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中国科学院上海药物研究所
Shanghai Institute of Materia Medica
Chinese Academy of Sciences
SIMM

UNNC – SIMM, CAS Doctoral Training Partnership

It's essential that you have contacted the UNNC and/or SIMM supervisors before applying.

Formal applications should follow the instructions in 'How to apply' section.

Research areas

- Pharmaceutical science and related fields

Available PhD topics

PhD topic	**AI-Driven Discovery of Broad-Spectrum Antiviral Molecules Targeting Viral Proteases**
SIMM Supervisor	Prof. Yechun XU Prof Haixia Su
UNNC Supervisor(s)	Dr Weihua MENG
Short introduction & description of PhD	Viral proteases are critical for the replication of many pathogenic viruses (e.g., SARS-CoV-2, HIV, HCV). Their conserved structural and functional characteristics, along with the well-established druggability, make them ideal targets for developing broad-spectrum antiviral therapeutics, which is crucial for combating pandemics like COVID-19. However, current antiviral development primarily targeting HIV, HCV, and coronavirus proteases, with many viral proteases still lacking effective small molecule inhibitors. In this context, a robust AI model/platform capable of accelerating the discovery of hit/lead compounds with broad-spectrum potential, providing a powerful tool for rapid therapeutic development against emerging and re-emerging viral threats. Therefore, this research aims to develop a novel AI model that integrates graph neural networks, convolutional neural networks, molecular docking, and contrastive learning within a multi-modal framework. This model is designed to efficiently identify small molecules with potent, broad-spectrum inhibitory activity against key viral proteases for which no effective inhibitors currently exist.
Contact points	Informal inquiries may be addressed to Dr/Prof Yechun Xu (ycxu@simm.ac.cn) and Dr/Prof Weihua Meng (Weihua.meng@nottingham.edu.cn).
PhD topic	**AI-driven rational design of novel antifungal peptides using LSTM model**
SIMM Supervisor	Professor Dr Changbin CHEN
UNNC Supervisor(s)	Dr Loh Teng-Hern TAN Dr. Jodi Woan-Fei LAW

	Professor Dr Learn-Han LEE
Short introduction & description of PhD	To address the growing clinical challenge of drug-resistant fungal infections, this study aims to develop novel antifungal peptides (AFPs) characterised by high efficacy, low toxicity, and a low propensity to induce resistance. Moving beyond traditional empirical screening, we have innovatively established an artificial intelligence-driven, integrated rational design platform following a "generation-evaluation" pipeline. This platform first employs a conditionally generative model (EvoGen-Pep), built upon a large-scale pre-trained protein language model and incorporating prior knowledge of antifungal functionality, to efficiently explore novel peptide sequence spaces. Subsequently, a Long Short-Term Memory (LSTM) network, specifically optimised for deciphering sequence-activity relationships, is utilised for the precise prediction of antifungal potency and virtual screening of the generated sequences. Through this strategy, a series of novel antifungal candidate peptides is designed, synthesised, and prioritised for experimental validation. The research will then conduct systematic and in-depth biological evaluations of the lead peptides. This includes: 1) analysis of the antifungal spectrum and kinetics in vitro according to international standards; 2) comprehensive assessment of *in vivo* efficacy using *Galleria mellonella* and various murine infection models; and 3) establishment of a reliable safety profile through hemolysis assays, cytotoxicity tests, and acute toxicity studies in animals. Mechanistic investigations will adopt a multi-scale approach: initial phenotypic events (e.g., membrane disruption, ROS generation) will be examined via scanning/transmission electron microscopy and specific fluorescence probes; the spatiotemporal dynamics within fungal cells will be tracked in real-time using fluorescent labeling and live-cell imaging; finally, key molecular targets and the multi-target mode of action (which may underlie the low resistance tendency) will be identified and validated through integrative techniques such as biotin pull-down coupled with mass spectrometry and molecular dynamics simulations. Ultimately, guided by the elucidated structure-activity relationships and mechanism, rational structural optimisation of the lead peptides will be performed. Furthermore, an intelligent nanoparticle-based delivery system, responsive to the fungal infection microenvironment, will be developed to enhance the therapeutic index and targeting specificity. By integrating cutting-edge technologies from computational biology, synthetic chemistry, microbial pharmacology, and nanoformulation, this project not only seeks to obtain promising drug candidates but also strives to establish a novel research paradigm for AFPs, encompassing intelligent design, functional validation, and mechanistic clarification, thereby contributing an innovative solution to the global threat of fungal resistance.
Contact points	Informal inquiries may be addressed to Prof Dr Changbin Chen (cbchen@ips.ac.cn) and Dr Loh Teng-Hern Tan (Loh-Teng-Hern.Tan@nottingham.edu.cn), Dr Jodi Woan-Fei Law (Jodi-Woan-Fei.Law@nottingham.edu.cn), Prof Dr Learn-Han Lee (Learn-Han.Lee@nottingham.edu.cn)
PhD topic	**Combating Antimicrobial Resistance: Developing Next-Generation Antibacterial Agents and Novel Therapeutic Strategies Against Priority Human Pathogens**
SIMM Supervisor	Prof. Yanjie CHAO
UNNC Supervisor(s)	Dr Loh Teng-Hern TAN

