THE UNIVERSITY of EDINBURGH
School of Chemistry

Unlocking Organic Chemical Reaction Prediction with Limited-Data Machine Learning

A PhD studentship is available in the group of Dr Emma King-Smith, School of Chemistry, University of Edinburgh, see https://www.ed.ac.uk/profile/dr-emma-king-smith.

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 2024-25 this is £19,237 per annum, for a candidate satisfying EPSRC residency criteria. For more details, see:

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

Project Summary

Synthetic organic chemistry plays a vital role in various industries (pharmaceuticals, perfumery, agrochemicals, cosmetics, etc.) and fundamental research (probe / linker, design, methodology development, etc.). However, despite our best experimental and computational efforts, many reaction outcomes are difficult to predict due to the complex interplay between reactants, solvent, and reagents. This has resulted in an empirical-first based approach to reaction design and investigation.

This project will focus on predictive modelling of C(sp^2/sp^3)-N bond formation reactions, a highly privileged reaction class exemplified by its various mechanistic modalities: catalytic, 2-electron based, and 1-electron based. A combination of in-house experimental validation and custom machine learning model development will be employed which will build upon Dr King-Smith's work in the field of modelling chemical outcomes in low-data environments.

The ideal candidate is enthusiastic about working at the intersection of machine learning and organic chemistry, gaining expertise in both experimental synthetic chemistry and computational approaches. Training will be provided in all necessary disciplines: synthetic chemistry, machine learning, and coding. There will also be opportunities to collaborate with industry leaders in chemistry and AI. Previous research and lab experience is advantageous, but not essential.

In the first instance, the initial application consisting of a cover letter and CV should be emailed to:

Dr Emma King-Smith, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK. Email: ekingsm@ed.ac.uk

The closing date is 15 November 2024.

References

King-Smith, E., Faber, F.A., Reilly, U., Sinitskiy A. V., Yang. Q., Liu, B., Hyek, D., & Lee, A. A.* "Predictive Minisci Late Stage Functionalization with Transfer Learning." Nat Commun. 2024, 15, 426.

King-Smith, E.* "Transfer Learning for a Foundational Chemistry Model" Chem. Sci. 2024, 15, 5143.

IMPORTANT

Before Submitting your cover letter and CV, please complete the online 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.

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