School of Pharmacy PhD Project 2017 / 2018

Computer simulations of hydrogels to improve drug delivery

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Hydrogels are water swollen polymer matrices, with huge tendency to absorb water. Their ability to swell, under physiological conditions, makes them an ideal material for drug delivery applications.
The overall goal of the project is to develop a computational framework for characterisation of polymer and peptide hydrogels, their material properties and interactions with drug molecules. We will establish two computational platforms to conduct atomistic and coarse grain molecular dynamics simulations of peptide hydrogels (1) and polymer-based hydrogels (2) using the examples of hydrogels provided by wet-lab-based supervisors.
The goals will be to identify suitable software and computational parameters for efficient and rapid simulation protocols (1); to develop computational tools for analysis of simulated trajectories to distil information such as flexibility, interaction with solutes, drug diffusion rates and mechanical strength (2); and to develop structure-properties relationships of hydrogels that could be used for specific drug delivery questions (3).
The proposed case studies include: (A) Molecular dynamics simulations of self-assembling of tetra- peptide-drug conjugates (e.g. Ibuprofen-FFKK) with antimicrobial activity; the computational work will be linked with Cryo-SEM, FTIR, CD spectroscopy and oscillatory rheology;
(B) Molecular dynamics simulations of drug-PEG, drug-cross-linked PEG/PMVE/MA hydrogels focusing on drug diffusion in mixed hydrogels. The project will facilitate design of hydrogel-based microneedles with advanced properties. Calculated drug diffusion rates will be compared with experimental values. Dynamics of interactions will be also linked with neutron scattering experiments. The project facilitates skills development in the area of drug delivery, which is applicable in academia and industry.

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How to Apply
Postgraduate applications should be made using Queen's University Direct Applications Portal. Please note that there are two application processes: one for admission to the university and another for postgraduate awards.

Further Information
Additional information for prospective postgraduate students can be found on the School of Pharmacy website and the Queen's Postgraduate website.

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