	Dr Jodi Woan-Fei LAW Professor Dr Learn-Han LEE
Short introduction & description of PhD	Antimicrobial resistance (AMR), marked by the alarming rise of drug-resistant bacteria, represents one of the most critical threats to public health. Classified by the World Health Organization (WHO) among the top 10 global health challenges, AMR was directly responsible for an estimated 1.27 million deaths in 2019 and contributed to approximately 5 million more. Projections suggest that by 2050, AMR could claim 10 million lives annually—surpassing cancer mortality. As traditional antibiotics have become increasingly ineffective, the demand for novel antimicrobial solutions has never been greater. This project aims to address this crisis by developing innovative antibacterial agents to combat priority human and animal pathogens, including carbapenem-resistant *Klebsiella pneumoniae*, *Salmonella enterica*, and *Vibrio parahaemolyticus*. The prospective student will employ cutting-edge approaches across molecular biology, synthetic biology, and pharmaceutical sciences, with a focused emphasis on large-molecule drugs and natural products. This research offers an exceptional opportunity to contribute to a field of paramount global importance and to develop expertise at the forefront of biomedical science.
Contact points	Informal inquiries may be addressed to Prof Yanjie Chao (yjchao@simm.ac.cn) and Dr Loh Teng-Hern Tan (Loh-Teng-Hern.Tan@nottingham.edu.cn), Dr Jodi Woan-Fei Law (Jodi-Woan-Fei.Law@nottingham.edu.cn), Prof Dr Learn-Han Lee (Learn-Han.Lee@nottingham.edu.cn)
PhD topic	**Endogenous peptide modulation and genetic variation of incretin GPCRs: from biased signalling to metabolic Disease**
SIMM Supervisor	Prof Dehua Yang
UNNC Supervisor(s)	Dr Weihua Meng
Short introduction & description of PhD	Incretin receptors GLP-1R, GIPR and GCGR are central drug targets for obesity and type 2 diabetes. Clinically successful GLP-1–based mono-, dual- and tri-agonists were largely inspired by endogenous peptides, yet we still know little about how different endogenous peptide families and their processed forms modulate these receptors in human tissues – and how this is further shaped by receptor splicing isoforms and SNPs. This project aims to build a multi-scale bridge from human biology to mechanism: 1) At the tissue and cell level, we will map where and how endogenous peptide precursors, processing enzymes and incretin receptors (including splicing variants) are co-expressed in human tissues relevant to energy balance; 2) At the mechanistic level, we will reconstruct key GLP-1R/GIPR/GCGR splice variants and genetic variants (SNPs) to explore multiplex GPCR signalling platforms (cAMP, Ca^{2+}, Gs/q, β-arrestin, internalisation); 3) We will connect variant-specific signalling and cell–cell communication changes to metabolic and pathophysiological readouts, providing mechanistic insight into how human GLP-1R/GIPR/GCGR variation modulates endogenous peptide actions.
Contact points	Informal inquiries may be addressed to Dr Weihua Meng (Weihua.meng@nottingham.edu.cn) and Prof Dehua Yang (dhyang@simm.ac.cn).
PhD topic	**Graph Foundation Models for Accelerated Drug Discovery**
SIMM Supervisor	Prof. Mingyue Zheng

