John C. Faver, Ph. D.

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EXPERIENCE

Relay Therapeutics — Cambridge, MA
Principal Scientist, Computation — 2021-2025
- Built informatics platform (analytical tools, web applications, statistical models) to enable hit finding with DNA-Encoded Chemical Libraries and Machine Learning (DEL+ML)
- Developed software infrastructure for analyzing NGS data from RNA-Display screening
- Automated processes to link data sources, build custom data sets, generate project dashboards, and build structure-activity models to drive drug discovery projects
- Designed novel compound libraries to sample unexplored in 3D pharmacophore spaces

ZebiAI Therapeutics (acquired by Relay Therapeutics 2021) — Waltham, MA
Principal Scientist, Scientific Computing and Informatics — 2020-2021
- Developed custom informatics platform for machine learning with DEL data
- Designed high fidelity DEL encoding/decoding strategy with built-in error correction
- Built informatics platform for project management and reporting

Baylor College of Medicine Center for Drug Discovery — Houston, TX
Assistant Professor and Cheminformatics Leader — 2015-2020
- Developed informatics infrastructure for DEL screening platform
- Led analysis and hypothesis generation from 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
- Guided compound design for 2 medicinal chemistry projects
- Developed web application for collaborative medicinal chemistry projects

University of Florida Quantum Theory Project — Gainesville, FL
Graduate Research Assistant with Kenneth M. Merz — 2007-2012
- Developed methods for on-the-fly error estimation in molecular modeling
- Built fast statistics-based models for quantum chemistry

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 simulation — 2012

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

TECHNICAL SKILLS

Programming/Scripting: Experienced in developing scientific, statistical, and web applications using Python, SQL, JavaScript, C++, FORTRAN, versioning with git, and deploying applications in cloud providers including AWS.

Chemistry-related: Experienced in developing and using cheminformatics methods, structure-based drug design, free energy calculations, quantum chemistry, Gaussian, Schrödinger, OpenEye, RDKit, Dotmatics/Vortex, Spotfire

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

HONORS

Crow Award for excellence in scientific publication	2012, 2011
Chemical Computing Group Research Excellence Award	2011

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. 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.
2. 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.
3. 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.
4. Newton, A. S., **Faver, J. C.**, et al. Structure-Guided Identification of DNMT3B Inhibitors. *ACS Medicinal Chemistry Letters* 2020 11(5) 971-976.
5. **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.
6. 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.
7. Cole, D. J., Janecek, M., Stokes, J. E., Rossmann, M., **Faver, J. C.**, McKenzie, G. J., Venkitaraman, A. R., Hyvonen, M., Spring, D. R., Huggins, D. G., Jorgensen, W. L. Computationally-guided optimization of small-molecule inhibitors of the Aurora A kinase–TPX2 protein–protein interaction. *Chemical Communications* 2017. 53, 9372-9375.
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.