John C. Faver, Ph. D.

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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
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
- Developed informatics infrastructure for DNA-Encoded chemical Library (DEL) 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
- Optimized target-specific protocols large virtual screens
- Developed web application to enhance 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
- 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 Arkansas Honors College Undergraduate Research Grant	2006

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 19 total)

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

1. 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. Article ASAP DOI: 10.1021/acsinfecdis.0c00015.
2. 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.
3. **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.
4. 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.
5. 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.
6. **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.
7. **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.
8. **Faver, J. C.** *et al.* The Energy Computation Paradox and ab initio Protein Folding. *PLoS ONE* 2011. 6(4): e18868.
9. **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.
10. **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.