

**PhD studentship (Full-time)**

Institution	Xi'an Jiaotong-Liverpool University, China
Department	Department of Biological Sciences
Supervisors	Principle supervisor: Dr. Xin Liu (XJTLU, BIO) Co-supervisor: Dr. Jia Meng (XJTLU, BIO) Co-supervisor: Professor Francesco Falciani (UoL, IIB)
Application Deadline	Open until the position is filled
Funding Availability	Funded PhD project (world-wide students)
Project Title	Construction of QSAR models for searching multi-target drug hits beyond similarity-based applicability domains 一种全新的基于机器学习算法的定量构效关系方法在多靶点药物设计中的应用
Contact	Please email <a href="mailto:Xin.Liu@xjtlu.edu.cn">Xin.Liu@xjtlu.edu.cn</a> with a subject line of the PhD project title

**Requirements:**

The candidate should have a first class or upper second class honours degree, or a master's degree (or equivalent qualification), in Bioinformatics/Computational Biology/Computational Chemistry. Experience in machine learning algorithms and drug design would be an advantage. Evidence of good spoken and written English is essential. The candidate should have an IELTS score of 6.5 or above, if the first language is not English. This position is open to all qualified candidates irrespective of nationality.

**Degree:**

The student will be awarded a PhD degree from the University of Liverpool (UK) upon successful completion of the program.

**Funding:**

The PhD studentship is available for three years subject to satisfactory progress by the student. The award covers tuition fees for three years (currently equivalent to RMB 80,000 per annum) and provides a monthly stipend of 5,000 RMB as a contribution to living expenses. It also provides up to RMB 16,500 to allow participation at international conferences during the period of the award. It is a condition of the award that holders of XJTLU PhD scholarships carry out 300-500 hours of teaching assistance work per year. The scholarship holder is expected to carry out the major part of his or her research at XJTLU in Suzhou, China. However,

he or she is eligible for a research study visit to the University of Liverpool of up to three months, if this is required by the project.

### **Project Description:**

Drugs designed to act against individual molecular targets cannot usually combat multigenic diseases such as cancers in which alternative or compensatory pathways are often activated. Thus, selection of proper multi-target combinations and prediction of new molecules against multi-targets are highly useful for discovering drugs with improved therapeutic efficacies. In silico methods have been extensively explored for the discovery of multi-target drugs. Apart from drug lead optimization, predictive quantitative structure-activity relationship (QSAR) models with well-defined applicability domains (ADs) have shown promising capability in virtual screening large chemical databases for drug candidate selection. However, these models are impeded by their inability in finding highly novel drug hits outside similarity-based ADs. The current project aims to develop an extended QSAR approach via chemspace-wide activity regression which can serve as an effective novel approach for finding novel drug hits outside the similarity-based ADs.

For more information about doctoral scholarship and PhD programme at Xi'an Jiaotong-Liverpool University (XJTLU): Please visit

<http://www.xjtlu.edu.cn/en/study-with-us/admissions/entry-requirements>

<http://www.xjtlu.edu.cn/en/admissions/phd/feesscholarships.html>

### **How to Apply:**

Interested applicants are advised to email [Xin.Liu@xjtlu.edu.cn](mailto:Xin.Liu@xjtlu.edu.cn) following documents for initial review and assessment (please put the project title in the subject line).

- CV
- Two reference letters with company/university letterhead
- Personal statement outlining your interest in the position
- Proof of English language proficiency (an IELTS score of 6.5 or above)
- Verified school transcripts in both Chinese and English (for international students, only the English version is required)
- Verified certificates of education qualifications in both Chinese and English (for international students, only the English version is required)
- PDF copy of Master Degree dissertation (or an equivalent writing sample) and examiners reports available

**Informal enquiries** may be addressed to Dr. Xin Liu ([Xin.Liu@xjtlu.edu.cn](mailto:Xin.Liu@xjtlu.edu.cn)), whose personal profile is linked below,

<https://www.xjtlu.edu.cn/en/departments/academic-departments/biological-sciences/staff/xin-liu>