

Yumeng Zhang

Ph.D. Candidate

Phone: (413)409-1164

Email: yumzhang@umass.edu

Address: 279 Amherst Rd, Sunderland, MA

EDUCATION

- 2015 - 2019 B.S. in Chemistry and Molecular Science, Wuhan University, China
2019 - Ph.D. in Chemistry, University of Massachusetts at Amherst, US (in progress)

RESEARCH EXPERIENCE

09/2019-present: Graduate Research Assistant, University of Massachusetts Amherst (Advisor: Jianhan Chen)

- Developed a novel coarse-grained (CG) protein model, **HyRes II**, for accurate CG simulation of the conformational ensemble and dynamic interaction of intrinsically disordered proteins (IDPs).
- Developed a new enhanced sampling method, **REST3**, that resolved the temperature segregation problem in the widely-used replica exchange with solute tempering (REST2) protocol. Demonstrated that REST3 achieved faster convergence and higher efficiency in IDP simulations.
- Applied multi-scale simulation techniques to investigate the physical basis of how several IDPs, including tumor suppressor p53, flaviviral proteases, ion channel KCNQ1 N-terminal tail, and staphylococcal peroxidase inhibitors (SPINs) dynamically interact with their biological targets.

07/2018-05/2019: Undergraduate Researcher, Wuhan University, China (Advisor: Fuan Wang)

- Constructed an enzyme-free, hybrid HCR-CHA DNA circuits to amplify the phosphorylase kinase signal detection in vitro?

07/2016-05/2018: Undergraduate Researcher, Wuhan University (Advisor: Qianghui Zhou)

- Developed total synthesis protocols of natural products such as DHP-vinylindole using metal-catalyzed (e.g., Pd^{II}) enzyme.

PUBLICATIONS

1. **Y. Zhang**, X. Liu* and J. Chen*, " Coupled binding and folding of SPIN N-terminal region in myeloperoxidase inhibition" (*in preparation, est. 2022*)
2. **Y. Zhang**, X. Liu* and J. Chen*, " Re-balancing Replica Exchange with Solute Tempering for Sampling Dynamic Protein Conformations" (*in preparation, est. 2022*)
3. **Y. Zhang**, X. Liu* and J. Chen*, "Towards Accurate Coarsed-Grained Simulations of Disordered Proteins and Their Dynamic Interactions", *J. Chem. Inf. Model* (2022).
4. J. Zhao, X. Liu, A. Blayney, **Y. Zhang**, L. Gandy, F. Zhang, R. J. Linhardt, J. Chen, C. Baines, S. N. Loh and C. Wang, "Intrinsically disordered N-terminal domain (NTD) of p53 interacts with mitochondrial PTP regulator Cyclophilin D" *J. Mol. Biol.* 434, 167552 (2022).
5. X. Gong#, **Y. Zhang**# and J. Chen, "Advanced Sampling Methods for Multiscale Simulation of Disordered Proteins and Dynamic Interactions" *Biomolecules*, 11, 1416 (2021).

TECHNICAL SKILLS

Computation and Molecular Modeling:

- High proficiency in Unix, bash, Jupyter-lab, and Python programing.
- High proficiency in VMD, CHARMM, and Gromacs. Proficiency in OpenMM.

Organic and Analytical Chemistry:

- Proficient in designing and optimizing synthetic pathways.
- Proficient in NMR characterization of natural product characterizations.
- Proficient in PCR, electrophoresis gel, UV, and fluorescence spectroscopy

HONORS AND AWARDS

- 2021- Referees for *Biophysical Journal*, *Scientific Reports*, *Proteins*.
2020 1st place prize in Chemistry ResearchFest poster presentation, UMass Amherst
2016 2nd Class Freshman Scholarship, Wuhan University, China
2015 Freshman Scholarship, Wuhan University, China