

**EPSRC Centre for Doctoral Training (CDT) in Molecular Sciences for Medicine (MoSMed)**

**Integrating computational physics-based simulation and machine learning with drug discovery pipelines**

**Newcastle University & Genesis Therapeutics**

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| **Supervisory Team** | * [**Dr Daniel Cole**](https://www.ncl.ac.uk/nes/people/profile/danielcole.html)**, Newcastle University** * [**Prof Martin Noble**](https://www.ncl.ac.uk/medical-sciences/people/profile/martinnoble.html)**, Newcastle University** * **Dr Simon Boothroyd,** [**Genesis Therapeutics**](https://www.genesistherapeutics.ai/) |

**Project overview/context**

Artificial intelligence and machine learning aim to transform the drug discovery landscape through the prediction of potential new therapeutics with unprecedented speed and accuracy. Yet these approaches work best when combined with physics-based modelling, in which the interactions between potential drugs and their target receptor are explicitly modelled at the atomic scale. Such computer simulation platforms enable us to account for the roles of, for example, protein flexibility and critical water molecules in binding.

**Research Project**

Modelling of the dynamics and interactions of molecules at the atomic scale is ideally performed using first principles quantum mechanics. However, these simulations are prohibitively expensive.

In our previous work, some of the supervisory team have shown that classical (force field) models with novel functional forms have the flexibility to model interactions in the condensed phase with higher accuracy than traditional (Lennard-Jones based) models.

Here, the student will further incorporate high level quantum mechanical data and machine learning to improve the design and scope of these models such that they accurately model interactions between proteins, small organic molecules and water, at a fraction of the cost of quantum mechanics. They will integrate the workflows into drug discovery pipelines, at Newcastle University and/or at the collaborating industry partner, and thereby showcase the potential for utilising physics-based modelling for design of future therapies.

This studentship is a collaboration between Newcastle University and [Genesis Therapeutics](https://www.genesistherapeutics.ai/).

**Further Reading**

[1] <https://pubs.rsc.org/en/content/articlelanding/2023/dd/d3dd00070b>

[2] <https://arxiv.org/abs/2312.15211>

[3] <https://pubs.acs.org/doi/10.1021/acs.jcim.2c01153>

**Training & Skills**

The supervisory team will provide highly sought-after training in the fields of computational medicinal chemistry, machine learning and molecular modelling. As such, this project is ideal for a candidate with ambitions towards a career in the pharmaceutical industry or academic drug discovery.

The student will benefit from bespoke research and life skills training programme through alignment with the Newcastle-Durham MosMed EPSRC Centre for Doctoral Training.

**Further Information**

**For further information, please contact the lead supervisor Dr Daniel Cole (daniel.cole@ncl.ac.uk)**

**How to Apply**

You must apply through the University’s [**Apply to Newcastle Portal**](https://applyto.newcastle.ac.uk/)

Once registered select **‘Create a Postgraduate Application’.**

**Use ‘Course Search’ to identify your programme of study:**

* search for the ‘Course Title’ using the programme code: **8100F**
* Research Area: Chemistry
* Select ‘PhD Chemistry (full time)’ or ‘PhD Chemistry (part time)’ as the programme of study, depending on your preference.

**You will then need to provide the following information in the ‘Further Details’ section:**

* a ‘Personal Statement’ (this is a mandatory field) - upload a document or write a statement directly in to the application form. Please include the full title of the studentship, the studentship code **(mos2\_03)**, and how your interests/experience relate to the project.
  + the relevant studentship code **(mos2\_03)** in the ‘Studentship/Partnership Reference’ field. **You must include the relevant code for your application to be considered.**
  + when prompted for how you are providing your research proposal - select ‘Write Proposal’. You should then type in the title of this project. You do not need to upload a research proposal.

**In the ‘Supporting Documentation’ section please upload:**

* An up to date CV.

Please upload all documents in PDF format.

**You must submit one application per studentship, you cannot apply for multiple studentships on one application.**

**Equality, Diversity and Inclusion (EDI)**

Within the MoSMed CDT we are committed to building a diverse community based on excellence and commitment. To that end, in our recruitment of Doctoral Researchers we welcome applications from outstanding candidates of all backgrounds regardless of ethnicity, disability, gender identity, sexual orientation and will consider all applications equally based on merit.

Should you have any queries regarding the MoSMed application process to Newcastle University please contact Craig Hinds, the MoSMed CDT Manager: [**mosmed.cdt@newcastle.ac.uk**](mailto:mosmed.cdt@newcastle.ac.uk)