Qianzhen Shao

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Education

B. Sc., Chemistry (Bolin Class),

Nankai University, Tianjin, China 09. 2017 – 06. 2021

Ph. D., Chemistry

Vanderbilt University, Nashville, TN, USA 09. 2021 – present

Research Experience

At **Vanderbilt University**, 09. 2021-present, supervisor: **Zhongyue (John) Yang**, as a graduate student.

- Developing EnzyHTP, the high-throughput computational platform for complete life-cycle of enzyme modeling.
- Developing EnzyToT, the downstream application of EnzyHTP, to identify rate-enhancing mutants for enzymes.
- Developing EnzyEFdesign, the downstream application of EnzyHTP, that designs the internal electric field of enzyme in a semi-rational manner.

At **Vanderbilt University**, 09. 2021-present, supervisor: **Jens Meiler**, as a co-advised graduate student.

- Developing RosettaQM that incorporates quantum mechanics (QM) into the Rosetta biomolecular modeling suite.
- Applying RosettaQM to build new energy functions for biomolecular modeling in Rosetta.

At **University of California, Los Angeles**, 07. 2019-09.2021, supervisor: **Kendall N. Houk**, as a visiting undergraduate student.

- QM, MD and QM/MM study of enzyme catalysis.
- Quasi-classical dynamic study of ambimodal reactions.
- Mechanism study of organic reactions and origin of selectivities.
- Theoretical study of the regioselectivity in radical based C-H functionalization.

At **Nankai University**, 06. 2017-09. 2021, supervisor: **Xiaosong Xue**, as an undergraduate student.

- DFT based mechanism and catalytic origin studies of organic reactions.
- Theoretical scale of the fluorinating power and a new kinetic equation bridging kinetic and thermodynamic.
- NMR prediction for the NMR based chiral sensing scaffold.

Publications

1. **Shao, Q.**, Jiang, Y. and Yang, Z. J. EnzyHTP: A High-Throughput Computational Platform for Enzyme Modeling *J. Chem. Inf. Model.* **62**, 647-655 (2022)
2. Jiang, Y., Stull, S. L., **Shao, Q.**, Yang, Z. J. Convergence in Determining Enzyme Functional Descriptors across Kemp Eliminase Variants *Electron. Struct.* in press (2022) https://doi.org/10.1088/2516-1075/acad51
3. Juarez, R. J., Tremblay, M., Jiang, Y., Shao, Q., Link, A. J., Yang, Z. J. LassoHTP: a High-throughput Computational Tool for Lasso Peptide Structure Construction and Modeling *J. Chem. Inf. Model.* Accepted Author Manuscript (2022)
4. Chen, Y.†, Gu, Y.†, Meng, H.†, **Shao, Q.†**, Xu, Z., Bao, W., Gu, Y., Xue, X. and Zhao, Y. Metal-Free C-H Functionalization via Diaryliodonium Salts with a Chemically Robust Dummy Ligand. *Angew. Chem. Int. Ed.* Accepted Author Manuscript. (2022) https://doi.org/10.1002/anie.202201240 ***(co-first author)***
5. Li, Y., **Shao, Q.**, He, H., Zhu, C., Xue, X.-S. and Xie, J. Highly selective synthesis of all-carbon tetrasubstituted alkenes by deoxygenative alkenylation of carboxylic acids *Nat. Comm.* **13**, 10 (2022)
6. Juliá, F.†, **Shao, Q.†**, Duan, M.†, Plutschack, M. B., Berger, F., Mateos, J., Lu, C., Xue, X.-S., Houk, K. N. and Ritter, T. High Site Selectivity in Electrophilic Aromatic Substitutions: Mechanism of C–H Thianthrenation *J. Am. Chem. Soc.* **143,** 16041–16054 (2021). ***(co-first author)***
7. Yan, B., Ran, X., Jiang, Y., Torrence, S. K., Li, Y., **Shao, Q.**, Yang, Z. J. Rate-Perturbing Single Amino Acid Mutation for Hydrolases: A Statistical Profiling. *J. of Phy. Chem. B* **125,** 10682–10691 (2021).
8. Yamano, M. M.†, Kelleghan, A. V.†, **Shao, Q.†** et al. Intercepting fleeting cyclic allenes with asymmetric nickel catalysis. *Nature* 586, 242–247 (2020) ***(co-first author)***
9. Quintela-Varela, H., Jamieson, C., **Shao, Q**., Houk, K. and Trauner, D. Bioinspired

Synthesis of (-) - PF - 1018. *Angew. Chem. Int. Ed.* 59, 5263. (2020)

10. Li, X., Duan, M., Deng, Z., **Shao, Q.**, Chen, M., Zhu, G., Houk, K. and Sun, J Catalytic Enantioselective Synthesis of Chiral Tetra-arylmethanes. *Nature Catalysis* 3, 1010–1019 (2020).
11. Shang, G.†, Duan, M.†, **Shao, Q.**, Houk, K. and Chen, M. Development of α,α-Disubstituted Crotylboronate Reagents and Stereoselective Crotylation via Brønsted or Lewis Acid Catalysis. *J. Am. Chem. Soc.* 142, 43, 18355–18368. (2020)

Honor & Awards

2016 30th Chinese Chemical Olympiad(Provincial level) First Prize (TOP 0.1% in China)

2016 30th Chinese Chemical Olympiad Silver award

2018 Gongneng Special Scholarship of Nankai University

2019 Gongneng Special Scholarship of Nankai University

2021 Yang Shixian scholarship of the best graduate of Year 2021 from College of Chemistry, Nankai University

2021 Award of excellent graduation thesis of Nankai University

2021 University Graduate Fellowship of Vanderbilt University