Lukas Jarosch

MS Student · Biochemistry

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Education

Heidelberg University *Heidelberg, Germany*

MS in Biochemistry *Oct. 2020 - Present*

- Current grade: 1.0
- Relevant courses: Bioinformatics, Foundations of machine learning, Comp. single-cell biology

Heidelberg University *Heidelberg, Germany*

BS in Biochemistry *Oct. 2017 - Oct. 2020*

- Grade: 1.5 (class rank: tied for 2nd)

Anna-Essinger-Gymnasium *Ulm, Germany*

High School *Sep. 2009 - Jul. 2017*

- A-levels: 1.0 (best in year)

German grading scale: 1.0 (best) - 5.0 (insufficient)

Research Experience

Columbia University - Dept. of Systems Biology *New York City, United States*

Supervisors: Prof. Mohammed AlQuraishi & Dr. Nazim Bouatta *Apr. 2023 - Present*

- MS Thesis: “OpenBind: Extending AlphaFold2 to protein-ligand co-folding”
- Working on an AlphaFold2-inspired deep learning model for structure prediction of protein-ligand complexes.

Roche - Dept. of Computational Engineering and Data Science (CEDS) *Penzberg, Germany*

Supervisor: Dr. Wing Ki (Catherine) Wong *May 2022 - Oct. 2022*

- Identified predictors of antibody affinity from phage and ribosome display affinity maturation NGS data.
- Implemented a Python library for interpretable and uncertainty-calibrated affinity prediction of experimentally unobserved sequences using Gaussian process models.

École Polytechnique Fédérale de Lausanne (EPFL) *Lausanne, Switzerland*

Supervisor: Prof. Bruno Correia *Nov. 2021 - Feb. 2022*

- Computationally designed helical peptide binders against amyloid fibrils and improved efficiency of the underlying Rosetta-based pipeline.
- Experimented with adapting a geometric deep learning framework for interaction site prediction (dMaSIF-site) to predict the secondary structure preference of binding sites.

European Molecular Biology Laboratory (EMBL) *Heidelberg, Germany*

Supervisor: Dr. Judith Zaugg *Mar. 2021 - Sep. 2021*

- Analyzed effects of aging on gene regulation in human mesenchymal stromal cells using single-cell transcriptomics data.
- Created computational workflow for identifying differentially active transcription factors (TFs), target gene enrichment analysis, and TF-TF network inference.

Heidelberg Institute for Theoretical Studies (HITS) *Heidelberg, Germany*

Supervisor: Prof. Rebecca Wade *Jul. 2020 - Oct. 2020*

- BS Thesis: “Computational modeling of SERCA interactions with S100A1ct and DWORF”
- Computationally modeled interactions of the SERCA ATPase with the regulatory peptides S100A1ct and DWORF using protein-protein docking tools and presented hypothesis for mode of action.

University of Oxford - Dept. of Biochemistry *Oxford, United Kingdom*

Supervisor: Prof. Maike Bublitz *Feb. 2020 - May 2020*

- Successfully crystallized the SERCA ATPase with three novel inhibitors and built a 3.6 Å X-ray structure model.
- Proved a novel mode of action for another inhibitor using tryptophan fluorescence measurements.

Publications

Accepted

Ahdritz, G., Bouatta, N., Kadyan, S., **Jarosch, L.**, Berenberg, D., Fisk, I., Watkins, A. M., Ra, S., Bonneau, R., & AlQuraishi, M. (2023). OpenProteinSet: Training data for structural biology at scale. *arXiv*. DOI: 10.48550/arXiv.2308.05326
Accepted for publication in NeurIPS 2023 Track Datasets and Benchmarks

In Review

(*: equal contribution)

Kehr, D.*, Ritterhoff, J.*, Glaser, M.*, **Jarosch, L.**, Salazar, R. E., Spaich, K., Varadi, K., Birkenstock, J., Egger, M., Gao, E., Koch, W. J., Katus, H. A., Frey, N., Jungmann, A., Busch, C., Mather, P. J., Ruhparwar, A., Völkers, M., Wade, R. C., & Most, P. (2023). S100A1ct: a synthetic peptide derived from human S100A1 protein improves cardiac contractile performance and survival in pre-clinical heart failure models. *bioRxiv*. DOI: 10.1101/2023.03.04.531024
Submitted to Circulation

Posters

Jarosch, L., Leisibach, D., Hanisch, L. J., Kroedel-Mueller, M., & Wong, W. K. (2023). Modeling NGS data from Display campaigns with Gaussian Processes. Poster presented at PEGS Boston Summit, May 15-19, 2023.

Scholarships & Awards

2019-2023 **Scholarship**, Friedrich Naumann Foundation for Freedom
Stipend awarded for academic excellence and commitment to liberal values and an open society

2017 **GDCh School Prize**, German Chemical Society
Prize for best Chemistry A-levels

Teaching Experience

Nov. 2022 **Python for Scientists**, Co-organizer and Co-instructor
Co-organized and co-led a four-day programming course for Biochemistry students focusing on data analysis with Python.
Topics: Python basics (data structures, functions, flow control), Data analysis (pandas, seaborn, matplotlib, Jupyter Notebook)

Oct. 2021 **Informatics in Biochemistry**, Co-organizer and Co-instructor
Co-organized and co-led a two-day seminar for Biochemistry students focusing on the intersection of Computer Science and Biochemistry and an introduction to Python.
Topics: Research in Computational Biology, Python basics (data structures, functions, flow control, plotting)

Skills

Programming Languages	**Python, R**
Machine Learning	**PyTorch, PyTorch Lightning, GPyTorch, scikit-learn**
Data Science	**pandas, seaborn, Matplotlib, plotly, dplyr, ggplot2**
High-Performance Computing	**SLURM, LSF**
Tools	**Git, Docker, Singularity**
Languages	**German, English**