UNNC Supervisor	Dr. Daokun Zhang
Short introduction & description of PhD project	This research will pioneer a novel architectural framework for **Graph Foundation Models (GFMs)**, specifically designed to address the multi-scale complexity of drug discovery. Moving beyond single-task, narrow-scope models, we will develop, pre-train, and systematically benchmark a family of GFM variants, each architected with distinct inductive biases and trained on large-scale, heterogeneous biological graph data—including molecular structures, protein interaction networks, and disease pathways. Our core innovations will include: (1) a hierarchical graph transformer architecture capable of natively modeling interactions from atomic to systems-level; (2) novel multi-modal and self-supervised pre-training objectives that jointly learn chemical, geometric, and biological semantics; and (3) a unified adaptation protocol for efficient downstream fine-tuning. The research program is structured to validate the versatility and robustness of the GFM family across the drug discovery pipeline. We will conduct extensive empirical studies to evaluate their performance on a carefully curated suite of tasks: de novo generation of synthesizable, property-optimized molecules; prediction of drug-target interaction and polypharmacology profiles; and identification of novel therapeutic repurposing candidates. A key deliverable will be an open-source toolkit encapsulating the pre-trained models and adaptation protocols, ensuring reproducibility and community adoption. The student will be jointly supervised by **Prof. Mingyue Zheng**, an expert in AI- and big data-driven drug design at the Shanghai Institute of Materia Medica (CAS), and the UNNC supervisor **Dr Daokun Zhang**, an internationally recognized researcher on graph machine learning and a national talent. The project offers a unique interdisciplinary training environment at the interface of **graph AI** and **computational drug discovery**, combining cutting-edge graph learning methodology with real-world pharmaceutical problems and data. The successful candidate will receive training in advanced machine learning (especially graph neural networks and graph foundation models), cheminformatics, computational drug design workflows and reproducible research practices. Depending on background and interests, the project can be tailored towards more methodological innovation, more application-driven translational work, or a balanced combination of both.
Contact points	Informal inquiries may be addressed to Prof. Mingyue Zheng, (myzheng@simm.ac.cn) and Dr. Daokun Zhang (daokun.zhang@nottingham.edu.cn).
PhD topic	**Paired Maternal–Preterm Neonatal Gut Microbiome Profiling in Neonatal Hematochezia: A Multi-Kingdom, Gestational-Age–Stratified Study**
SIMM Supervisor	Prof. Dr. Changbin CHEN
UNNC Supervisor(s)	Assistant Prof. Dr. Jodi Woan-Fei LAW Assistant Prof. Dr. Loh Teng-Hern TAN Prof. Dr. Learn-Han LEE
Short introduction & description of PhD project	Haematochezia in preterm infants is a clinical dilemma because the differential diagnosis ranges from benign conditions (e.g., allergic proctocolitis) to life-threatening diseases such as necrotising enterocolitis (NEC) and sepsis, while current diagnostic approaches may be nonspecific and sometimes require invasive evaluation. Meanwhile, the neonatal gut microbiome develops dynamically after

