

BioAID BBSRC Doctoral Training Programme:

Dynamic tools for enzyme design

Supervisor: Sofia Oliveira

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Application deadline: 30th April 2026

A PhD studentship is available in the group of Sofia Oliveira on computational enzyme design and engineering. This project will develop and apply advanced dynamics methods for enzyme design, collaborating with experiments. This project part of the new BBSRC-funded BioAID Doctoral Focal Award programme in AI-driven enzyme design for biocatalysis.

About the Project

This BioAID PhD project will develop and apply methods to predict target sites for mutations and modification to inform and accelerate experimental programmes of enzyme design, evolution and engineering. The targets will be natural and designed enzymes relevant for biocatalysis. Dynamical-nonequilibrium molecular dynamics (D-NEMD) simulations are emerging as a powerful method to identify functionally relevant sites in enzymes, including sites far from the active site that are often modified by natural or directed evolution of enzyme activity. D-NEMD simulations will probe and predict effects of mutation, and tests effects of different physical conditions on enzymes. The results will be used to train machine learning models. These methods will be combined with other simulation methods and AI tools for enzyme design. This project will apply these combined methods to inform and accelerate experimental evolution and engineering in enzyme design. 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.

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 Dr. Sofia Oliveira sofia.oliveira@bristol.ac.uk if you have any queries or would like to discuss the project.

How to Apply

Apply online at: [How to apply | Study at Bristol | University of Bristol](#)

References

1. B. Balega, B. *et al.* *Molecular Physics* 123(7–8) (2025) <https://doi.org/10.1080/00268976.2024.2428350>
2. C. Acevedo-Rocha *et al.* *Faraday Discussions* 252, 127-156 (2024) <https://doi.org/10.1039/D4FD90022G>
3. M. Beer *et al.* *Chemical Science* 15, 17232-17244 (2024) <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>
5. HA Bunzel *et al.* *Current Opinion in Structural Biology* 67, 212-218 (2021) <https://doi.org/10.1016/j.sbi.2020.12.015>