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John C. Faver, PhD

EXPERIENCE

Relay Therapeutics — Cambridge, MA
Principal Scientist, Computation — 2021-2025

- Built informatics platform (databases, web applications, analytical tools) to enable drug discovery with DNA-Encoded Chemical Libraries and Machine Learning (DEL+ML)
- Managed statistical and chemical data analysis for hundreds of DEL screens
- Developed software infrastructure for analyzing sequencing data from mRNA-Display to identify bioactive peptides
- Automated ETL pipelines to link data sources, build ML data sets, generate interactive project dashboards, and build structure-activity models to drive drug discovery projects
- Designed DEL screening libraries to sample unexplored 3D pharmacophore spaces

ZebiAI Therapeutics (acquired by Relay Therapeutics) — Waltham, MA
Principal Scientist, Scientific Computing and Informatics — 2020-2021

- Designed high fidelity DEL encoding/decoding methodology with built-in error correction
- Built informatics platform and analytical pipeline for DEL+ML hit finding
- Built research informatics platform and web applications for project management and reporting to track millions of datapoints across multiple collaborations

Baylor College of Medicine Center for Drug Discovery — Houston, TX
Assistant Professor and Cheminformatics Leader — 2015-2020

- Developed computational infrastructure for DEL screening platform
- Led statistical and chemical data analysis and hypothesis generation from DEL screening data against dozens of therapeutic targets
- Developed novel statistics for normalized enrichment in analyzing DEL screening data
- Taught graduate courses in computational methods for biomedical research

Yale University Department of Chemistry — New Haven, CT
Postdoctoral Associate with William Jorgensen — 2012-2015

- Led compound design for two medicinal chemistry projects (virtual screening, molecular docking, FEP)
- Developed database and web application for tracking medicinal chemistry projects

TECHNICAL SKILLS

Software Development: Experienced in developing scientific, statistical, data science, and web applications using Python (and common libraries including Django, pandas, scikit-learn, numpy, scipy, matplotlib, etc.), SQL, JavaScript, versioning (git), testing (pytest), workflow orchestration (prefect), infrastructure as code (pulumi), and deploying containerized (docker) applications in cloud environments (AWS).

Chemistry-related: Experienced in developing and using cheminformatics methods including chemical fingerprints (2D/3D), molecular shape and pharmacophore-based modeling, virtual library enumeration and molecular diversity/property analysis, structure-based drug design, free energy calculations, quantum chemistry, Schrödinger, OpenEye, RDKit, Dotmatics/Vortex, Spotfire

EDUCATION

Yale University — New Haven, CT
Postdoctoral Associate Chemistry – Computer-aided drug design — 2012-2015

University of Florida — Gainesville, FL
PhD Computational Chemistry – Statistical models for biomolecular modeling and quantum chemistry — 2012

University of Arkansas Fayetteville, AR
BS Chemistry – Synthesis of natural product analogs 2007

CONTRIBUTIONS

Co-organized symposium at the American Chemical Society National Meeting 2013
Developed the Biomolecular Fragment Database web application for benchmarking molecular models 2012
Reviewer for scientific journals 2012-Present

HIGHLIGHTED TALKS AND PRESENTATIONS

1. "Drug Discovery with DNA-Encoded Chemical Libraries" Invited talk at SLAS2020 conference, San Diego, CA 2020.
2. "Quantitative Comparisons of Enrichment from DNA-Encoded Library Selections" Poster presentation, 9th International Symposium on DNA-Encoded Chemical Libraries. Zurich, Switzerland 2019.
3. "Development of a Cheminformatics Platform for DNA-Encoded Library Screening" Poster presentation. NICHD Contraceptive Development Meeting. Minneapolis, MN 2018.
4. "Dotmatics and DNA-Encoded Chemical Libraries" Invited talk at Dotmatics User Group Meeting. Boston, MA 2017

HIGHLIGHTED PUBLICATIONS

ORCiD: https://orcid.org/0000-0002-0181-9283
Google Scholar: https://scholar.google.com/citations?user=ngoqSMgAAAAJ

1. **Faver, J. C.**, Sundersingh, F., Viarengo-Baker, L. A., Chen, Ying-Chu, Billings, K., Riley, P., Tsai, C., Kollmann, C. S., DNA-Encoded Chemical Library Screening with Target Titration Analysis: DELTA. Preprint online at ChemRxiv. 2025; doi:10.26434/chemrxiv-2025-tqmnj
2. Yu, Z., Ku, A.F., Anglin, J.L., Sharma, R., Ucisik, M.N., **Faver, J. C**., et al. Discovery and characterization of bromodomain 2–specific inhibitors of BRDT. *Proceedings of the National Academy of Sciences*. 2021 118(9), e2021102118.
3. Dawadi, S., Simmons, N., Miklossy, G., Bohren, K.M., **Faver, J. C.,** et al. Discovery of potent thrombin inhibitors from a protease-focused DNA-encoded chemical library. *Proceedings of the National Academy of Sciences*. 2020 117(29) 16782-16789.
4. Taylor, D.M., Anglin, J., Park, S., Ucisik, M.N., **Faver, J. C.,** *et al.* Identifying OXA-48 Carbapenemase Inhibitors using DNA-Encoded Chemical Libraries. *ACS Infectious Diseases*. 2020. 6(5) 1214-1227.
5. Newton, A. S., **Faver, J. C.**, et al. Structure-Guided Identification of DNMT3B Inhibitors. *ACS Medicinal Chemistry Letters* 2020 11(5) 971-976.
6. **Faver, J. C.**, Riehle, K., Lancia, D. R., Milbank, J. B. J., Kollmann, C. S., Simmons, N., Yu, Z., Matzuk, M. M. Quantitative Comparison of Enrichment from DNA-Encoded Chemical Library Selections, *ACS Combinatorial Science* 2019. 21(2) 75-82.
7. Burns, L., **Faver, J. C.**, Zheng, Z., Marshall, M., Smith, D., Vanommeslaeghe, K., MacKerrell, A., Merz, K. M., Sherrill, C. D. The BioFragment Database (BFDb): An Open-Data Platform for Computational Chemistry Analysis of Noncovalent Interactions. *Journal of Chemical Physics* 2017. 147, 161727.
8. **Faver, J. C.**, Yang, W., Merz, K. M. The Effects of Computational Modeling Errors on the Estimation of Statistical Mechanical Variables. *Journal of Chemical Theory and Computation* 2012. 8(10), 3769–3776.
9. **Faver, J. C.**, Zheng, Z., Merz, K. M. Statistics-based Model for Basis Set Superposition Error Correction in Large Biomolecules. *Physical Chemistry Chemical Physics* 2012. 14, 7795-7799.
10. **Faver, J. C.** *et al.* Formal Estimation of Errors in Computed Absolute Interaction Energies of Protein-ligand Complexes. *Journal of Chemical Theory and Computation* 2011. 7(3), 790-797.