	birth and is strongly influenced by prematurity, delivery mode, feeding practices, and antibiotic exposure; disrupted colonisation has been linked to NEC and late-onset sepsis. While the gut microbiome is widely implicated in neonatal intestinal health, existing studies are fragmented. Fungal gut communities are comparatively understudied, although Candida colonisation is common in preterm infants and has been associated with adverse outcomes. The maternal–infant microbial transmission and gestational-age–dependent gut ecosystem development may contribute to disease susceptibility, yet paired analyses of maternal–neonatal microbiome data remain limited. This study aims to characterise the bacterial and fungal gut microbiome in preterm infants with haematochezia and their mothers, employing a paired maternal–infant design. Maternal and preterm neonatal stool samples will be collected concurrently under standardised SOPs. Bacterial and fungal community profiles will be generated using 16S rRNA gene sequencing and ITS sequencing, respectively, with uniform DNA extraction and quality control procedures. Microbiome features (e.g., diversity metrics, taxonomic composition, and derived community signatures) will be integrated with structured clinical metadata (perinatal factors, feeding practices, medication/antibiotic exposure, relevant laboratory indices, and clinical course variables). Analyses will include confounder-aware association testing across gestational-age strata and development of internally validated predictive models for clinically relevant endpoints, emphasising model interpretability and reproducibility. This study design expects to yield gestational-age–specific microbial biomarkers that support early risk stratification in preterm haematochezia. The resulting paired maternal–infant microbiological framework may guide preventive maternal interventions and enable more precise design of future therapeutic trials, advancing toward personalised care for preterm infants.
Contact points	Informal inquiries may be addressed to Prof. Dr. Changbin CHEN (cbchen@ips.ac.cn), Assistant Prof. Dr. Jodi Woan-Fei LAW (jodi-woan-fei.law@nottingham.edu.cn), Assistant Prof. Dr. Loh Teng-Hern TAN (loh-teng-hern.tan@nottingham.edu.cn), and Prof. Dr. Learn-Han LEE (learn-han.lee@nottingham.edu.cn).
PhD topic	**To explore the pathogenesis of cardiovascular diseases and find new therapeutic targets based on modern medical biotechnology. This will encompass, drug screening, developing novel drug delivery systems, and evaluating biological mechanisms for the treatment of cardiovascular diseases**
SIMM Supervisor	Prof. Hanbin Lin
UNNC Supervisor(s)	Prof. Yong Ren
Short introduction & description of PhD project	Cardiovascular disease is a prevalent and progressively worsening condition, with its incidence and death rates consistently rising and affecting individuals at younger ages. Currently, cardiovascular disease has surpassed cancer as a leading cause of mortality globally. This underscores the importance of exploring the pathological mechanism and developing new therapeutic targets to aid the diagnosis, prognosis, and treatment of cardiovascular diseases. As such, our study will aim to investigate pathological mechanisms of cardiovascular disease and develop new therapeutic targets and drug delivery systems via technologies including microfluidics. This will encompass the

	utilization of multi-omics and molecular biotechnology to examine and validate novel targets and biological mechanisms of cardiovascular diseases. In vivo and in vitro models will be established to study the biological mechanisms of cardiovascular disease through cardiac function, including histopathological changes, and myocardial enzymes. Furthermore, novel therapeutic targets will used to evaluate the attenuation of cardiovascular disease in vitro and in vivo. In addition, our study will investigate novel drug delivery systems to improve drug bioavailability and achieve targeted treatment of cardiovascular diseases. This major involves pharmacodynamics, pharmacology, histopathology, materials science, nanomedicine pharmaceutics, and other disciplines. Candidates should be self-motivated and have a strong background in pharmacology, pathology, or materials science. This Ph.D. program is multi-disciplinary, which covers broad fields of pharmacology, pharmacodynamics, pharmaceutics, and histopathology and materials science. The potential candidate should be self-motivated and have strong background in material sciences, pharmacological sciences or pathological sciences.
Contact points	Informal inquiries may be addressed to Prof. Hanbin Lin (linhanbin@simm.ac.cn), and Prof. Yong Ren (Yong.ren@nottingham.edu.cn).

Other potential supervisors

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