

Candidate Information

Position: Research Fellow Chemoinformatics (Future Medicines Institute)
School/Department: Faculty Office MHLS
Reference: 25/112511
Closing Date: Monday 12 May 2025
Salary: £39,922 - £43,605 per annum.
Anticipated Interview Date: Thursday 22 May 2025
Duration: 12 months

JOB PURPOSE:

The newly funded Future Medicines Institute (FMI) will be a collaborative innovation centre developed as a focal point to enable industry, academia and health professionals to drive research and development in the Life and Health Sciences (LHS) sector. It will build upon and exploit Northern Ireland's recognised capabilities and strengths in oncology and digital health to accelerate the development of biomarker-led products. The Institute's vision is a partnership of Northern Ireland's leading pharmaceutical, diagnostics and health analytics companies, alongside academic institutions and government agencies.

The post holder will develop computational drug discovery techniques for FMI. Working across project teams, this Research Fellow role will involve the use of cutting-edge computational methods (structure/ligand-based design, AI/ML, virtual screening, chemo/bioinformatics, data-mining etc) to effectively advance programs with creative solutions and insights. The post will require a dynamic self-starter with an eagerness to learn who will be an integral member of the FMI team. They must exhibit excellent people skills, accountability and the ambition to thrive within a highly interactive, fast-paced team.

MAJOR DUTIES:

1. Build a Chemoinformatics platform that incorporates the latest computational, AI/ML and cheminformatics technologies.
2. Develop computational and chemoinformatic tools that assess target druggability, compound selectivity, affinity and SAR.
3. Perform the design, evaluation, and prioritisation of new targeted analogues and focused libraries across FMI projects using state-of-the-art computational methods and technologies.
4. Rationally identify and acquire new screening compound collections and implement virtual screening opportunities.
5. Develop and implement the latest generative AI approaches alongside gold standard ML methods to ligand design, property prediction and PPI prediction methods.
6. Effectively communicate project results, strategies and objectives with internal and external partners.
7. Ensure state-of-the-art software, hardware and computational infrastructure is maintained that will maximise impact across FMI programs.
8. Present regular progress reports on research to members of the research group.
9. Develop collaborative links with external academic/industrial partners with the aim of creating new opportunities and driving FMI programs.
10. Prepare, often in consultation with supervisor, material for publication in national and international journals and presentations at international conference.
11. Carry out routine administrative tasks associated with the research project/s to ensure that project/s are completed on time and within budget. These might include organisation of project meetings and documentation, financial control, risk assessment of research activities.
12. Carry out occasional undergraduate supervision, demonstrating or lecturing duties within the post holder's area of expertise and under the direct guidance of a member of academic staff.
13. Read academic papers, journals and textbooks to keep abreast of developments in own specialism and related discipline.
14. Carry out any other duties designated by a line manager and which fall within the general ambit of the post.

ESSENTIAL CRITERIA:

1. Degree in chemistry, biochemistry, computer science or mathematics.
2. Have or be about to obtain a relevant PhD.(must be obtained within 3 months of date of interview).
3. Significant, relevant research experience.
4. Experience in Chemoinformatics in a University, academic institute, or industrial setting.
5. An expert level user of HPC infrastructure / Linux systems.
6. Able to implement key R and / or Python packages.
7. An expert level user of CADD software e.g. MOE or Schrodinger.
8. Track record of publications commensurate with stage of career.
9. Experience in lab project supervision.
10. Ability to plan and manage own workload and contribute to requisite administrative tasks.
11. Sufficient breadth and depth of specialist knowledge in the discipline and of research methods and techniques to work within established research programmes.
12. Ability to work across multidisciplinary teams.
13. Ability to communicate complex information clearly.
14. Ability to build contacts and participate in internal and external networks.
15. Ability to assess and organise resources according to adjusting priorities.
16. Team player, proactive, highly motivated and supportive of other team members.
17. Interest in driving research focussed programmes.
18. Willingness to travel to partner sites and collaborate with industry partners.

DESIRABLE CRITERIA:

1. Drug discovery experience in an academic or industrial setting.
2. Experience in working within industry.
3. Experience working with next-generation structural design tools such as AlphaFold2.
4. Data handling expertise e.g. cloud storage and SQL.

ADDITIONAL INFORMATION:

Informal enquiries can be directed to: James Mawhinney - j.mawhinney@qub.ac.uk.