''Advancing structure-based drug design with novel binding free-energy calculations methods''

3-year fully funded PhD studentship, September 2018, stipend ca. £14.5k pa,

Supervisor: Dr Julien Michel, School of Chemistry, University of Edinburgh.

Applications are invited for a PhD studentship in the Michel lab (http://www.julienmichel.net) in the area of biomolecular simulations and computer-aided drug design. The EaStCHEM school of Chemistry at the University of Edinburgh is among the top ranked departments within the EU.

The prediction of protein-ligand binding affinities is a major goal of modern computer-aided drug design. Among existing computational techniques, alchemical free energy methods are currently receiving considerable interest from the industry to support structure-based drug design campaigns. However significant obstacles remain before alchemical free energy methods can be widely applied to the full breadth of protein-ligand complexes of pharmaceutical interest.

This project will focus on considerably enhancing the efficiency and scope of alchemical free energy methods for structure-based drug design problems. This will be achieved by implementing and validating novel algorithms that substantially decrease the computing time needed to identify promising ligands among large datasets of putative drug-like molecules. This project will be carried out in close collaboration with a leading computational chemistry software company. This is an exciting opportunity to develop, validate and apply next-generation computer-aided drug design software and methodologies. Upon completion of the studentship, the successful applicant will have gained strong technical expertise in molecular modelling and learned to work closely with the software and pharmaceutical industry sectors. This will prepare him or her well for a future career in academia or industry.

Applicants with an excellent academic record in a chemistry/biochemistry/physics/high performance computing degree are encouraged to apply. The ideal candidate will have: strong knowledge in physical chemistry and/or biophysical chemistry; relevant research experience; excellent written and oral communication skills; enthusiasm for rational drug design, computational chemistry and scientific computing. Previous experience in computer programming (Python, C++) is desirable but not essential, provided the applicant is keen to develop skills in this area during the studentship.

Applications will be considered until an excellent candidate has been identified. Candidates should normally be UK resident, with or about to obtain a 2.i or 1st class degree in a relevant discipline. EU candidates may be considered, provided they demonstrate an outstanding academic record (within top 5% of your class) and strong written/spoken English language skills.

To apply, please submit initially by email a CV, covering-letter describing your previous research experience, reasons to apply and justifying your eligibility, as well as the names and email address of two referees in pdf format to Dr. Julien Michel julien.michel@ed.ac.uk. Informal enquiries are encouraged.