

## Candidate Information

<b>Position:</b>	Research Fellow in Molecular Modelling
<b>School/Department:</b>	School of Pharmacy
<b>Reference:</b>	19/107968
<b>Closing Date:</b>	Thursday 2 January 2020
<b>Salary:</b>	£33,797 - £34,804 per annum
<b>Anticipated Interview Date:</b>	Wednesday 15 January 2019
<b>Duration:</b>	19 months or until 30 September 2020 <sup>1</sup> (whichever is sooner).

### 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 study Bile Salt Hydrolase structure and function and use the gained information for structure-based drug design. Techniques will include molecular dynamics simulations (NAMD, GROMACS or AMBER), enhanced sampling simulations, 3D-GRID-based analysis, docking, scoring, virtual screening, substructure search, machine learning and 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 experimental chemists and biologists 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 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 about to obtain a PhD in computer-aided drug design or a closely related area.
2. At least 3 years recent research experience in computer-aided structure-based drug design.
3. Strong background in structure-based ligand design methods.
4. Proficiency in Schrodinger Small Molecule Drug Discovery suite and OpenEye.
5. Proficiency in at least one MD simulation program, i.e. NAMD, Gromacs, or Amber.
6. Experience in structure-based virtual screenings.
7. Recent high-quality original research publications in reputable peer-reviewed journals, commensurate with career stage.
8. Ability to prioritise research and experiments in order to meet deadlines and targets.
9. Methodical approach to project & data management and meticulous in regards to 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 structure-based virtual screening protocols.
13. Competent in maintaining knowledge of cutting-edge of field of expertise.
14. Excellent verbal and written communication skills.
15. Competent in giving effective and informative oral and poster presentations.
16. Competent in communicating stipulated research.
17. High quality manuscript, report and abstract writing experience.
18. Highly ambitious, motivated, efficient, organised and show a commitment to, and interest in, research topic.
19. Strong ability to work from own initiative.
20. Excellent team working skills in multiple internal and external team settings.
21. Leadership qualities.
22. Excellent problem-solving skills.
23. Demonstrable intellectual ability.
24. Ability to assess and organise resources.
25. Must be willing to travel to national and international meetings and collaborative laboratories.

#### **DESIRABLE CRITERIA:**

1. Experience in modelling of enzymes.
2. Experience in scripting language for specific tasks.
3. Experience in machine learning.
4. Experience in using and maintaining Linux supercomputer network environment.
5. Experience in teaching/supervising/mentoring postgraduate/undergraduate/school students and visiting researchers in the laboratory.

6. Experience in teaching lab members as well as undergraduate lectures/tutorials/practicals.
7. Research project management skills.
8. Experience working in outreach settings.
9. Up-to-date knowledge of fields of computational chemistry.
10. Knowledge of chemoinformatics techniques.
11. High quality grant writing experience.