

HU Ziheng

BSc (Hons) Pharmaceutical Sciences, Xi'an Jiaotong-Liverpool University

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RESEARCH INTERESTS

Protein therapeutics design, computational drug design (molecular dynamics, virtual screening, and binding free energy analysis), and protein nanoparticle engineering for intracellular delivery, with an emphasis on connecting computational prediction and experimental validation. A developing interest in allosteric regulation and how conformational dynamics shape protein function.

EDUCATION

BSc (Hons) Pharmaceutical Sciences

Sep 2023 – Jul 2027 (expected)

Xi'an Jiaotong-Liverpool University (XJTLU)

Suzhou, China

Academy of Life and Natural Sciences (AoLNS); dual degree from Xi'an Jiaotong-Liverpool University and the University of Liverpool.

AoLNS was formed in September 2026 through the merger of XJTLU's School of Science and Wisdom Lake Academy of Pharmacy.

First Class Honours (on track); overall average 74% (year-on-year: 68% → 76% → 78%).

Selected coursework: Chemistry for Pharmacy (92%), Drug Action (85%), Advanced Chemistry for Pharmacy (82%), Pharmaceutical Analysis (82%), Introduction to Physiology & Pharmacology (82%), Principles of Pharmacology (79%).

PUBLICATIONS

- [J1] Peirun Yang, **Ziheng Hu**, Panxi Xu, Xinyu He, Jiaxuan Wu, Xiaotian Kong, Bin Guo, Daiyun Huang, Chun Chan*, Jun Yang*, and Sijin Wu*. "Computational Exploration of ActRII-Coupled Conformational Dynamics during Myostatin Activation." *Journal of Chemical Information and Modeling* (American Chemical Society), 2026. Under review. (* Corresponding authors.)

CONFERENCE PRESENTATIONS

- [C1] **Ziheng Hu**, Peirun Yang, and Sijin Wu*. "Mechanism of Action and Rational Design of Small-Molecule Inhibitors Targeting Myostatin." The 35th CCS Congress, Chinese Chemical Society, Chongqing, China, April 11–14, 2026. Session 26: Quantum and Classical Dynamics. Poster (Paper No. 26-P-022).

RESEARCH EXPERIENCE

Final Year Project – Protein Nanoparticle Engineering

Aug 2026 – Present

XJTLU Peptide and Drug Research Group (XPad), Xi'an Jiaotong-Liverpool University
Suzhou, China

Supervisors: Dr. Shining Loo & Dr. Antony Kam

- Re-engineering protease-driven encapsulin nanoparticles with dual orthogonal conjugation handles (Sortase A and SnoopLigase) for modular, dual-functionalised intracellular protein delivery.
- Assembling cargo-loaded nanoparticles via TEV protease-triggered self-assembly, followed by surface functionalisation with affibody ligands and small-molecule labels.
- Characterising particles by DLS, TEM, blue native gel, and HPLC-SEC; evaluating HER2-dependent cell penetration in HER2-positive versus HER2-negative cell lines.

Summer Undergraduate Research Fellowship (SURF)

Jun 2026 – Aug 2026

XJTLU Peptide and Drug Research Group (XPad), Xi'an Jiaotong-Liverpool University
Suzhou, China

Supervisors: Dr. Shining Loo & Dr. Antony Kam

- Trained in the wet-lab pipeline for protein engineering: molecular cloning, protein expression, IMAC purification, and buffer exchange.
- Produced recombinant proteins in bacterial systems and performed quality control for downstream nanoparticle assembly.
- Gained hands-on experience with protein characterisation techniques.

Undergraduate Researcher – Computer-Aided Drug Design

Apr 2025 – Jul 2026

ATOMs Lab, Xi'an Jiaotong-Liverpool University

Suzhou, China

Supervisor: Dr. Sijin Wu

- Worked on small-molecule inhibitors targeting myostatin (MSTN) using structure-based drug design and molecular dynamics simulations.
- Ran virtual screening and molecular docking to identify candidate compounds.
- Performed binding free energy analysis and protein–ligand stability assessment to help prioritise lead compounds.
- Co-author of a manuscript under review at the Journal of Chemical Information and Modeling.

AWARDS & HONOURS

- Dean's List, Wisdom Lake Academy of Pharmacy, Xi'an Jiaotong-Liverpool University – Academic Year 2025–26 (top 10% by academic performance)
- Dean's List, Wisdom Lake Academy of Pharmacy, Xi'an Jiaotong-Liverpool University – Academic Year 2024–25 (top 10% by academic performance)
- Summer Undergraduate Research Fellowship (SURF), Xi'an Jiaotong-Liverpool University, 2026

TECHNICAL SKILLS

Computational: molecular dynamics, virtual screening, molecular docking, structure-based drug design, binding free energy analysis, protein–ligand interaction analysis

Experimental: molecular cloning, protein expression, affinity chromatography (IMAC), size-exclusion chromatography, binding assays, SDS-PAGE, western blot

Software: Python, PyMOL, AutoDock, GROMACS, Schrödinger Suite, AlphaFold2, RoseTTAFold

Languages: Chinese (native); English (academic proficiency); IELTS (in progress)

REFERENCES

Dr. Sijin Wu – Associate Researcher / Assistant Professor, AI Therapeutics & Molecular Simulation Lab (ATOMs Lab), Xi'an Jiaotong-Liverpool University

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Dr. Shining Loo – Assistant Professor, XJTLU Peptide and Drug Research Group (XPad), Xi'an Jiaotong-Liverpool University

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Dr. Antony Kam – Assistant Professor, XJTLU Peptide and Drug Research Group (XPad), Xi'an Jiaotong-Liverpool University

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