



QUEEN'S UNIVERSITY BELFAST

*Title of studentship	The importance of pre-nucleation aggregates for guiding crystallisation outcome
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 £14,553
Awarding body	Department of Education
Number of studentships	1
*Summary descriptive text / Example of research project	<p>Crystal polymorphism, i.e. the ability of a molecule to crystallise in different molecular arrangements, is a real-world problem to the pharmaceutical industry due to the inherently varied physico-chemical characteristics (melting point, stability, solubility) of the different crystal forms. The pathway, through which molecules interact and come together in order to form a stable crystal nucleus, will play a crucial role in determining the resulting molecular arrangement. This step will be influenced not only by the method of crystallisation, but also by the solvent used and supersaturation levels.</p> <p>In order to better understand and thus control the formation of different crystal forms, this project will investigate the drug-drug and drug-solvent interactions before the crystallisation event. As the first step, the student will extensively characterise model compounds by solid-state analytical techniques. This will give a holistic understanding of the crystallisation behaviour from solution and the melt as well as an insight into the stability of the resulting crystal forms. On parallel, the student will use NMR and IR spectroscopic techniques in highly controlled solution titrations to gain information about the dominant interactions in the crystallisation environments. The compounds will also be investigated with the use of neutron total scattering techniques and connected reverse Monte-Carlo simulations to give a structural snapshot of the amorphous phase. Connecting the gathered knowledge on the solid state and the amorphous phases will enable us to generate a better understanding, and thus control, of the factors leading to the crystallisation of multiple crystal forms.</p>
*Supervisor(s)	Dr Katharina Edkins Dr Victoria Kett
*Eligibility / residence Status	UK/EU only

Country	Northern Ireland
*Start date and duration	1 October 2018 Funding covers a three-year full-time PhD.
*Faculty	MHLS
*Research centre / School	Pharmacy
Subject area	Pharmaceutics
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, Psychology, Social Sciences 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	31 January 2018
*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	Crystallisation, solid state, NMR, diffraction, thermal analysis
Training provided through the research project	The student will gain highly-sought after expertise in pre-formulation, the standard solid state techniques along with solution based spectroscopy. Training will be provided in (thermo-) microscopy, DSC, TGA, X-ray and neutron diffraction, IR and NMR spectroscopy, crystal structure determination and total scattering techniques. In addition to the topic specific expertise, the student will also be trained in presentation techniques, verbal and written, of complex information, information mining, networking and time-management. Additional training courses in transferrable skills are offered through the School of Pharmacy or the wider university.
Expected impact activities	The student will be participating and presenting on at least one national and one international conference ranging from PharmSci, BCA spring meeting and BACG to IUCr and ECM meetings, AAPS, Gordon Conference etc. depending on the results. In addition, a research visit to a collaborating group in academia and/or industry is planned. The group has a long standing in outreach and STEMnet related activities and the student will be encouraged to join this activity. Outreach will range from school visits to public lectures in a Café Scientific style. Additional activities at local

	science festivals or national actions, e.g. 3 minute thesis challenge, dance your PhD, I'm a scientist get me out of here, are encouraged and will be actively supported.
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