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EDUCATION

2008 Ph.D. Chemistry, Duke University, Advisor: Weitao Yang
2001 M.S. Chemistry, Southern Methodist University, Advisor: George P. Ford
1999 B.S. Chemistry, Texas Christian University

PROFESSIONAL POSITIONS

2020 – present Senior R & D Staff and Group Leader, Molecular Biophysics, Biosciences Division, Oak Ridge National Laboratory
2015 – 2020 R & D Staff, Biosciences Division, Oak Ridge National Laboratory
2015 – 2021 Adjunct Assistant Professor, Genome Science and Technology Graduate Program, University of Tennessee
2009 – 2015 R & D Associate, Biosciences Division, Oak Ridge National Laboratory
2008 – 2009 Postdoctoral Research Associate, Center for Molecular Biophysics, Biosciences Division, Oak Ridge National Laboratory, Advisor: JC Smith

AWARDS

2020 ORNL Director's Award for Outstanding Team, Science and Technology Category "for revolutionary advancements in the area of microbial isolation techniques that promise to usher in a new era for microbiome studies, an area of current significant interest in both health and agriculture"
2020 UT-Battelle Award for Outstanding Scholarly Output, Science and Technology Category
2014 ORNL Nominee for the Blavatnik Award for Young Scientists, Chemistry Category
2013 ORNL Director's Award for Outstanding Team Accomplishment "for groundbreaking research in biotic and abiotic mechanisms of mercury methylation in the environment, leading to high-impact publications in *Science* and *Nature Geoscience*"
2013 UT-Battelle Team Award for Scientific Research
2013 ORNL Significant Event Award – For the discovery of genes and proteins required for bacterial mercury methylation

Journal review

Journal of Physical Chemistry • *Journal of Chemical Information and Modeling* • *Theoretical Chemistry Accounts* • *Journal of Applied and Analytical Pyrolysis* • *European Journal of Cell Biology* • *Cellulose* • *PNAS* • *Acta Crystallographica D: Biological Crystallography* • *Applied and Environmental Microbiology* • *Nature Geoscience* • *Crystal Growth and Design* • *Inorganic*

Chemistry • Environmental Science and Technology • Journal of Geochemical Exploration • PeerJ • ACS Earth and Space Chemistry • Journal of Molecular Structure • ACS Catalysis • Frontiers in Microbiology • ISME J • Science of the Total Environment • ACS Sustainable Chemistry and Engineering • International Journal of Biological Macromolecules • Molecular Physics • Phytochemistry • J Am Chem Soc • BBA General Subjects • ChemComm • Frontiers in Immunology • Frontiers in Chemistry • ACS Infectious Diseases • PLOS ONE • ACS Omega • Trends in Pharmacological Sciences • Journal of Molecular Modeling • Bioorganic and Medicinal Chemistry • Scientific Reports • iScience • PLOS Neglected Tropical Diseases • J Biomolec Struct Dyn • Current Opinion in Microbiology • Journal of Chemical Theory and Computation

PUBLICATIONS

Journal articles

96. Lewis BR, Uddin MR, Moniruzzaman M, Kuo KM, Higgins AJ, Shah LMN, Sobott F, Parks JM, Hammerschmid D, Gumbart JC, Zgurskaya HI, and Reading E. Conformational restriction shapes inhibition of a multidrug efflux adaptor protein. *Nat Commun.* **2023**, 14, 3900. DOI: 10.1038/s41467-023-39615-x
95. Shen Y, Parks JM, Smith JC. HLA-Clus: HLA class I clustering based on 3D structure. *BMC Bioinf.* **2023**, 24, 189. DOI: 10.1186/s12859-023-05297-x
94. Sanders BC, Pohkrel S, Labbe AD, Mathews II, Cooper CJ, Davidson RB, Phillips G, Weiss KL, Zhang Q, O'Neill H, Kaur M, Ferrins L, Schmidt JG, Reichard W, Surendranathan S, Parvathareddy J, Phillips L, Rainville C, Sterner DE, Kumaran D, Andi B, Babnigg G, Moriarty NW, Adams PD, Joachimiak A, Hurst BL, Kumar S, Butt TR, Jonsson CB, Wakatsuki S, Galanie S, Head MS, and Parks JM. Potent and selective covalent inhibition of the papain-like protease from SARS-CoV-2. *Nat Commun.* **2023**, 14, 1733. DOI: 10.1038/s41467-023-37254-w
93. Gionfriddo C, Soren A, Wymore A, Hartnett DS, Podar M, Parks JM, Elias DA, and Gilmour CC. Transcriptional regulation of *hgcAB* by an ArsR-like regulator in *Pseudodesulfovibrio mercurii* ND132. *Appl Environ Microbiol.* **2023**, 89, e01768-22. DOI: 10.1128/aem.01768-22
92. Shen Y, Parks JM, and Smith JC. HLA Class I Supertype Classification Based on Structural Similarity. *J Immunol.* **2023**, 210, 103–114. DOI: 10.4049/jimmunol.2200685
91. Moniruzzaman M, Cooper CJ, Uddina MR, Walker JK, Parks JM, and Zgurskaya HI. Analysis of Orthogonal Efflux and Permeation Properties of Compounds Leads to the Discovery of New Efflux Pump Inhibitors. *ACS Infect Dis.* **2022**, 8, 10, 2149–2160. DOI: 10.1021/acsinfecdis.2c00263
90. Drago VN, Dajnowicz S, Parks JM, Blakeley MP, Keen DA, Coquette N, Weiss KL, Gerlits O, Kovalevsky A, and Mueser TC. An N···H···N low-barrier hydrogen bond pre-organizes the catalytic site of aspartate aminotransferase to facilitate the second half-reaction. *Chem Sci.* **2022**, 13, 10057-10065. DOI: 10.1039/d2sc02285k
89. Pal D, De K, Shanks CM, Feng K, Yates TB, Morrell-Falvey J, Davidson RB, Parks JM, and Muchero W. Core cysteine residues in the PAN domain are critical for HGF/c-MET signaling. *Comm Biol.* **2022**, 5, 646. DOI: 10.1038/s42003-022-03582-8
88. Leus IV, Weeks JW, Bonifay V, Shen Y, Yang L, Cooper CJ, Nash D, Duerfeldt A, Smith JC, Parks JM, Rybenkov VV, and Zgurskaya HI. Property space mapping of small molecule permeabilities in *Pseudomonas aeruginosa*. *Sci Rep.* **2022**, 12, 8220. DOI: 10.1038/s41598-022-12376-1

