

|  |  |
| --- | --- |
| **\*Title of studentship** | Molecular Modelling and Pharmacology of G protein-coupled Receptors |
| **Value / what is covered?**  | Fully funded  100% of UK/EU tuition fees paid and an annual stipend for UK residents only (living expenses), currently at **£15,285** |
| **Awarding body** |  |
| **Number of studentships** | 1 |
| **\*Summary descriptive text / Example of research project**  | Many physiological processes are controlled through the activation of G protein-coupled receptors (GPCRs). 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. A recent breakthrough in structural biology disclosed the 3D structures of several GPCRs and provided opportunities to develop computational technologies for allosteric medicine discovery in GPCRs. In this PhD, you will study a GPCR using molecular dynamics simulations and cheminformatics approaches and predict novel allosteric binders. You then validate the developed protocols via mutagenesis and functional assays. 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 drug design research, which is applicable in academia and industry.  |
| **\*Supervisor(s)** |  Dr. Irina Tikhonova and Dr. Bianca Plouffe |
| **\*Eligibility / residence Status** | UK, overseas |
| **Country** | Northern Ireland |
| **\*Start date and duration**  | 1 October 2022 |
| **\*Faculty** | MHLS |
| **\*Research centre / School** | Pharmacy + Wellcome Wolfson Institute for Experimental Medicine.  |
| **Subject area** | Molecular modelling, pharmacology, biochemistry, 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, 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** | September 2022 |
| **\*How to apply / contacts** | Postgraduate Research applicants must have applied to Queen’s, via the Direct Applications Portal.<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** |  |