



PhD Studentship in Soft Matter/Lipid Membranes (Dr John Sanderson, Prof. Mark Wilson)

Applications are invited for a 39-month joint PhD Studentship funded by the EPSRC in the Chemistry Department at Durham University on:

Structure-Function Relationships for Drug Reactivity in Lipid Membranes

The successful applicant will have the unique opportunity to work at the interface of experimental and theoretical chemistry alongside researchers within the Departments of Chemistry and the Durham Centre for Soft Matter. The project, with an anticipated start date of October 2021, will involve:

- **Analysis of drug-membrane binding**
- **Determination of drug-lipid reactivity profiles**
- **Atomistic and coarse grained molecular modelling**
- **Free energy calculations**

For further details of the project, please contact: Dr John Sanderson (j.m.sanderson@durham.ac.uk) or Professor Mark Wilson (mark.wilson@durham.ac.uk).

Further information:

Recent work has demonstrated that small organic molecules possess unexpected reactivity with lipid membranes (doi: 10.1126/sciadv.aaz8598, Science Advances) and that this reactivity has functional consequences (doi: 10.1039/c8sc04831b, Chem. Sci.). Many of the factors that control this reactivity are poorly understood: mechanistic aspects of the reactivity, including the rate determining step, have not been characterised. Preliminary data have revealed that how a molecule partitions into the membrane interface is likely to be crucial in dictating reactivity – specifically the orientation and depth of binding. This project will use a combination of reactivity and binding measurements on model organic molecules in liposomes to probe the factors that control reactivity. Molecular modelling at atomistic and coarse-grained levels will be used to understand how partitioning depth and orientation affect reactivity, and to model the transition state of the rate determining step. The combination of experimental data and modelling will ensure that the work is both robust and insightful.

For more information on the Department of Chemistry:

<http://www.durham.ac.uk/chemistry>

<https://www.dur.ac.uk/chemistry/staff/profile/?id=206>

<https://www.dur.ac.uk/chemistry/staff/profile/?id=198>

Applicants should have, or expect to obtain, a First class or a minimum of an Upper Second class (2.1) Honours degree, MSci, MChem or equivalent qualification in Chemistry or a related subject.