***Title of studentship**	Rational design of novel peptide hydrogels for drug delivery
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 £14,777
Awarding body	DFE
Number of studentships	1
***Summary descriptive text / Example of research project**	**The Problem**: A significant number of medical conditions such as Alzheimer's disease, alcohol withdrawal, schizophrenia, malaria prophylaxis and contraceptive cover suffer from complex drug treatment regimens that patients find difficulty complying with. This negatively influences therapeutic outcomes. Long-acting injectable nano-suspensions, which are colloidal dispersions of nano-sized water-insoluble drug particles stabilized by surfactants are commonly used for the treatment. Nevertheless, difficulties in manufacturing scale-up, amorphous drug formation and drug load restrictions make nano-suspensions often costly and inefficient in usage. As a result, there is a clear need to develop alternative formulations. This project will explore peptide hydrogels as a new technology platform for development of medicines within these healthcare areas. **What will we do?** Dr Garry Laverty has extensive expertise in construction and characterization of hydrogels and their validation *in vitro* and *in vivo* experiments. The team has recently developed several hydrogels based on peptide-drug conjugates. Dr. Tikhonova has multiscale simulation expertise to study the behaviour of peptide molecules and their properties at an atomic level and, using the gained insights, to predict novel medical interventions. The first-hand expertise in experiment and computation provides an exciting opportunity for our teams to rationally design novel peptide hydrogel systems as an alternative to nano-suspensions to carry water-insoluble drugs and to be administrated via subcutaneous injection. **How will we do it?** Self-assembling peptides represent an efficient, selective and inexpensive formulation for sustained release of insoluble drugs. At the start, self-assembling of peptide-drug conjugated systems will be designed, modelled and studied using atomistic and coarse grain computer simulations. Physico-chemical and dynamic properties of peptide-drug hydrogels will be characterized. Calculated drug diffusion rates, mechanical strength and other parameters will be compared with corresponded values obtained experimentally. Insight gained from computer

	simulations will inform the experiment on the most stable hydrogel systems. Next, the rationally selected hydrogels will be synthetized and characterized in vitro and in vivo drug release. Drugs will be selected based on their association with complicated drug treatment regimens and would therefore provide maximal therapeutic benefit in a long-acting formulation (e.g. once monthly administered).
***Supervisor(s)**	Dr Irina Tikhonova; Dr Garry Laverty
***Eligibility / residence Status**	UK/EU only
Country	Northern Ireland
***Start date and duration**	1 October 2019 Funding covers a three-year full-time PhD.
***Faculty**	MHLS
***Research centre / School**	Pharmacy
Subject area	Drug Delivery, Computational Chemistry
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.
***Deadline for applications**	7th January 2019
***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	Drug delivery, hydrogels; peptide; molecular modelling, molecular dynamics; rational design
Training provided	This research will be conducted at the School of Pharmacy Queen's University Belfast which in 2018 was ranked 2nd in the UK for Pharmacy and Pharmacology

through the research project	according to the Guardian University Guide 2018, underpinning the school's investment in and commitment to world-class facilities and staff, with internationally leading research programmes. The School of Pharmacy Queen's University Belfast was particularly outstanding ranking as first amongst Pharmacy submissions in REF 2014. The School of Pharmacy is a leading UK centre for pharmaceutical research and has been supported by philanthropic donations of more than £7 million for strategic research developments. The School's research strategy has focused on developing high profile projects, including in cancer and dermatological therapies that ultimately have the potential to meet identified clinical needs and, consequently, also have high priority status with the pharmaceutical industry. As a member of the Russell Group, Queen's University Belfast which is consistently recognised as one of the leading universities for knowledge exchange in the UK, thus ensuring research is creating jobs, wealth, skills and innovation. The Postgraduate Research Committee (PGRC) advises and supports all PGR students, ensures appropriate training is provided, considers all matters relating to recruitment, admission, progress and examination for postgraduate degrees, monitors and reviews supervision, appoints external examiners, reviews complaints, refers student appeals to the University Postgraduate Appeals Committee and also submits an annual report to the University Postgraduate Office. The School of Pharmacy expects monthly meetings with students where electronic records must be kept. Students must also complete a three-month initial review and annual progress review to proceed to years two and three. The annual progress review involves written work, presentation and/or mini viva. These are the standard management and monitoring arrangements that must be adhered to by the academic partners. As such the School of Pharmacy has the best PhD completion rates within Queen's University Belfast. Each PhD student must also complete the centrally organised Queen's University Belfast researcher development framework program consisting of 30 days of training. These have been created by vitae, and endorsed by the QAA and Research Councils UK. Dr. Tikhonova will supervise the computational work of the project. Dr Lavery will provide Cryo-SEM, FTIR, CD spectroscopy and oscillatory rheology for peptide hydrogels. The supervisors will form a scientific advisory board to evaluate the execution of the project and help the PhD student in meeting all the objectives. The training areas include four domains that encompass: (A) knowledge and intellectual abilities, (B) personal effectiveness, (C) research governance and organisation and (D) engagement influence and impact. For this studentship the student will be trained in the following generic skills; developing writing skills, developing presentation skills, power point for academic presentations and posters, communication skills, introduction to research design, academic plagiarism, basic and advanced statistics, networking and negotiating, lab demonstrating and introduction to ref works. Students are also encouraged to use the Personal Development Planning (PDP) process to build a portfolio on learning, performance and achievement. PDP encourages the students to adopt a good work practice and supports the timely submission of thesis. The student will receive formal training in the following specialist skills necessary for this project- molecular modelling and dynamics, atomistic trajectory analyses, date mining, peptide synthesis, drug release protocols, confocal microscopy, scanning and transmission electron microscopy, tissue culture, HPLC, Fourier Transform infra-red spectrometry, circular dichroism, Mass Spectroscopy, and NMR. The combination of these skills is highly

	transferable and should give the student a distinct advantage either in academia or industry.
Expected impact activities	Simulations and design of hydrogels for drug delivery lies within the Smarter Materials Priority Area. The short-term goal is to establish an *in silico* platform for modelling of hydrogels and prediction of their properties, which could be used efficiently by PRP experimentalists. In the long-term, the developed platform will play a critical role in rapid and cost-effective design of novel materials for unmet medical needs. It is envisaged that the data generated will lead to significant funding income from RCUK. Furthermore, it facilitates skills development in the area of therapeutics research, which is applicable in academia and industry. -Involved in development of intellectual property - first *in silico* platform to model various peptide hydrogels for drug delivery -Attendance at relevant conferences -Engagement with industry, patients and key stakeholders -Generation of publications