Curriculum Vitae

Name
Chia-Ru Chung

Current Position
Assistant Professor
Department of Computer Science & Information Engineering

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Education & Professional Experiences (Times New Roman, 11 point)

- (2021) Ph. D of Engineering in Computer Science and Information Engineering National Central University
- (2022/08 ~ 2023/07) Postdoctoral Researcher in Kobilka Institute of Innovative Drug Discovery, The Chinese University of Hong Kong
- (2021/09 ~ 2022/07) Postdoctoral Researcher in Department of Computer Science and Information Engineering, National Central University

Research Interests (Times New Roman, 11 point)

- Rapid antibiotics susceptibility prediction to bacteria based on mass spectra data
- Deep learning techniques for antimicrobial peptides prediction and generation
- Integrated multi-omics and deep learning approach for kinase activity and pan-cancer analysis
- Exploration of spatial transcriptomics for enhanced molecular profiling
- Computational analysis and tool development for microbiota research in disease contexts

Selected Publications (※3-5 major papers)

- **Chia-Ru Chung**, et al. (2024, Nov). dbPTM 2025 update: comprehensive integration of PTMs and proteomic data for advanced insights into cancer research. Nucleic Acids Research, gkae1005.
- Lantian Yao[†], Jiahui Guan[†], Peilin Xie[†], **Chia-Ru Chung**[†], et al. (2024, Nov). dbAMP 3.0: updated resource of antimicrobial activity and structural annotation of peptides in the post-pandemic era. Nucleic Acids Research, gkae1019.
- Zhuo Wang[†], Yuxuan Pang[†], **Chia-Ru Chung**[†], et al. (2023, Sep). A risk assessment framework for multidrug-resistant Staphylococcus aureus using machine learning and mass spectrometry technology. Briefings in Bioinformatics, 24(6), 1-13.
- **Chia-Ru Chung**, et al. (2022, Oct). An intelligent motor assessment method utilizing a bi-lateral virtual-reality task for stroke rehabilitation on upper extremity. IEEE Journal of Translational Engineering in Health and Medicine, 10, 1-11.
- **Chia-Ru Chung**, et al. (2020, May). Characterization and identification of antimicrobial peptides with different functional activities. Briefings in Bioinformatics, 21 (3), 1098-1114.

Lecture Title

AI-Driven Sequence Optimization for Antimicrobial Peptide Discovery

Abstract (500 words maximum)

The rapid emergence of multidrug-resistant pathogens necessitates the development of novel therapeutic agents such as antimicrobial peptides (AMPs). However, the de novo computational design of AMPs is fundamentally challenged by the vast combinatorial sequence space and the complexity of jointly optimizing antimicrobial efficacy and host safety. To navigate this

complex landscape, this talk presents an AI-driven sequence optimization framework that employs surrogate-guided self-play Monte Carlo tree search. By utilizing explicit look-ahead planning and policy-value learning, this reinforcement learning algorithm strategically explores the peptide sequence space over multi-step mutation trajectories. The optimization is driven by a unified surrogate-ensemble reward system that scalarizes multiple predictive evaluations into a single fitness score. Deep learning surrogate models continuously evaluate and guide candidate sequences based on predicted antimicrobial potency, structural folding confidence, and minimized hemolytic toxicity. Crucially for translation into functional peptides, the AI-optimized sequences are subjected to rigorous in silico validation. Protein-protein docking is utilized to evaluate the binding propensity of the generated peptides against key bacterial resistance targets, such as MurA and PBP2a. Furthermore, molecular dynamics simulations within explicit lipid bilayer models are employed to assess membrane insertion and confirm structural stability via backbone root mean square deviation. This integrated computational pipeline highlights how advanced AI search algorithms, surrogate modeling, and rigorous structural simulations can be bridged to establish a robust in silico workflow for discovering and optimizing therapeutically viable peptides.