# 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)
AoLNS was formed in September 2026 through the merger of XJTLU's School of Science and Wisdom Lake Academy of Pharmacy.
University of Liverpool degree; 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

[1] 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. In press. (*Corresponding authors.)

## CONFERENCE PRESENTATIONS

[1] **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.

## RESEARCH EXPERIENCE

**Final Year Project — Protein Nanoparticle Engineering** Aug 2026 – Present
XJTLU Peptide and Drug Research Group (XPad) Suzhou, China

Supervisors: Dr. Shining Loo & Dr. Andony 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) Suzhou, China

Supervisors: Dr. Shining Loo & Dr. Andony 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
AI Therapeutics & Molecular Simulation Lab (ATOMs Lab) 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-first author of a manuscript accepted by 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)