# John C. Faver, Ph. D.

352.327.8314
jfaver@posteo.net | Residence:
http://johncfaver.com | Houston, TX

## EXPERIENCE

**Relay Therapeutics** — Cambridge, MA
*Senior Scientist II, ML Discovery* — 2021-Present
- Platform development for machine learning with DNA-Encoded Chemical Libraries (DEL)

**ZebiAI Therapeutics** (acquired by Relay Therapeutics 2021) — Waltham, MA
*Principal Scientist, Scientific Computing and Informatics* — 2020-2021
- Platform development for machine learning with DEL
- 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

**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

**University of Arkansas** Department of Chemistry — Fayetteville, AR
*Undergraduate Research Assistant* with Matthias McIntosh — 2005-2007
- Synthesized analogs of natural products with anti-leukemia activity

**University of Arkansas for Medical Sciences** Department of Pharmacology & Toxicology — Little Rock, AR
*Undergraduate Research Fellow* — 2006
- Conducted binding assays of monoclonal antibodies as therapies for drug overdose

## 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 and web applications using Python, SQL, JavaScript, C++, FORTRAN, Java, Git

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

## 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 |

## RECENT INVITED 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

## RECENT AND HIGHLIGHTED PUBLICATIONS (of 25 total)


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



1. Dawadi, S., Simmons, N., Miklossy, G., Bohren, K.M., **Faver, J.C.,** Ucisik, M.N., Nyshadham, P., Yu, Z. and Matzuk, M.M., 2020. 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.
2. 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.
3. Newton, A. S., **Faver, J. C.**, Micevic, G., Muthusamy, V., Kudalkar, S. N., Bertoletti, N., Anderson, K. S., Bosenberg, M. W., Jorgensen, W. L. Structure-Guided Identification of DNMT3B Inhibitors. *ACS Medicinal Chemistry Letters* 2020 11(5) 971-976.
4. **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.
5. 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.
6. 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.
7. **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.
8. **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.
9. **Faver, J. C.** *et al.* The Energy Computation Paradox and ab initio Protein Folding. *PLoS ONE* 2011. 6(4): e18868.
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.