

Candidate Information

Position:	Research Fellow in Molecular Modelling (Maternity Cover)
School/Department:	Pharmacy
Reference:	20/108194
Closing Date:	Monday 20 April 2020
Salary:	£33,797 per annum.
Duration:	This post is available until 30 September 2020

JOB PURPOSE:

To be an active member of the molecular modelling group to assist in planning and delivery of research within the area of structure-based drug design methods so that the overall research objectives of the project/school are met.

MAJOR DUTIES:

1. Develop, plan and deliver an area of personal research and expertise, and/or undertake research under supervision within a research programme aimed at understanding allosteric drug binding to membrane proteins. Techniques may include molecular dynamics simulations (NAMD, GROMACS or AMBER), enhanced sampling simulations, allosteric network analysis, 3D-GRID-based analysis, docking, scoring, virtual screening, substructure search, machine learning as well as sequence analysis.
2. Develop and implement, with support, a highly ambitious personal career development plan in the course of the post.
3. Maintain up-to-date knowledge of the field of interest at the cutting edge and communicate same to the group.
4. Design, develop and refine computational protocols in order to obtain reliable and reproducible data from computer simulations.
5. Carry out analyses, critical evaluations and interpretations of simulation data and the literature using methodologies and other techniques appropriate to area of research.
6. Collaborate effectively with pharmacologists from Dr McCormick's lab by making on-time predictions for mutagenesis and compound screening.
7. Present regular progress reports on research to members of the research group, other groups within the School/University, to external audiences nationally and internationally to disseminate and publicise research findings.
8. Prepare, always in consultation with supervisor, material for publication in national and international journals and presentations at international conferences.
9. Assist grant holder in the preparation of funding proposals by generating preliminary data and applications as well as project progress reports to external bodies.
10. Carry out routine administrative tasks associated with the research projects/group to ensure that projects are completed on time and within budget and that the group functions efficiently. These might include organisation of project/group meetings and documentation, financial control, stock management/procurement and risk assessment of research activities.
11. Carry out school/undergraduate/post-graduate student and visiting researcher training and supervision, demonstrating, tutoring or lecturing duties within the post holder's area of expertise and under the guidance of a member of academic staff.
12. Participate, and in some cases lead, outreach activities on behalf of the group/School.
13. Participate in local research-related activities such as journal clubs, training sessions, seminar series etc.
14. Assist in assessment of research communications and data, particularly within the group.
15. Additional research and/or laboratory related duties within the general range of the post and competence of post holder.

Planning and Organising:

1. Plan for specific aspects of research programme. Timescales range from 1-18 months in advance and may contribute to overall research group planning.
2. Plan for access to, and use of, research resources, computer clusters (local and ARCHER) and workshops where appropriate.

3. Plan own day-to-day activity within framework of the agreed research programme as well as communal activities (e.g. meetings) were appropriate.
4. Plan up to one year in advance to meet deadlines for grant applications, journal publications and to prepare presentations and papers for conferences and meetings.
5. Coordinate and liaise with other members of the research group and collaborative research groups regarding work progress and stock management.
6. Assist in training other group members on effective planning and organisation.

Resource Management Responsibilities:

1. Ensure research resources are used in an effective and efficient manner including liaising with vendors and collaborators.
2. Provide guidance as required to support staff and any post-graduate/under-graduate students and visiting researchers who may be assisting with work of the group.

Internal and External Relationships:

1. Liaise on a regular basis with supervisor, colleagues, students and collaborators.
2. Communicate appropriately and effectively with lab colleagues topics such as latest research findings/results within the group and field.
3. Build internal contacts and participate in internal networks for the exchange of information and to form relationships for future collaboration.
4. Travel to, and present at scientific meetings and work in collaborative laboratories when necessary.
5. Join external networks to share information and ideas and help develop and maintain external collaborations, as appropriate.
6. Contribute to the School's outreach programme by developing links with local community groups, industries etc.

ESSENTIAL CRITERIA:

1. Have or be about to obtain a PhD in computational chemistry, computational biophysics, molecular modelling, computer-aided drug design or a closely related area.
2. At least 3 years recent research experience in computational chemistry or related field with proficiency in molecular simulation and molecular docking methods.
3. Strong background in structure-based ligand design methods.
4. Proficiency in at least one standard scientific package, i.e. Schrodinger Small Molecule Drug Discovery suite, OpenEye or MOE.
5. Proficiency in at least one MD simulation program, i.e. NAMD, Gromacs, Amber or ACEMD.
6. Experience in molecular docking: Glide, Autodock, Dock and etc.
7. Experience with high-performance computing.
8. Recent high-quality original research publications in reputable peer-reviewed journals, commensurate with career stage.
9. Methodical approach to project & data management and meticulous in regards to computational and safety procedures and record keeping.
10. Ability to contribute to broader management and administrative processes.
11. Contribute to the School's outreach programme by links with industry, community groups etc.
12. Knowledge of molecular dynamics simulations of membrane proteins.
13. Knowledge of force fields.
14. Competent in maintaining knowledge of cutting-edge of field of expertise.
15. Excellent verbal and written communication skills.
16. Competent in giving effective and informative oral and poster presentations.
17. Competent in communicating stipulated research.
18. High quality manuscript, report and abstract writing experience.
19. Highly ambitious, motivated, efficient, organised and show a commitment to, and interest in, research topic.
20. Strong ability to work from own initiative.
21. Excellent team working skills in multiple internal and external team settings.
22. Leadership qualities.
23. Excellent problem-solving skills.
24. Demonstrable intellectual ability.
25. Ability to assess and organise resources.
26. Must be willing to travel to national and international meetings and collaborative laboratories.

DESIRABLE CRITERIA:

1. Experience in modelling of GPCRs.
2. Experience in scripting language for specific tasks.
3. Experience in virtual screening.
4. Experience in machine learning.
5. Experience in using and maintaining Linux supercomputer network environment.
6. Productive PhD/postdoctoral experience as evidenced by a strong publication record commensurate with career stage.
7. Experience in teaching/supervising/mentoring postgraduate/undergraduate/school students and visiting researchers in the laboratory.
8. Experience in teaching lab members as well as undergraduate lectures/tutorials/practicals.
9. Ability to prioritise research and experiments in order to meet deadlines and targets.
10. Research project management skills.
11. Experience working in outreach settings.
12. Up-to-date knowledge of fields of computational chemistry and GPCR pharmacology.
13. Knowledge of chemoinformatics techniques.
14. High quality grant writing experience.