Gao Zhang

No. 37 Yongwang Road, Daxing District, Beijing, China
Tel: +86 15829780925; E-mail: gao.zhang2000@outlook.com; 102629

EDUCATION

Peking Union Medical College, Tsinghua University (The best university in China*) **Beijing, China**
PhD candidate in Medicinal Chemistry **Sept. 2021–Present**

Xi'an Jiaotong University (Top 10 universities in China*) **Shaanxi, China**
Bachelor of Science in Pharmacy **Sept. 2017–Jun. 2021**
• **GPA**:3.78 (Top 1% of students)

RESEARCH EXPERIENCE

1. Identify novel chemotypes of LpxH inhibitors using computer-aided drug design (CADD) technique **Sept. 2023–present**
PI of a special student research fund; Collaborated with Prof. Pei Zhou in Duke University

- Search of novel LpxH inhibitors through a multistage virtual screening.
- CADD techniques: pharmacophore modelling, 3D-shape similarity, molecular docking, etc.
- Identified a novel chemotype of LpxH inhibitor (IC_{50} < 0.17 μM) (**Gao#** et al, *J. Med. Chem.*, **Revision**).

2. Design and synthesis of LpxH inhibitors to combat Gram-negative bacteria **Sept. 2023–present**

- Rational drug design and synthesis sulfonylpiperazine derivatives as LpxH inhibitors.
- Practiced CADD techniques, including molecular docking and molecular dynamics.
- Deep understanding for non-covalent molecular interactions. (In preparation)

3. Design and synthesis of novel GyrB inhibitors to combat MRSA infection **Sept. 2021–present**

- Design and synthesis of 4-hydroxy-2,5-dihydrothiazole derivatives (**Gao#** et al, *Eur. J. Med. Chem.*, published).
- Identifying the target of 1,4-dicarbonylthiosemicarbazides (**Gao#** et al, *Eur. J. Med. Chem.*, published).
- CADD techniques: substructure search, 2D similarity, molecular docking and molecular dynamics.

4. Key synthetic process of anti-schistosomiasis drug: praziquantel **Sept. 2020–Jul. 2021**
Bachelor's Degree Project; Supervisor: Prof. Yuan Huang, Xi'an Jiaotong University

- Research for a key synthetic process.
- Practiced synthesis technique.

PUBLICATIONS

1. **Gao Zhang**, et al. Structure-based discovery of a new LpxH-targeted chemotype with activity against *Klebsiella pneumoniae*, *J. Med. Chem.*, (Revision).
2. Rui Teng#, **Gao Zhang#**, et al. 4-Hydroxy-2,5-dihydrothiazole derivatives as a new class of small-molecule antibiotics for MRSA: AI-integrated design, chemical synthesis and biological evaluation, *Eur. J. Med. Chem.*, 302 (**2026**) 118266.
3. **Gao Zhang**, et al. Discovery of novel 1,4-dicarbonylthiosemicarbazides as DNA gyrase inhibitors for the treatment of MRSA infection, *Eur. J. Med. Chem.*, 280 (**2024**) 116905.
4. **Gao Zhang**, et al. Research progress on LpxH-targeted antibacterial drugs, *Acta Pharm. Sin.*, 60 (**2025**), 1616-1630. (Review)
5. Tao Shen, Jiale Guo, Zunsheng Han, **Gao Zhang**, et al. AutoMolDesigner for Antibiotic Discovery: An AI-Based Open-Source

* According to QS World University Rankings 2026 (https://www.topuniversities.com/world-university-rankings), Tsinghua Univ. is ranked 17th and Xi'an Jiaotong Univ. is ranked 305th

Software for Automated Design of Small-Molecule Antibiotics, *J. Chem. Inf. Model*., 64 (**2024**) 575-583.

6. Lei Xu, …, **Gao Zhang**, et al. Discovery of Metabolic Reprogramming 2-Quinolones as Effective Antimicrobials for MRSA-Infected Wound Therapy, *J. Med. Chem.*, 68 (**2025**) 3004-3019.
7. Wei Chen, Fangming Chen, **Gao Zhang**, et al. Fabrication of cellulose nanocrystal composite filter papers for rapid and highly efficient removal of bacteria from aqueous solutions, *Cellulose*, 26 (**2019**) 7027-7035.

shared first author position

HONORS & GRANTS

1. National Scholarship for PhD Students, the Ministry of Education of the People's Republic of China, 2025
2. Fundamental Research Funds for the Central Universities of Ministry of Education of China (student project PI), 2024–2025
3. Merit Poster Award, Asia Hub for e-Drug Discovery 2025 (AHeDD2025)
4. The First Prize, the National Third Simulation Innovation Application Competition, 2024
5. The First Prize Scholarship, Peking Union Medical College, 2024
6. Outstanding Students, Peking Union Medical College, 2024
7. The Third Prize Scholarship, Peking Union Medical College, 2023
8. Freshman Scholarship, Peking Union Medical College, 2021
9. Outstanding Graduates, Xi'an Jiaotong University, 2021
10. The Third Prize Scholarship, Xi'an Jiaotong University, 2020
11. National Scholarship for Undergraduate Students, the Ministry of Education of the People's Republic of China, 2019
12. The Second Prize Scholarship, Xi'an Jiaotong University, 2018
13. Outstanding Students, Xi'an Jiaotong University, 2018, 2019, 2020

SKILLS & INTERESTS

Research Skills:

1. **Computer-Aided Drug Design (CADD):** Proficient in protein–ligand interaction analysis, molecular docking, molecular modeling, and molecular dynamics simulations. Skilled in using PyMOL, Discovery Studio, Schrödinger, OpenEye software, Autodock, and Gromacs, etc. Solid understanding of non-covalent molecular interactions and structure–activity relationships.
2. **Synthetic Chemistry:** Organic synthesis and compound purification. Designing and optimizing synthetic routes, analyzing reaction mechanisms, and interpreting spectroscopic data (^{1}H NMR, ^{13}C NMR, MS).
3. **Programming:** Linux and basic Python scripting for data analysis and cheminformatics applications.

Interests:

• Computer-aidded drug design (CADD), medicinal chemistry, and molecular design.

Personal hobbies:

Runing, playing badminton, cooking.

Referees:

Name	Institute	Contact
Igor V. Tetko	Helmholtz Munich, Germany	itetkoai@gmail.com
Jie Xia (Co-Supervisor)	Peking Union Medical College, China	jie.william.xia@hotmail.com
Song Wu (Co-Supervisor)	Peking Union Medical College, China	ws@imm.ac.cn

* According to QS World University Rankings 2026 (https://www.topuniversities.com/world-university-rankings), Tsinghua Univ. is ranked 17th and Xi'an Jiaotong Univ. is ranked 305th