

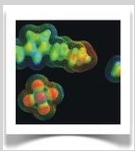
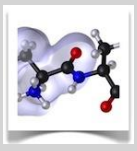
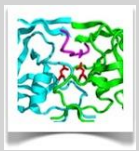

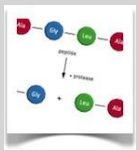
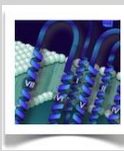

School of Pharmacy PhD Projects 2015/16

Project Title

Analysis of receptor dynamic conformational ensembles with machine learning algorithms for drug discovery

Supervisors

Dr. Irina Tikhonova

Description

Computer simulations provide easy means to explore protein flexibility in order to guide structure-based drug design efforts. However, the standard analysis of computer simulations trajectories for drug discovery can be complicated and time consuming. It is therefore essential to develop novel fast methodologies in analyzing high-dimensional conformational space for drug discovery. Here, we aim to merge computer simulations and pattern recognition methods to address the drug discovery issues across the bioamine receptors, which are the targets for depression and schizophrenia. The main aim of this research is therefore to develop a computational methodology that will enable preclinical antipsychotic drug discovery by incorporating flexible protein methodologies to computer-aided approaches.
Upon completion of this project, you will have gained knowledge and experience in multi-scale modelling, machine learning and computational drug design. As a result, you will graduate with a comprehensive series of *in silico computational biology/chemistry* skills and the expertise that enables you to forge a career in either the academic or pharmaceutical sectors.

Start Date

October 2015

Keywords

Multi-scale modeling, machine learning, drug design

Contact Details
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How to Apply
Postgraduate applications should be made using Queen's Online:
http://go.qub.ac.uk/pgapply

Please note that there are two application processes: one for admission to the university and another for postgraduate awards.

Further Information
Additional information for prospective postgraduate students can be found on the School of Pharmacy website:
http://www.qub.ac.uk/pha
and the Queen's Postgraduate website:
http://www.qub.ac.uk/home/ProspectiveStudents/PostgraduateStudents/