

Peter Eckmann

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Research Interests

Machine learning for drug discovery, deep generative modeling, molecular dynamics

Education

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

B.S. Computer Science

3.896 GPA

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

4.86 GPA

Honors and Awards

NSF Research Experiences for Undergraduates Award (*June - Sept. 2022*)

Regents Scholarship, UC San Diego (*2021*)

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 Dr. Michael Gilson (Skaggs School of Pharmacy) to develop machine learning methods for drug discovery. Especially focused on generative modeling for small-molecule drug discovery and few-shot compound activity prediction.

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, Remote

(*June 2022 - September 2022*)

Researched and developed few-shot learning techniques for scoring candidate compounds in drug discovery. Submitted work resulting from this effort to the *International Conference on Machine Learning (ICML) 2023*.

Visiting researcher, Charité and Berlin Institute of Health, Berlin, Germany (June 2022 - September 2022)

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

Conference Publications

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/>

Eckmann P, Anderson J, Gilson M, Yu R (2023). Target-Free Compound Activity Prediction via Few-Shot Learning. Manuscript in review at *40th International Conference on Machine Learning (ICML 2023)*.

Journal Publications

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.

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.

Schulz R, Barnett A, Bernard R, Brown NJ, Byrne JA, **Eckmann P**, ..., Weissgerber TL (2022). Is the future of peer review automated? *BMC Research Notes*, 15(1), 1-5.

Eckmann P, Bandrowski A (2022). PreprintMatch: a tool for preprint publication detection applied to analyze global inequities in scientific publishing. *Public Library of Science (PLOS) One*, in press.

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.

Conference Abstracts

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

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, 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>

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**