Candidate Information

Position:	Research Fellow
School/Department:	School of Pharmacy
Reference:	26/113143
Closing Date:	Monday 2 March 2026
Salary:	£41,519 per annum
Anticipated Interview Date:	Friday 13 March 2026
Duration:	18 Months

JOB PURPOSE:

To lead the computational chemistry aspects of a BBSRC-funded collaborative project 'Unlocking GPCR Signalling Bias: A Multiscale Approach to GPR84 and Beyond'. The role-holder will work closely with medicinal chemists at University of Oxford and pharmacologists at University of Glasgow, applying virtual screening, machine learning, AI-driven generative chemistry, pharmacophore modelling, and molecular dynamics simulations to design novel GPR84 ligands with predictable signalling bias profiles.

MAJOR DUTIES:

1. Lead computational drug design activities within the GPR84 project, developing and applying virtual screening, machine learning, generative AI, and pharmacophore modelling approaches to design novel ligands with predictable signalling bias profiles.
2. Perform large-scale virtual screening of compound libraries (ZINC20, Enamine REAL) using docking methods and utilize AI-driven generative chemistry platforms (GENTRL, Reinvent 4, AutoGrow, LiGAND) for de novo ligand design.
3. Develop machine learning frameworks to predict ligand bias and build pharmacophore models for biased GPR84 agonists. Conduct molecular dynamics simulations to support ligand design and validate binding hypotheses.
4. Collaborate closely with medicinal chemists at University of Oxford (Prof. Russell) providing computational predictions to guide synthesis priorities, and with pharmacologists at University of Glasgow (Prof. Milligan) to interpret experimental validation data.
5. Prepare manuscripts for publication in high-impact journals, taking lead authorship where appropriate. Present research findings at national and international conferences.
6. Contribute to BBSRC progress reports and assist in preparation of follow-on funding proposals. Extend GPR84 findings to other Class A GPCRs including FFA4/GPR120.
7. Manage computational workflows on HPC systems (QUB Kelvin-2, ARCHER2). Organize multi-site consortium meetings between QUB, Oxford, and Glasgow. Maintain detailed computational workflow documentation.
8. Train and supervise students on computational methods. Provide training to team members at partner institutions on molecular modelling techniques.
9. Keep up-to-date with current literature in GPCR drug discovery, biased signalling, computational chemistry, and generative AI. Communicate advances to the consortium team.
10. 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.
11. Read academic papers, journals and textbooks to keep abreast of developments in own specialism and related disciplines.

ESSENTIAL CRITERIA:

1. Hold or be about to obtain* (must be obtained* within 3 months of start date in post) PhD in computational chemistry, computational biology, structural biology, biophysics, pharmacology or related discipline.
2. Significant experience in virtual screening and molecular docking.
3. Experience with machine learning/AI approaches in drug discovery.
4. Familiarity with generative chemistry platforms.

5. Experience with pharmacophore modelling.
6. Experience with molecular dynamics simulations.
7. Strong scripting skills (Python, Bash).
8. Experience with HPC environments.
9. Knowledge of GPCR structure, function, and signalling pathways.
10. Ability to manage computational workflows and storage on HPC systems (Kelvin-2, ARCHER2).
11. Understanding of structure-based drug design and medicinal chemistry principles.
12. Ability to communicate computational concepts to chemists and biologists.
13. Excellent problem-solving skills.
14. Ability to communicate complex computational concepts to chemists and biologists.
15. Excellent verbal and written communication skills.
16. High-quality manuscript writing experience.
17. Ability to work effectively in interdisciplinary teams.
18. Highly motivated, ambitious, and efficient.
19. Ability to work independently and as part of a team.
20. Scientific creativity in hypothesis generation.
21. Strong organizational skills managing multiple computational workstreams.
22. Willingness to travel between QUB, Oxford, and Glasgow.

DESIRABLE CRITERIA:

1. Experience with enhanced sampling MD methods.
2. Free energy calculations (FEP, MM-PBSA).
3. GPCR/membrane protein modelling.
4. Knowledge of GPCR pharmacology and biased signalling.
5. Experience with cell-based assays (cAMP, Î²-arrestin recruitment).
6. Wet lab experience in pharmacology.
7. Combined expertise in both molecular modelling AND pharmacology.
8. Knowledge of biased signalling and operational models.
9. Experience interpreting cryo-EM structural data.

ADDITIONAL INFORMATION:

Informal enquiries may be directed to: Dr Yiwei Tian at y.tian@qub.ac.uk.