



Modelling allosteric modulation of protein function

A PhD studentship is available in the group of Professor Julien Michel (School of Chemistry, The University of Edinburgh; <https://www.julienmichel.net/>)

The studentship is fully funded for 42 months by the University of Edinburgh and covers tuition fees and an annual stipend (starting at £17,668 per annum) for a candidate satisfying EPSRC residency criteria. <https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/#contents-list>

Project Summary

This project will focus on developing computational methodologies grounded in molecular simulation and machine learning for predicting how the binding of a ligand to the surface of a protein will modulate its biological function. Such capability may facilitate the rational design of allosteric modulators of protein function which of enormous importance in drug discovery. This work builds on Markov State Modelling methodologies and alchemical free energy calculation methodologies that the Michel research group has recently developed to simulate large scale conformational changes in protein structures (*Chem. Sci.*, 11, 2670-2680, 2020) and to estimate protein-ligand binding affinities (*Chem. Sci.*, 13, 5220-5229, 2022). Throughout the project there will be opportunities to interact with pharmaceutical companies interested in such 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 pharmaceutical industry sector. 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 are encouraged to apply. The ideal candidate will have: interest in computer programming (Python) and evidence of strong programming abilities, 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.

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. International candidates may be considered, provided they demonstrate an outstanding academic record (within top 10% of your class) and strong written/spoken English language skills.

In the first instance, the initial application (including cover letter and CV) should be directed to: Professor Julien Michel School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK.

Email: julien.michel@ed.ac.uk

Informal enquiries are encouraged. The position will remain open until filled. It is anticipated that interviews will be arranged in late January 2023 and applicants are encouraged to make contact as soon as possible.

IMPORTANT

Before Submitting your cover letter and CV, please complete the online [School of Chemistry Equality, Diversity and Inclusion Form 2023](#) (link shorturl.at/nvGTY). The form will automatically generate a unique "Receipt Number" that you **MUST** include in your cover letter.

Equality and Diversity

The School of Chemistry holds a Silver Athena SWAN award in recognition of our commitment to advance gender equality in higher education. The University is a member of the Race Equality Charter and is a Stonewall Scotland Diversity Champion, actively promoting LGBT equality. The University has a range of initiatives to support a family friendly working environment. See our University Initiatives website for further information. University Initiatives website: <https://www.ed.ac.uk/equality-diversity/help-advice/family-friendly>