXiv.2407.14968

Eckmann P, Wu D, Heinzelmann G, Gilson MK, Yu R (2024). MFBind: a Multi-Fidelity Approach for Evaluating Drug Compounds in Practical Generative Modeling. *arXiv*:2402.10387v1 [q-bio.BM]. DOI: 10.48550/arXiv.2402.10387

PATENTS

Yu R, **Eckmann P**, Sun K, Zhao B, Feng M, Gilson MK (2023). Computational architecture to generate representations of molecules having targeted properties. United States patent pending US20240005179A1. June 16, 2023. [Link]

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]

REVIEW ACTIVITY

Reviewer, *International Conference on Learning Representations* (ICLR) 2025