87. Davidson RB, Woods J, Effler TC, Thavappiragasam M, Mitchell JC, Parks JM, Sedova S. OpenMDlr: Parallel, open-source tools for general protein structure modeling and refinement from pairwise distances. *Bioinformatics*. **2022**, 38, 3297–3298. DOI: 10.1093/bioinformatics/btac307
86. Glaser J, Sedova A, Galanie S, Kneller DW, Davidson RB, Maradzike E, Del Galdo S, Labbé A, Hsu DJ, Agarwal R, Bykov D, Tharrington A, Parks JM, Smith DMA, Daidone I, Coates L, Kovalevsky A, and Smith JC. Hit expansion of a non-covalent SARS-CoV-2 main protease inhibitor. *ACS Pharmacol Transl Sci*. **2022**, 2022, 5, 4, 255–265. DOI: 10.1021/acspsci.2c00026
85. Gao M, An DN, Parks JM, and Skolnick J. AF2Complex predicts direct physical interactions in multimeric proteins with deep learning. *Nat Commun*. **2022**, 13, 1744. DOI: 10.1038/s41467-022-29394-2
84. Gumbart JC, Ferreira JL, Hwang H, Hazel AJ, Cooper CJ, Parks JM, Smith JC, Zgurskaya HI, and Beeby M. Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. *Biophys J*. **2021**, 120, 3973–3982. DOI: 10.1016/j.bpj.2021.08.016
83. D’Cunha N, Moniruzzaman M, Haynes K, Malloci G, Cooper CJ, Margiotta E, Vargiu AV, Uddin MR, Leus IV, Cao F, Parks JM, Rybenkov VV, Ruggerone P, Zgurskaya HI, and Walker JK. Mechanistic duality of efflux substrates and inhibitors: Example of simple substituted cinnamoyl and naphthyl amides. *ACS Infect Dis*. **2021**, 7, 9, 2650–2665. DOI: 10.1021/acsinfecdis.1c00100
82. Cooper CJ, Bu L, Patil R, Mou Z, Turpin DB, van Heiningen ARP, Parks JM, and Knott BC. Pretreatment with sodium methyl mercaptide increases carbohydrate yield during kraft pulping. *ACS Sust Chem Eng*. **2021**, 9, 34, 11571-11580. DOI: 10.1021/acssuschemeng.1c04332
81. Davidson RB, Thavappiragasam M, Effler TC, Woods J, Elias DA, Parks JM, and Sedova A. Modeling protein structures from predicted contacts with modern molecular dynamics potentials: Accuracy, sensitivity, and refinement. BCB '21: Proceedings of the 12th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics, 2021, 21, 1-10. DOI: 10.1145/3459930.3469510
80. Lian P, Mou, Z, Johnston RC, Cooper CJ, Brooks SC, Gu B, Govind N, Jonsson S and Parks JM. Mechanisms of dimethylmercury formation facilitated by nanoparticles. *J Phys Chem A*. **2021**, 125, 24, 5397–5405. DOI: 10.1021/acs.jpca.1c04014
79. Mishra S, Cooper CJ, Parks JM, and Mitchell JC. Hotspot coevolution at protein-protein interfaces is a key identifier of native protein complexes. *J Phys Chem B*. **2021**, 125, 6058–6067. DOI: 10.1021/acs.jpccb.0c11525
78. Pavlova A, Zhang Z, Acharya A, Lynch DL, Pang YT, Mou Z, Parks JM, Chipot C, and Gumbart JC. Machine learning reveals the critical interactions for SARS-CoV-2 spike protein binding to ACE2. *J Phys Chem Lett*. **2021**, 12, 5494–5502. DOI: 10.1021/acs.jpcllett.1c01494
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76. Zgurskaya HI, Walker JK, Parks JM, and Rybenkov VV. Multidrug efflux pumps and the two-faced Janus of substrates and inhibitors. *Acc Chem Res*. **2021**, 54, 4, 930–939. DOI: 10.1021/acs.accounts.0c00843

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66. Cooper CJ, Alam S, Nzuwah Nziko VP, Johnston RC, Ivanov A, Mou Z, Turpin DB, Rudie AW, Elder TJ, Bozell JJ, and Parks JM. Co(salen)-catalyzed oxidation of lignin models to form benzoquinones and benzaldehydes: A computational and experimental study. *ACS Sust Chem Eng.* **2020**, 8, 18, 7225-7234. DOI: 10.1021/acssuschemeng.0c01970
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