

Project Title: Design and Synthesis of Peptide-derived Receptors for Binding Small Molecules

A PhD studentship is available in the groups of Prof. Scott Cockroft and Dr Annamaria Lilienkampf School of Chemistry, The University of Edinburgh, <a href="https://www.cockroft.chem.ed.ac.uk">https://www.cockroft.chem.ed.ac.uk</a> in collaboration with DSTL.

The studentship is fully funded for 48 months by DSTL and covers tuition fees and an annual stipend (starting at £19,237 per annum) for a candidate satisfying EPSRC residency criteria. <a href="https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/#contents-list">https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/#contents-list</a>

## **Project Summary**

The ability to detect, identify and quantify small molecules is critical in field and laboratory sensing applications. To yield new capabilities and meet future technology requirements, the development of new approaches affinity-based detection is desirable.

This project will design novel synthetic peptide binding partners for the detection and quantification of various small molecules. We seek to exploit quantum chemical calculations (e.g. Gaussian, Spartan), molecular dynamics simulations (e.g. *Gromacs*, *Autodock*), and emerging machine-learning tools (e.g. *alphafold*, *roseTTAFold*) to design the binding partners. We will then synthesise the designs using a combination of conventional organic synthesis and solid-phase peptide synthesis. The binding of the synthetic receptors to the target small molecules will be validated using NMR binding titrations or other spectroscopic approaches. There is the opportunity for a research placement at Dstl Porton Down.

In the first instance, the initial application (including cover letter and CV) should be directed to: Prof. Scott Cockroft, School of Chemistry, University of Edinburgh, David Brewster Road, Edinburgh EH9 3FJ, UK. Email: scott.cockroft@ed.ac.uk

Prior experience in organic synthesis or peptide synthesis, and/or computational chemistry are desirable.

The position will remain open until filled; prompt applications are encouraged.

## References

https://www.cockroft.chem.ed.ac.uk/publications-0

## **IMPORTANT**

Before Submitting your cover letter and CV, please complete the online <u>School of Chemistry</u> Equality, Diversity and Inclusion Form 2024.

The form will automatically generate a unique "Receipt 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. See our

University Initiatives website for further information. University Initiatives website: <a href="https://www.ed.ac.uk/equality-diversity/help-advice/family-friendly">https://www.ed.ac.uk/equality-diversity/help-advice/family-friendly</a>