BioAID BBSRC Doctoral Training Programme:
Machine learning models for enzyme catalysis and design
Supervisor: Adrian Mulholland
Centre for Computational Chemistry, University of Bristol

Application deadline: 30th April 2026

A PhD studentship is available in the groups of Adrian Mulholland on enzyme design and engineering, developing and applying methods to model enzyme-catalysed reactions, , collaborating with experiments. This project is part of the new BBSRC-funded BioAID Doctoral Focal Award programme in AI-driven enzyme design for biocatalysis.

About the Project
This PhD project will develop and apply computational methods for modelling enzyme catalytic mechanisms, for enzyme design and engineering. You will develop methods using machine learning, applying outstanding advanced computer resources. This project will provide excellent training in a range of advanced computational methods, ranging from machine learning to AI design tools to multiscale molecular simulations.

The ability to design new protein catalysts for specific transformations will revolutionize pharmaceutical synthesis and the chemical industry, and provide green routes to synthesis, sustainable manufacturing and diagnostics. Simulations of enzyme-catalysed reactions can identify reaction mechanisms and predict effects of mutations, accelerating enzyme design and engineering. Simulations are also crucial in providing transition state structures as "theozyme" templates for design.

Machine learning models allow accurate, efficient simulations of enzyme-catalysed reactions in atomic detail. In this project, you will develop and apply machine learning models for target reactions in biocatalysis, and contribute to enzyme design. Models will be trained on datasets from quantum mechanical density functional calculations and combined quantum mechanics/molecular mechanics (QM/MM) methods. They will be applied in molecular dynamics simulations of enzyme-catalysed reactions, and combined with AI tools for enzyme design. This project will apply advanced computational resources including Isambard-AI and Isambard-3. It will apply machine learning potentials with flexible electrostatic embedding for multiscale molecular dynamics simulations. The models will be used to investigate and predict catalytic effects of mutations, in collaboration with experimental work across the BioAID programme, contributing to practical catalyst design and development.

This project will provide outstanding training in enzyme design and a wide range of computational methods from machine learning, to molecular simulation to AI, interactive virtual reality and data analysis, and experience of world-class advanced computation. It will also provide experience of working in internationally leading groups on enzyme simulation and design, closely integrated with experiments. You will also benefit from training and interaction across the whole BioAID programme.

About the Programme

BioAID: AI-Driven Enzyme Design for Industry Biocatalysis is a new BBSRC Doctoral Focal Award training programme. BioAID brings together world-leading experts from Queen's University Belfast (QUB), University of Manchester (UoM), University of Edinburgh (UoE) and University of Bristol (UoB). BioAID will train the next generation of scientists in Artificial Intelligence and Data-Driven approaches for translational biocatalysis, addressing critical needs in the development of sustainable biotechnologies.

Eligibility

Applicants should have, or expect to achieve, at least a 2.1 honours degree or a master's (or international equivalent) in chemistry, biochemistry or a related subject.

Funding Notes

This 4-year PhD project is fully funded and home students, and EU students with settled status, are eligible to apply. The successful candidate will receive an annual tax-free stipend set at the UKRI rate (£20,780 for 2025/26) and tuition fees will be paid. We expect the stipend to increase each year. The start date is September 2026.

More information

We encourage you to make informal enquiries to Prof. Adrian.Mulholland@bristol.ac.uk if you like more information on the project.

How to Apply

Apply online at: How to apply|Study at Bristol|University of Bristol

References

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2. LP Merlicek *et al. Angewandte Chemie International Edition* 64, e202507031 (2025) https://doi.org/10.1002/anie.202507031
3. SL Lovelock *et al. Nature* 606, 49-58 (2022) https://doi.org/10.1038/s41586-022-04456-z
4. HA Bunzel *et al. Nature Chemistry* 13, 1017-1022 (2021) https://doi.org/10.1038/s41557-021-00763-6