

Candidate Information

Position: School/Department: Reference: Closing Date: Salary: Research Assistant School of Chemistry and Chemical Engineering 18/106983 Tuesday 18 December 2018 £27,831 - £32,236 per annum (potential to progress to £35,210 per annum through sustained exceptional contribution) Monday 7 January 2019 Available until 30 March 2019

Anticipated Interview Date: Duration:

JOB PURPOSE:

The work encompasses developing and applying computational chemistry/biology approaches to engineer enzymes to achieve desirable functions, in support of multiple enzyme evolution projects with close collaboration with biologists and chemists. Additionally, the successful applicant will be expected to contribute to the day to day running of the computer laboratory. The successful applicant will be expected to work at Almac Sciences Ltd. in Craigavon, as required by the project.

The position has specifications on the following topics:

- Protein structure prediction and refinement;
- Molecular dynamics simulations of biomolecules;
- Free energy calculation in MD simulation;
- Calculation of enzymatic reactions.

MAJOR DUTIES:

- 1. To contribute to the maintenance of lab computing resource and network as appropriate.
- Conduct research activity in the area of computational chemistry approaches to engineer biotechnology-related enzymes, with the aim to achieve desirable functions.
- 3. Perform protein structure simulations and bio-catalytic mechanism studies.
- 4. Rational design of enzyme libraries.
- 5. The individual will be expected to work as part of a team of researchers composed of biologists and chemists at all stages of the program.
- 6. Make periodic presentations and contribute actively to the overall discussion on the directions of the projects as his/her input will be critical to the projects' success.
- 7. To attend and present findings at research group meetings and other relevant local, national and international meeting.
- 8. Prepare, in consultation with the team leader, material for publication in high quality peer-reviewed journals.

Planning and Organising:

- 1. Prioritise and reprioritisation of research in order to meet deadlines and targets.
- 2. Organise informal meetings communicate directly with other lab members or with team leader.

Resource Management Responsibilities:

- 1. Support the development and training of support staff and students by making available their research experience and expertise.
- 2. Take shared responsibility for maintenance of lab computer network and parallel computing environment.

ESSENTIAL CRITERIA:

- 1. An Honours degree or equivalent in Chemistry or a closely related area.
- 2. At least 1 years' relevant experience in protein structure simulation and enzymatic mechanism calculation.

- 3. Linux and network environment experience
- 4. Scripting skills (e.g Python, Perl)
- 5. Must display clarity of thinking and ability to address a variety of research topics.
- 6. Organised and attentive to detail and ability to meet deadlines.
- 7. Excellent communication skills.
- 8. Must demonstrate good team working skills.
- 9. Must demonstrate a true commitment to and interest in research
- 10. Must be willing to work irregular hours when necessary for the progress of the research project.
- 11. Must be willing to work closely with industrial partners as required.
- 12. Must be willing and able to travel to national and international meetings.

DESIRABLE CRITERIA:

- 1. Appropriate MSc (awarded) or PhD (awarded or about to be awarded) in Computational Chemistry or Computational Biology or Biophysics or Bioinformatics.
- 2. At least 3 years' post-graduate experience in protein structure simulation and enzymatic mechanism calculation.
- 3. Experience in one or more of the following:
 - Experience in homology modelling. Experience in using various biological molecular modelling software package.
 - Extensive expertise in molecular dynamics including free energy calculation and coarse-grained MD simulation.
 - Experience in QM/MM calculations.
 - Experience in machine learning techniques.
 - Experience in using scripting language for specific tasks.
 - Experience in using and maintaining Linux supercomputer network environment.
 - Knowledge of enzymatic reaction and evolution
 - Biotech Industrial experience in multidisciplinary team
- 4. Evidence of project completion.
- 5. Ability to prioritise research/experiments in order to meet deadlines and targets.
- 6. Good communication/verbal skills with an ability to clearly explain experimental results to a non-subject specialist audience.