Zhaoqi SHI

(+86) 18058740766 | wuguojia@tmu.edu.cn | github.com/wunaiwuhuang

 https://github.com/wunaiwuhuang | AIB_001

Zhejiang University(ZJU), Hangzhou, Zhejiang - 310058, China

RESEARCH INTEREST

As a candidate with a strong foundation in both life sciences and physics, I specialize in applying molecular simulation techniques such as Molecular Dynamics and Free Energy Perturbation. My research interests focus on computational biophysics, with a particular emphasis on biomolecular studies. I am keen to explore applications in computer-aided drug design and engage in theoretical investigations like phase separation.

EDUCATION

- **Chu Kochen Honor College, Zhejiang University** *Sep. 2021 - Jun. 2025 (Expected)*

  *Bachelor of Science in **Biological Sciences and Physics (Double Major)*** Hangzhou, China

  ◦ **GPA:** 3.96/4.00 (overall) and 3.99/4.00 (third year); **RANKING :** 1st out of 104 students;

  ◦ **TOEFL:** 104 (Best Score, R:28, L:28, S:23, W:25);

RESEARCH PROJECTS

- **Molecular Simulation-Driven Optimization of CDK7 Inhibitors (Independent project)** *Jul. 2023 - Jun. 2024*

  *Supervisor: **Prof. Ruhong Zhou** Supported by ZJU Key Research Project Fund (50,000 RMB, 10 people total);* [ ]

  ◦ **Developed a covalent model** for the THZ1-CAK complex (PDBID: 6XD3) incorporating non-standard amino acids, using CHARMM-GUI with the CHARMM force field for proteins and CGenFF for the small molecule.

  ◦ Implemented virtual screening utilizing Smina, **identified 147 potential positive fragments using Smina's scoring function**, and generated linkers between selected fragments and the stable core-fragment of THZ1.

  ◦ Conducted molecular dynamic with NAMD3 to relax the conformation of the generated links, selecting stable ligands and identifying 17 candidate ligands for further evaluation.

  ◦ **Employed Free Energy Perturbation (FEP) calculations** to identify the top three ligands with superior free energy profiles compared to the original small molecules.

- **Molecular Dynamics Simulation for NMR Order Parameter (Collaborate project)** *Jul. 2024 - Now*

  *Supervisor: **Prof. Ruhong Zhou** Collaborator: **Prof. Ann E. McDermott from Columbia University*** [ ]

  ◦ Developed ubiquitin protein (PDBID: 3ONS) model for molecular simulation under different force field, including AMBER-99/SB, OPLS-AA/S and CHARMM-36m;

  ◦ Implemented both time average method and iRED method for calculating of order parameter, comparing between different bond-related order parameter (C-N, N-H, etc.);

  ◦ Created benchmark for different force field, comparing to the experimental result;

  ◦ Utilized Replica Exchange Molecular Dynamics (REMD) with GROMACS to enhance conformational sampling, performing under different temperature interval (300-400K, 300-450K, etc.).

- **FEBuilder: Tools to streamline the FEP modeling procedure (Collaborate project)** *Mar. 2024 - Aug. 2024*

  *Supervisor: **Prof. Ruhong Zhou** Collaborator: **Xufan Gao*** [ ]

  ◦ Contributed to the development of algorithms incorporating distance-based mapping and charge modification techniques to enhance simulation accuracy.

  ◦ Selected and studied systems such as Hif-2α, T4-lysozyme, and p38α-kinase; conducted benchmarking using FEBuilder for model establishment and utilized NAMD3 to perform free energy perturbation (FEP) calculations.

- **Coarse-Grained Molecular Dynamics of FUS Phase Separation (Independent project)** *Sep. 2024 - Now*

  *Supervisor: **Rui Shi*** [ ]

  ◦ Simulated single and dual-chain systems using both all-atom (AMBER force field) and HPS models (Open-ABC toolkit), benchmarked performance with REE and R_g metrics.

  ◦ Developed a coarse-grained model of 100 FUS monomers using OpenABC and conducted simulations with OpenMM.

○ Expanded the aggregated system from 100 to 500 chains to observe droplet coalescence in the coarse-grained model.

