BioProcess: Advanced tools for enzyme design and engineering

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Application deadline: 30 April 2026

About the Project

This BioProcess IDLA PhD project will develop and apply computational methods for design and engineering de novo protein catalysts and engineering of natural enzymes for biocatalysis. You will develop and apply computational workflows applying outstanding advanced computer resources. Models and predictions will be tested in collaborative experimental work. This project will provide excellent training in a range of advanced computational methods, ranging from 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. This interdisciplinary project will develop methods to (re)design and engineer enzymes for specific activities, tested in collaborative experiments. to predict enzyme activity and effects of mutation on catalysis and specificity. It will deliver new integrated methods to design enzymes and predict their activity. We will develop and apply advanced computational tools for enzyme design and engineering, going beyond the current state of the art. Most current design tools provide static structures, missing the complex dynamics that are crucial to protein function (and which are modulated and optimized by evolution). Engineering functional dynamics requires other approaches such as molecular dynamics (MD) simulations. Natural and directed evolution also optimizes active site electric fields for catalysis. We will develop workflows to incorporate these crucial dynamic and physical features in enzyme engineering and combine them with AI protein design tools.

This project will provide outstanding training in a wide range of computational methods, and experience of world-class advanced computation. It will also provide experience of working in internationally leading groups in enzyme simulation and design, closely integrated with experiments.

About the programme

Join experts in industry and academia working to sustainably manufacture the complex and diverse molecules needed by modern society.

Industrial manufacturing is at a turning point. Many conventional production routes rely on non-renewable resources, harmful chemicals, and energy-intensive steps. Biocatalysis using engineered enzymes offers a proven solution.

Led by The University of Manchester in collaboration with AstraZeneca, The Universities of Bristol and York alongside other leading industrial partners, BioProcess aims to train the next generation of scientists in the skills needed to realise full the potential of biocatalysis, protein engineering and biomanufacturing for the UK bioeconomy.

Training

BioProcess aims to train the next generation of bio-innovators. Our interdisciplinary programmes prepare PhD students and researchers with the real-world skills to apply biocatalysis, protein engineering and sustainable manufacturing in industry. Alongside the training on the specific project described above,

We offer:

- advanced theoretical and practical skills training provided by a mixture of industry and academic project partners covering structural biology; biophysical and analytical methods; computational modelling; directed evolution; process modelling and development; digital skills
- Access to a network of elite partners and mentors
- A strong track record of impact, including a free online course in industrial biotechnology with over 10,000 learners to date.

Strong foundations in Biocatalysis:

Formerly CoEBio3, our centre has a focus on delivering solutions with real impact in pharmaceutical and chemical manufacturing with our industry partners. Our work has already enabled major industrial advances

Commercialised over 1,000 enzymes

Covering 20+ reaction types, significantly expanding biocatalytic options for manufacturing.

Pioneered metal-free processes

- Reducing reliance on costly and hazardous precious metal catalysts.

Delivered high-performing biocatalysts

- Engineered industry-ready enzymes suitable for large scale pharmaceutical manufacturing.

We've also helped shape national policy. In 2018, our researchers co-authored the UK strategy report Growing the UK Industrial Biotechnology Base, supporting government plans for a £440 billion bio-economy by 2030.

Eligibility

Applicants should have, or expect to achieve, at least a 2.1 honours degree or a master's (or international equivalent) in chemistry and ideally with some experience of organic synthesis.

How to apply

To be considered for this project you'll need complete a formal application through our online application portal.

Applications should be submitted through the BioProcess IDLA Website (https://www.mib.manchester.ac.uk/research/centres/coebio3/), where you can find a step-by-step guide to the process.

For informal enquiries about this particular project please contact Prof Adrian Mulholland, Adrian.Mulholland@bristol.ac.uk

Informal enquiries about the programme and application process can be made by emailing sarah.shepherd@manchester.ac.uk.

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.

References

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2. A. J. Devine, A. E. Parnell, C. R. Back, N. R. Lees, S. T. Johns, A. Z. Zulkepli, R. Barringer, K. Zorn, J. E. M. Stach, M. P. Crump, M. A. Hayes, M. W. van der Kamp, P. R. Race and C. L. Willis, *Angew. Chem. Int. Ed.*, 2023, **62**, e 202213053.
3. 3. S. Z. Mbatha,C. R. Back, A. J. Devine, H. M. Mulliner, S. T. Johns, H. Lewin, Kaiman A. Cheung, K. Zorn, J. E. M. Stach, M. A. Hayes, M. W. van der Kamp, P. R. Race and C. L. Willis *Chem. Sci.* **2024**, *15*, 14009.
4. 4. J. Russell, C. R. Back, C. Perry, K. Cheung, L. Maschio, N. R. Lees, M. A. Hayes, M. van der Kamp, P. R. Race and C. L. Willis, *Chem. Sci*, **2025**, *16*, 1993.