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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** – Statistics-based methods in biomolecular modeling — 2012

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

## RESEARCH EXPERIENCE

**Baylor College of Medicine** Center for Drug Discovery — Houston, TX
*Programmer Analyst II* — 2015-Present

- Analyzed large data sets and generated hypotheses concerning the screening of DNA-encoded chemical libraries
- Developed customized workflows for data visualization and analysis

**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 (SciPy, NumPy, Pandas, scikit-learn, etc.), Bash, SQL (PostgreSQL, SQLite, MySQL), R, Fortran, C++, PHP, JavaScript, 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

## SCIENTIFIC 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 |
| Serves as reviewer for the Journal of Chemical Theory and Computation and Journal of Chemical Information and Modeling | 2012-Present |

## AWARDS AND 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. 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
2. **Faver, J. C.**, Merz, K. M. Fragment-Based Error Estimation in Biomolecular Modeling. *Drug Discovery Today* 2014. 19(1), 45-50.
3. **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.
4. **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.
5. **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.
6. 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.
7. **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.
8. 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.
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.
11. **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.