# Candidate Information

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| **Position:** | Research Assistant - Computational Chemist |
| **School/Department:** | Chemistry and Chemical Engineering |
| **Reference:** | 21/109398 |
| **Closing Date:** | Sunday 2 January 2022 |
| **Salary:** | £28,756 - £33,309 per annum |
| **Anticipated Interview Date:** | Friday 14 January 2022 |
| **Duration:** | Until 31 March 2024 |

## JOB PURPOSE:

The work forms part of the Invest Northern Ireland-funded INSIGHT (IN Silico Informed metaGenomic Harvesting Technology) project which is an exciting academia-industry collaboration between Queen's University (the academic partner) and Almac Sciences Ltd (the industrial partner). The position will be based primarily at the School of Chemistry and Chemical Engineering at Queen's University in Belfast, Northern Ireland, although the successful candidate will also be expected to spend some time at the Almac Sciences Ltd site in Craigavon, Northern Ireland.. The research assistant will work on multidisciplinary high impact research projects, which involve close collaboration with experimentalists from Almac and Queen's. It also offers exceptional opportunities to meet industrial clients and expedient knowledge transfer.

### MAJOR DUTIES:

1. To contribute to the maintenance of lab computing resource and network as appropriate.
2. Conduct research activity in computational study of the structure-properties relationship of various enzymes, and developing machine learning models for the design/discovery of new enzyme biocatalysts.
3. Perform binding free energies calculations and QM/MM calculations.
4. Develop machine learning models for rapid screening of enzyme libraries.
5. The individual will be expected to work as part of a multidisciplinary 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. Write up results of own work and contribute to the production of research reports, publications and proposals.
8. In consultation with the team leader, assist with preparation of material for publication in high quality peer-reviewed journals.

### Planning and Organising:

1. Plan own day to day activity within the framework of the agreed research programme. Timescales range from 1-6 months in advance and contribute to research group planning.
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, Biochemistry, Biotechnology, Bioengineering, Pharmaceutical Engineering or a closely related area.

2. At least 1 years' relevant experience in MD simulations, QM calculations and applications of machine learning in one or more of the following areas:
   • potential energy surface
   • chemical reactivities
   • free energy simulation
   • protein function prediction
   • substrate space
   • enzyme engineering.
3. Evidence of HPC experience/application.
4. Demonstrable evidence of python programming skills.
5. Sufficient breadth or depth of specialist knowledge in the discipline and of research methods and techniques to work within own area.
6. Demonstrate a significant interest in algorithm development, chemical reactions, structure-function relationship, catalyst design.
7. Must display clarity of thinking and ability to address a variety of research topics.
8. Organised and attentive to detail and ability to meet deadlines.
9. Excellent communication skills.
10. Must demonstrate good team working skills.
11. Must demonstrate a true commitment to and interest in research.
12. Must be willing to work irregular hours when necessary for the progress of the research project.
13. Must be willing to work closely with industrial partners as required.
14. Must be willing and able to travel to national and international meetings.

**DESIRABLE CRITERIA:**

1. Have or about to obtain a Postgraduate qualification and/or PhD Degree in the field of Computational Chemistry, Computational Biology, Biotechnology, Computational Biochemistry or Computational Biophysics.
2. Experience, evidenced by relevant output in peer-reviewed academic journals commensurate with career stage.
3. Proven experience in one or more of the following:
   • Experience in using various biological molecular modelling software packages including Gaussian, Amber or Gromacs, ChemShell, etc.
   • Experience in prediction of protein sequence /structure function relationship
   • Experience in database and data mining
   • Extensive expertise in molecular dynamics
   • Experience in free energy calculations
   • Experience in SMILES representations of small molecules
   • Experience in metadynamics
   • Experience in QM/MM calculations
   • Experience in machine learning potential.
4. Demonstrable experience in using and maintaining Linux supercomputer operation environment.
5. Knowledge of enzymatic reactions and directed evolution.
6. Biotech Industrial experience in a multidisciplinary team.
7. Evidence of project completion.
8. Ability to prioritise research/experiments in order to meet deadlines and targets.
9. Excellent communication/verbal skills with an ability to clearly explain experimental results to a non-subject specialist audience.