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John C. Faver, Ph. D.

Baylor College of Medicine
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Houston, TX 77030

EDUCATION

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

University of Florida — Gainesville, FL
PhD Chemistry – Statistical error estimation in biomolecular modeling — 2012

University of Arkansas — Fayetteville, AR
BS 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 compound hypotheses from DNA-encoded chemical library screening
- Developed custom software and workflows for data analysis and visualization
- 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 using computational modeling (molecular docking, free energy calculations, molecular dynamics, ADMET modeling)
- Optimized target-specific protocols for screening large virtual compound libraries
- Developed open source web application for team-based compound/assay data management and analysis

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

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++, 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

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
Reviewer for the Journal of Chemical Theory and Computation, Journal of Chemical Information and Modeling, Scientific Reports, and ACS Combinatorial Science	2012-Present

HONORS

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

SELECTED PUBLICATIONS

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

1. 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. Article ASAP DOI: 10.1021/acsmedchemlett.0c00011.
2. **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.
3. 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.
4. 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.
5. 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. 10(3) 1314-1325.
6. **Faver, J. C.**, Merz, K. M. Fragment-Based Error Estimation in Biomolecular Modeling. *Drug Discovery Today* 2014. 19(1), 45-50.
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.** *et al.* The Energy Computation Paradox and ab initio Protein Folding. *PLoS ONE* 2011. 6(4): e18868.
11. **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.
12. **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.