## PhD Studentship in Computational Biological Chemistry: Unveiling the functional dynamics underpinning allostery and drug resistance in proteins

Supervisors: Dr Sofia Oliveira and Prof Adrian Mulholland

## About the Project:

Proteins and related biomolecules are not static entities. In fact, it is the opposite; they are inherently dynamic, continuously moving and switching between different conformations, with the intricate balance between their multitude of conformations ultimately determining their macroscopic properties. Therefore, understanding these functional dynamics in detail is essential for comprehending protein function.

This project aims to investigate the functional dynamics of therapeutically significant targets, from enzymes linked to drug resistance to human receptors involved in neurotransmission, using state-of-the-art computational approaches and digital technologies, aligning with the broader research programme in the Centre for Computational Chemistry at the University of Bristol. Specifically, this project will employ advanced biomolecular simulation techniques, virtual reality, AI, and machine learning to unravel the dynamic basis underpinning allosteric modulation and the effect of drug-resistance-causing mutations in various biomedically relevant proteins. The Oliveira and Mulholland groups are at the forefront of developing innovative computational methods to investigate these effects and predict activity changes in enzymes. This PhD project sits at the interface between Chemistry, Data Science, Biology, Physics and Computer Science, thus providing the successful candidate with a comprehensive understanding across these different but highly interconnected fields.

We will leverage the world-class High-Performance Computing facilities at the University of Bristol, including the TOP500-class supercomputers IsambardAI and Isambard3. The project will be conducted in close collaboration with experimental groups in the UK and abroad, who will subsequently test the key biological findings from the computational studies.

**Requirements:** Candidates who aspire to work in a multidisciplinary project are encouraged to apply. Applicants must have obtained, or be about to obtain, a First or Upper Second Class UK degree, or the equivalent qualifications gained outside the UK, in Chemistry or a related discipline (such as Biology, Biochemistry, Chemical engineering, Life sciences, Physics). The successful candidate will be based in the School of Chemistry in the Faculty of Science and Engineering at the University of Bristol.

## Start date: Sept 2025

**Funding Notes:** A full studentship will cover tuition fees, a training support fee and a stipend (£20,780p.a. in 2025/26, updated each year) for 4 years.

**How to Apply:** Please make an online application for this project at the following page <u>How to apply | Study at Bristol | University of Bristol</u>. **Diversity and Inclusion:** We are committed to advancing issues of equality, diversity, and inclusion. We recognise the benefits of working in diverse teams and, therefore, encourage applications from highly talented individuals across a wide range of backgrounds.

**Getting in Contact:** Please contact <u>chem-pg-admissions@bristol.ac.uk</u> with any queries about the application process. For questions about the project, please make an informal enquiry to Dr Sofia Oliveira (<u>sofia.oliveira@bristol.ac.uk</u>).