“Explaining allosteric modulation of protein function by energy/entropy localization”

4-year fully funded PhD studentship, stipend ca. £17,863 pa, BBSRC eligible applicants only

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

**Industrial Supervisor:** Dr Benjamin Cossins, UCB Ltd.

Applications are invited for a prestigious 4-year CASE PhD studentship in the Michel lab in collaboration with UCB and in the area of biomolecular simulations and computer-aided drug design. The Michel lab ([http://www.julienmichel.net](http://www.julienmichel.net)) is based at the EaStCHEM school of Chemistry at the University of Edinburgh, which is among the top ranked departments within the EU. UCB is a global biopharmaceutical company ([http://www.ucb.com](http://www.ucb.com)).

In this project new molecular simulation methods will be developed and implemented to elucidate the mechanisms of allosteric modulation of protein function by small molecules. This will be achieved by researching new theoretical and computational approaches to relate ligand binding energetics to changes in structure and dynamics.\(^{1-4}\) The student will be based at the University of Edinburgh but the training will include a 3-6 month placement spent at UCB, Slough. On successful completion, the student will receive a doctorate from the University of Edinburgh.

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 exposure to collaborative multi-disciplinary research. Applicants with an excellent academic record in a chemistry/physics/biochemistry degree are encouraged to apply. The ideal candidate will have: strong knowledge in biophysical/medicinal chemistry, structural biochemistry or chemical physics; relevant research experience; excellent written and oral communication skills; enthusiasm for rational drug design and for chemical theory, computational chemistry and Linux scientific computing skills. Previous experience in computer programming (e.g. Python, C++) is desirable but not essential, provided the applicant has a keen interest in developing his/her computer programming skills.

**Applications must be submitted by January 4\(^{th}\) 2015 at the latest.** Interviews with short-listed candidates will be organised in mid-January. The starting date of the project is October 1\(^{st}\) 2015. **Candidates must satisfy BBSRC eligibility criteria to be considered for this position.** To apply, please submit initially by email a CV, covering-letter describing your previous research experience and reasons to apply, and the names and email address of two referees in pdf format to Dr. Julien Michel (julien.michel@ed.ac.uk) and Dr Ben Cossins (ben.cossins@ucb.com). Informal enquiries are encouraged.

**Representative references**