YUMENG ZHANG

PH.D CANDIDATE

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EDUCATION

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

RESEARCH INTERESTS

2019-present: University of Massachusetts, Amherst (Ph.D. study)

- **Graduate Research Assistant (Advisor: Jianhan Chen).**
  - Coarse-grained model (HyRes II) optimization for IDP studies.
    Re-parametrize the HyRes protein model to achieve accurate CG simulations of disordered proteins and dynamic interactions. The optimized HyRes II model has been applied to study
    - We succeeded in determining the relationship between the inhibitory ability and the domain stability. We offered the molecular insights on how the bacteria homogeneous function differently on inhibit the immune enzyme.
    - The revealed immunity mechanism can guide the next drug targeting program on prevent the inflammation from *Staphylococcus.*
  - The cellular regulation of the mitochondrial via CypD (2020).
    - Characterizing the dynamics between the disordered N-terminal domain of p53 and Cyclophilin (CypD), which regulate the opening of the mitochondrial permeability pore. With the coarse-grained simulations, we successfully locate the highly consistent binding surface on CypD.
    - The hot spots between CypD and p53-NTD indicate an electrostatic-driven process between two proteins, both identified by simulations and experiments.
  - The active states of the membrane protein KCNQ (2021).
    - Aim1: Characterize the conformational dynamics between two significant active states of KCNQ: Intermediate open state (IO) and Active open state (AO).
    - Aim2: Locating how the N-terminal domain on KCNQ will co-operatively interact with the calmodulin (CAM) in different states using coarse-grained simulations. Revealing the mechanism on how CAM regulates the conformational transitions of KCNQ.
  - The conformational dynamics of the Flavivirus Proteases (2021-*ongoing*).
    - Aim1: Offering the molecular insights of the conformational dynamics of Proteases in ClyA nanopore using coarse-grained simulations. (Done)
    - Aim2: Help to engineering the *typhi* ClyA nanopore to stably trap the proteases. (Done)
    - Aim3: Using the engineered pore to detect the ligand-bound state and open state conformational dynamics with simulation and experiments.

- Aim4: Scan the potential drugs that may help inhibit the Proteases.

❖ **Multi-scale method developments for MD.**

➢ The HyRes II coarse-grained force field development (2021-2022).
- Optimizing the HyRes CG model to solve the over-compaction problem by re-balancing the intra-molecular interactions and implement SASA model.
- We succeeded in re-capitulating the globular conformational and the 2nd structure propensities of IDPs, which was hard to be re-produced by the current CG models.
- We accurately simulated the intermolecular dynamics between IDP and other proteins.

➢ Optimizing the REST2 method (2021-2022).
- We did exhausted analysis of the old RSET2 (replica-exchange with solute tempering) method, and unreal an artificial but unexpected over-compaction condition under high temperature conditions.
- We optimized the solute-solvent interactions and developed the new REST3 method to solve the high temperature chain collapse, which is particularly unfavored in IDP simulations.
- We realized more efficient simulations with the new protocol tested by two model IDPs. We conclude the hidden disadvantage of the over-compaction in T-REX methods.

2015-2019: Wuhan University, Wuhan (B.S. Study)

❖ **Organic synthesizing of the aatural product synthesis (2015-2017).**

➢ Metal-catalyzed enyne cycloisomerization in natural product total synthesis.
- Organic synthesis of some natural product like DHP-vinylindole via metal-catalyzed enyne.
- Optimizing the reaction path to improve the production rate.
- Product characterizations using NMR.

❖ **Construction of the enzyme-free DNA circuit for signal amplification (2018-2019).**

➢ Hybrid HCR-CHA circuits for phosphorylase kinase signal amplifications.
- Develop the HCR-CHA circuits to amplify the FRET signal during a continuous chain reaction.
- Using the circuits to detect the interactions between phosphorylase kinase with inhibitors.

HONORS AND AWARDS

Freshman Scholarship of Wuhan University	**2015**
2nd Class Freshman Scholarship of Wuhan University	**2016**
1st place prizes in 2022 ResearchFest poster presentation of UMass Chemistry	**2020**

TEACHING EXPERIENCE

Support Teaching in Guiyang, China	2018
CHEM111 TA in UMass Amherst Chemistry department.	2019-2020

Mentoring experience for junior students From 2021

PUBLICATIONS

1. X. Gong#, **Y. Zhang#** and J. Chen, "Advanced Sampling Methods for Multiscale Simulation of Disordered Proteins and Dynamic Interactions" *Biomolecules*, 11, 1416 (2021) (Invited Review). MDPI
2. 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). JMB
3. **Y. Zhan**g, X. Liu* and J. Chen*, "Towards Accurate Coarsed-Grained Simulations of Disordered Proteins and Their Dynamic Interactions", *J. Chem. Inf. Model* (2022). ACS

CO-WORKERS

- Chen Lab
- Wang Lab
- Geisbrecht Lab

SKILLS

Organic Chemistry:

- Proficient in optimizing the synthetic path, basic purification skills.
- Proficient in basic product characterizations by NMR.

Analytical and Biochemistry:

- Proficient in PCR, UV spectrum, Fluorescence spectrum, and Gel purification.

Computation and Physics Chemistry:

- High proficiency in CHARMM and Gromacs
- Proficient in multi-scale methodology developments.

Computer Software:

- High proficiency in bash, python language.
- Proficiency in VMD, Jupyter-lab, and Unix.