



QUEEN'S UNIVERSITY BELFAST

*Title of studentship	Molecular interactions in solution for multi-component crystallisation
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	<p>Crystallisation is probably one of the most important unit operations in pharmaceutical industry for purification, as well as the generation of materials appropriate for formulation and application to the patient. Whilst most research activity currently is focused on generating crystal forms of the active pharmaceutical ingredient (API) showing physicochemical characteristics ideal for formulation and treatment, very few studies report findings on the molecular interaction of different species in solution before crystallisation. This knowledge, though, feeds into the rational design of crystallisation experiments towards co-crystal formation or for the use of crystallisation as purification tool. In this project, we will concentrate on interaction between two or more related components in solution and determining the strength of their interaction. Using model systems based on pharmaceutical compounds, we will concentrate on interactions leading to the co-crystallisation of two or more components (API and co-former/impurity), concentrating primarily on strong directed interactions based on hydrogen bonding. The main analytical tools will be infrared and nuclear magnetic resonance spectroscopy with their ability to qualitatively gauge interactions on complementary timescales as well as quantitative information about the energy of the interactions. In addition, we will use X-ray and neutron total scattering in combination with Monte-Carlo simulations to build a structural model of the solution state. These models will be verified by Molecular Dynamics simulations. Finally, the solution structure and interactions therein will be compared to the crystal structures resulting from these solutions, enabling us to tailor the solution environment to the intended crystallisation outcome.</p>

*Supervisor(s)	Dr Katharina Edkins Dr John Holbrey
*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	Physical 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, 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	7 th 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	<p>http://www.qub.ac.uk/schools/SchoolofPharmacy/Research/PostgraduatePositions/</p> <p>http://www.qub.ac.uk/schools/SchoolofPharmacy/Research/</p> <p>https://www.qub.ac.uk/schools/SchoolofPharmacy/Research/ResearchThemes/PharmaceuticalMaterialsScienceandFormulation/DrKatharinaEdkins/</p>
Keywords for search filters	<p>Crystallisation, co-crystal, pre-nucleation aggregates, molecular recognition, pharmaceuticals</p>
Training provided through the research project	<p>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. Computational techniques covered will be Monte-Carlo and Molecular Dynamics simulations.</p> <p>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. Training courses in transferrable skills are offered through the School of Pharmacy or the wider university.</p>
Expected impact activities	<p>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 record in outreach and STEMnet related activities and the student will be encouraged to join these activities. Outreach will range from school visits to public lectures in a Café Scientific style. Participation 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.</p>