***Title of studentship**	Computer Simulations of G protein-coupled Receptors
Value / what is covered?	
Awarding body	
Number of studentships	
***Summary descriptive text / Example of research project**	Many physiological processes are controlled through the activation of G protein-coupled receptors (GPCRs) by regulatory peptides, making peptide GPCRs particularly useful targets for major human diseases such as diabetes and CNS diseases. It has become widely accepted that most GPCRs possess spatially distinct allosteric sites that can be targeted by small molecule ligands to modulate the receptor biological state. Allosteric binding sites offer advantages over orthosteric binding sites in identifying drugs with increased selectivity and structural novelty. However, the discovery of allosteric sites and modulators has been largely serendipitous, achieved through high-throughput screening. A recent breakthrough in structural biology disclosed the crystal structures of several GPCRs has provided opportunities to develop computational technologies for allosteric medicine discovery in GPCRs. In this PhD, we will develop a computer methodology to map allosteric binding sites in GPCRs using molecular dynamics simulations and chemoinformtics approaches. You then validate the developed protocols via compound screening and mutagenesis. You will learn cutting-edge computational approaches in data collection, mining and analysis at the interface of chemistry and biology. The project facilitates skills development in the area of drug design research, which is applicable in academia and industry.
***Supervisor(s)**	Dr Irina Tikhonova
***Eligibility / residence Status**	UK, Overseas
Country	Northern Ireland
***Start date and duration**	1 October 2020
***Faculty**	MHLS

***Research centre / School**	Pharmacy
Subject area	Chemistry, biochemistry, computational biology, medicinal computational chemistry, drug design
Candidate requirements / Key skills required for the post	Applicants should have a 1st or 2.1 honours degree (or equivalent) in a relevant subject. Relevant subjects include Pharmacy, Molecular Biology, Pharmaceutical Sciences, Biochemistry, Biological/Biomedical Sciences, Chemistry, Engineering, or a closely related discipline. Students who have a 2.2 honours degree and a Master's degree may also be considered, but the School reserves the right to shortlist for interview only those applicants who have demonstrated high academic attainment to date
***Deadline for applications**	January 2020
***How to apply / contacts**	Postgraduate Research applicants for Pharmacy who are interested in applying for a fully funded DFE studentship must have applied to Queen's, via the Direct Applications Portal, and submitted all required supporting documents by the closing date, which will be announced later in the Academic year. https://dap.qub.ac.uk/portal/user/u_login.php
Relevant links / more information	http://www.qub.ac.uk/schools/SchoolofPharmacy/Research/PostgraduatePositions/ http://www.qub.ac.uk/schools/SchoolofPharmacy/Research/
Keywords for search filters	
Training provided through the research project	
Expected impact activities	