THE UNIVERSITY of EDINBURGH
School of Chemistry

Machine Learning-Guided Synthetic Strategies for Natural Product Synthesis
A joint PhD studentship is available in the groups of Professor Andrew L. Lawrence and Dr Emma King-Smith at the University of Edinburgh School of Chemistry.

The studentship is fully funded for 42 months by the University of Edinburgh and covers tuition fees and an annual stipend at the UKRI rate, for 2025-26 this is £20,780 per annum, for a candidate satisfying EPSRC residency criteria, see:

https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/#contents-list

Project Summary
Natural products serve as a rich source of therapeutic agents, but their structural complexity presents challenges in synthesis. However, this complexity also allowed these scaffolds to become fruitful environments for new chemical discovery, providing rigorous "testing grounds" for methodology. In turn, this yielded better syntheses to a wider variety of targets.

Machine learning (ML) has seen advances in synthesis prediction and planning however, ML methods are typically built for, and applied to, simpler molecules. ML methodology forged in the intricate chemical setting of natural product synthesis will yield streamlined syntheses whilst also advancing the field of data-driven chemistry. In conjunction with the novel ML development, the student will be guiding model training with experimental validation in the lab. This work builds upon the work from Prof. Lawrence's group in biomimetic total synthesis and Dr King-Smith's work in data-driven chemistry.

Candidates should have a keen interest in both organic synthesis and machine learning with some research experience in either field. This is an interdisciplinary post and will provide an unparalleled opportunity for a student to gain expertise in total synthesis and deep machine learning.

References
J. S. Bestwick, D. J. Jones, H. E. Jones, P. G. Kalomenopoulos, R. Szabla, A. L. Lawrence*, *Angew. Chem. Int. Ed.* **2022**, *61*, e202207004.

E. King-Smith*, *Chem. Sci.* **2024**, *15*, 5143.

How to apply
In the first instance, the initial application of cover letter and CV should be directed to:
Dr Emma King-Smith School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK. Email: emma.king-smith@ed.ac.uk

The closing date for applications is 4 April 2025.

IMPORTANT
Before Submitting your cover letter and CV, please complete the online form at:

School of Chemistry Equality, Diversity and Inclusion Form, entry 2025-26.

The form will automatically generate a unique 'Response ID number' that you must include in your cover letter.

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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. For further information, please see our University Initiatives website: https://equality-diversity.ed.ac.uk/inclusion/family-and-carer