• **Synthesis of Low-dose X-ray Responsive Nanocarriers (Collaborate project)** *Mar. 2022 - Jun. 2023*
*Supervisor: **Prof. Ruhong Zhou** Collaborator: **Lianxue Zhang*** [O]
• Demonstrated that in high reactive oxygen species (ROS) environments, such as in tumors, selenium radicals are rapidly oxidized into selenic acid, allowing efficient drug release, advancing its application in tumor radiotherapy.

• Led the cell experiments and part of the synthesis experiments, successfully validating the mechanism where the Se-Se bond absorbs X-ray energy leading to bond breakage and radical formation

PATENTS AND PUBLICATIONS C=CONFERENCE, P=PUBLICATION, S=IN SUBMISSION

[S.1] Zhaoqi Shi, et al. (2024). **Molecular Dynamics Simulation-Based Optimization of CDK7 Inhibitors for Enhanced Cancer Therapy**. Manuscript submitted for publication in *BioArxiv*.

[C.1] Gao, X., **Shi, Z.**, Zhou, R. (2024). FEbuilder: A comprehensive webserver to streamline FEP simulation setup in drug discovery. American Chemical Society (ACS) Conference, 2024 Fall (ACS Fall 2024), Denver. Zenodo. https://doi.org/10.5281/zenodo.14059079

SKILLS

• **Programming Languages:** C, C++, Python, R, Shell, Assembler language (x86 architecture)
• **Molecular Dynamic Software:** NAMD, GROMACS, OpenMM, AmberTool, CHARMM-GUI, Smina, Autodock Vina, MDAnalysis, Rdkit
• **Molecular Visualization:** Pymol, VMD, ChimeraX
• **Biological Experiment and Techniques:** Surface Plasmon Resonance(SPR), Transmission Electron Microscopy(TEM), Determination of IC50, Common biochemical experiment like Western Blot, PCR, etc.
• **Research Skills:** Biorender, LaTeX, familiar with PowerPoint and PhotoShop for research drawing and academic poster production

HONORS AND AWARDS

• **National Scholarship** *Oct. 2024*
Zhejiang University [⊕]
○ Ranked in the top 2% of students in China.

• **Zhejiang University Scholarship – First Prize** *Oct. 2022 & Oct. 2023 & Oct. 2024*
Zhejiang University [⊕]
○ Merit-Based scholarship for top 10% student in Zhejiang University

• **The China Optical Valley Scholarship** *Oct. 2023*
Zhejiang University [⊕]
○ The Highest External Corporate Scholarship

○ Awarded to only one student in the entire *College of Life Science* for outstanding academic achievement and leadership potential

• **Provincial Government Scholarship** *Oct. 2022*
Government of Zhejiang Province [⊕]
○ Merit-Based scholarship for top 5% student in Zhejiang Province

• **Scholarship for Pursuit Science Class** *Oct. 2022 & Oct. 2023 & Oct. 2024*
ChuKoChen Honor College [⊕]
○ Merit-Based scholarship for student in Chu Kochen Honor College, especially for fundamental subjects

LEADERSHIP, SOCIAL ENGAGEMENT, AND OTHER ACHIEVEMENTS

• **Teaching Assistant in Molecular Pathology** *Apr. 2024- Jun. 2024*
*Zhejiang University, College of Life Sciences in association with **Prof. Yiping Li** at Tulane University*
• **Head of Department, Life Sciences Student Association** *Sep. 2022 - Jun. 2024*
College of Life Science, Zhejiang University [⊕]
○ Organized and coordinated all volunteer activities in College of Life Science, including social practice and community service; Responsible for recruiting and training volunteers, enhancing their skills and engagement in projects

○ Designed and developed college web pages, improving overall user experience and site accessibility

• **Second Prize in the Physics Competition** *Oct. 2023*
Zhejiang Physical Society [⊕]
• **Third Prize in the Chinese Mathematics Competitions** *Oct. 2022*
Chinese Mathematical Society [⊕]
• **Fifth place in mixed doubles table tennis, Zhejiang University** *Oct. 2022*
Table Tennis Association of Zhejiang University [⊕]