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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

## UNNC-SIMM, CAS Doctoral Training Partnership

### Available PhD research topics

#### 1. Novel drug delivery system for encapsulating multiple components using microfluidics

<b>SIMM Supervisor</b>	<a href="#">Prof Youhong Hu</a>
<b>UNNC Supervisor(s)</b>	<a href="#">Dr Yong Ren</a> & Prof Pavel Gershkovich (UNUK)
<b>Short introduction &amp; description of PhD</b>	This project will aim to develop a facile microfluidic technology to synthesize highly monodispersed microcapsules with multi-cores, the microcapsules will be incorporated with certain functional groups, and the core/shell structured microcapsules can be applied as highly functional carriers with notable advantages for co-encapsulation of diverse incompatible ingredients without cross-contamination, and this will significantly enhance the loading capacity. The intrinsic good size monodispersity of microcapsules will enable exquisite control over drug release kinetics. The capsules can lead to broader biomedical applications including cancer therapy and new route of drug delivery for insulin or protein as well as multiple components with contrasting pH values.
<b>Contacts</b>	Prof Youhong Hu ( <a href="mailto:yhhu@simm.ac.cn">yhhu@simm.ac.cn</a> ) Dr Yong Ren ( <a href="mailto:Yong.ren@nottingham.edu.cn">Yong.ren@nottingham.edu.cn</a> )

#### 2. AI Enabled Chemistry for Drug Candidates

<b>SIMM Supervisor</b>	<a href="#">Prof Xiaojie Lu</a>
<b>UNNC Supervisor(s)</b>	<a href="#">Dr Bencan Tang</a> & Prof Jonathan Hirst (UNUK)
<b>Short introduction &amp; description of PhD</b>	Machine learning is an interdisciplinary study of statistical model that solves problems by making data-based predictions and deductions. The significance of machine learning and artificial intelligence used in chemistry research has been emphasized by recent papers published in high ranking journals. This research aims to develop advanced machine learning algorithms for the prediction of chemical reaction profiles. It involves bench chemistry as well as artificial intelligence.
<b>Contacts</b>	Prof Xiaojie Lu ( <a href="mailto:xjlu@simm.ac.cn">xjlu@simm.ac.cn</a> ) Dr Bencan Tang ( <a href="mailto:bencan.tang@nottingham.edu.cn">bencan.tang@nottingham.edu.cn</a> )

3. Development highly efficient MD simulation method for predicting drug affinity to target protein and its application

<b>SIMM Supervisor</b>	<a href="#">Prof Weiliang Zhu</a>
<b>UNNC Supervisor(s)</b>	<a href="#">Dr Hainam Do</a> & Dr Bencan Tang
<b>Short introduction &amp; description of PhD</b>	Based on the 3 methods (NUMD, vsREMD and ossPTMetaD) we developed for predicting protein conformation change and associated energy profile, the PhD candidate is expected to develop new method for predicting the binding affinity and kinetics of drug to protein, as well as to perform application study of the new method on designing novel ligands for important target proteins.
<b>Contacts</b>	Prof Weiliang Zhu ( <a href="mailto:wlzhu@simmm.ac.cn">wlzhu@simmm.ac.cn</a> ) Dr Hainam Do ( <a href="mailto:Hainam.Do@nottingham.edu.cn">Hainam.Do@nottingham.edu.cn</a> )

4. Drug Discovery of Anti-cancer Drugs

<b>SIMM Supervisor</b>	<a href="#">Dr Bing Zhou</a>
<b>UNNC Supervisor(s)</b>	<a href="#">Dr Bencan Tang</a> & Dr Binjie Hu
<b>Short introduction &amp; description of PhD</b>	The project involves computer chemistry design, synthesis and biology.
<b>Contacts</b>	Dr Bin Zhou ( <a href="mailto:zhoubing@simmm.ac.cn">zhoubing@simmm.ac.cn</a> ) Dr Bencan Tang ( <a href="mailto:bencan.tang@nottingham.edu.cn">bencan.tang@nottingham.edu.cn</a> )

5. The impacts of novel compound CPX-065 and its vehicles on hepatocytes plasticity from ADMET perspectives

<b>SIMM Supervisor</b>	<a href="#">Prof Guoyu Pan</a>
<b>UNNC Supervisor(s)</b>	<a href="#">Dr Chengheng Pang</a> & Dr Zheyang Zhu
<b>Short introduction &amp; description of PhD</b>	This project will focus on the impacts of novel drug candidate and its vehicles on the plasticity of hepatocytes. The change of hepatocytes fate will influence their metabolic capacities and responses to toxic liver microenvironment, which may lead to potential liver toxicity issues and other risks.
<b>Contacts</b>	Prof Guoyu Pan ( <a href="mailto:gypan@simmm.ac.cn">gypan@simmm.ac.cn</a> ) Dr Chengheng Pang ( <a href="mailto:ChengHeng.Pang@nottingham.edu.cn">ChengHeng.Pang@nottingham.edu.cn</a> )