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# John C. Faver, Ph. D.

Baylor College of Medicine
1 Baylor Plaza
Houston, TX 77030

## EDUCATION

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

**University of Florida** — Gainesville, FL
**Ph. D. Chemistry** – Statistical error estimation in biomolecular modeling — 2012

**University of Arkansas** — Fayetteville, AR
**B.S. Chemistry** – Synthesis of natural product analogs — 2007

## EXPERIENCE

**Baylor College of Medicine** Center for Drug Discovery — Houston, TX
*Instructor and Cheminformatics Leader* — 2015-Present
- Analyzed large data sets and generated hypotheses concerning screens of DNA-encoded chemical libraries
- Developed custom software and workflows for data visualization and analysis
- Taught graduate level 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 using computational modeling (molecular docking, free energy calculations, molecular dynamics, ADMET modeling)
- Optimized protocols for generating and screening virtual compound libraries fit for specific targets
- Developed open source software for managing and analyzing data in collaborative drug design projects through a web application

**University of Florida** Quantum Theory Project — Gainesville, FL
*Research Assistant* with Kenneth M. Merz — 2007-2012
- Developed novel methodologies for error estimation in molecular simulations (statistical modeling, machine learning, Monte Carlo simulation)
- Fast statistics-based models for quantum chemistry
- Published strategies for free energy estimation in community prediction challenges
- Generated QSAR models using descriptors from 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

## TECHNICAL SKILLS

**Programming/Scripting:** Python, SQL, JavaScript, C++, R, Fortran, Java, Git
**Computational Chemistry:** Virtual screening, molecular docking, structure-based drug design, QSAR, statistical mechanics, molecular dynamics, Monte Carlo simulations, free energy calculations, linear-scaling QM, Gaussian, Schrödinger, OpenEye, AMBER, MCPRO, Dotmatics/Vortex, RDKit

## CONTRIBUTIONS

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| Open source software contributions at https://github.com/johncfaver | 2014-Present |
| Co-organized symposium at the American Chemical Society National Meeting | 2013 |
| Developed the Biomolecular Fragment Database web application for benchmarking molecular models | 2012 |
| Served as reviewer for the Journal of Chemical Theory and Computation, Journal of Chemical Information and Modeling, and Scientific Reports | 2012-Present |

## HONORS

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|---|---|
| Crow Award for excellence in scientific publication | 2012, 2011 |
| Chemical Computing Group Research Excellence Award | 2011 |
| University of Florida College of Liberal Arts and Sciences Graduate Student Travel Award | 2011 |
| University of Florida Open Access Publishing Fund | 2011 |
| University of Arkansas Honors College Undergraduate Research Grant | 2006 |

## PUBLICATIONS

1. **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 DOI: 10.1021/acscombsci.8b00116
2. 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.
3. 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.
4. Ucisik, M. N., Zheng, Z., **Faver, J. C.**, Merz, K. M. Bringing Clarity to the Prediction of Protein-Ligand Binding Free Energies via “Blurring”. *Journal of Chemical Theory and Computation* 2014. Advance online publication. DOI: 10.1021/ct400995c
5. **Faver, J. C.**, Merz, K. M. Fragment-Based Error Estimation in Biomolecular Modeling. *Drug Discovery Today* 2014. 19(1), 45-50.
6. **Faver, J. C.**, Ucisik, M. N., Yang, W., Merz, K. M. Computer-aided Drug Design: Using Numbers to your Advantage. *ACS Medicinal Chemistry Letters* 2013. 4(9), 812–814.
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. Benson, M. L., Dashti, D. S., **Faver, J. C.**, *et al*. Prediction of Trypsin/Molecular Fragment Binding Affinities by Free Energy Decomposition and Empirical Scores. *Journal of Computer-Aided Molecular Design* 2012. 26(5), 647-659.
10. **Faver, J. C.**, Zheng, Z., Merz, K. M. Model for Fast Estimation of Intramolecular Basis Set Superposition Error in Macromolecules. *Journal of Chemical Physics* 2011. *135,* 144110.
11. Ucisik, M. N., Dashti, D., **Faver, J. C.**, Merz, K. M. Pairwise Additivity of Energy Components for Protein-Ligand Binding: HIV II Protease-Indinavir Case. *Journal of Chemical Physics* 2011. *135,* 085101.
12. **Faver, J. C.** *et al.* The Energy Computation Paradox and ab initio Protein Folding. *PLoS ONE* 2011. 6(4): e18868.
13. **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.
14. **Faver, J.**, Merz, K. M. The Utility of the HSAB Principle via the Fukui Function in Biological Systems. *Journal of Chemical Theory and Computation* 2010. 6(2), 548–559.