COMPUTATIONAL MODELLER

ABOUT RXCELERATE

The RxCelerate group is an out-sourced drug development platform and is one of the fastest growing companies in the UK. We design and deliver complete drug development programs and project management for our clients, from inception through to Phase II clinical studies, offering services to the pharmaceutical industry across small molecule and biologic development. Our team is dedicated to applying the most innovative methods to accelerate drug discovery paradigms.

THE ROLE

We are currently looking to recruit a computational modeller to expand our group. Computational design is at the forefront of our approach, driving projects with innovative methodologies and solving challenging problems for our clients. As part of our success and continued expansion, we are looking to add a new member to our in-silico discovery team.

The team designs both small molecules and biologics, often on completely novel targets, which require an appetite for the application and development of innovative methods to achieve project goals.

In the role of computational chemist or protein modeller you will be involved in a variety of scientific activities and will have a significant degree of input into any project you work on. It is important that you are self-motivated and have the determination to solve complex problems whilst working as part of team.

Key requirements

- You will ideally have a PhD or MSc with a chemistry background
- >1 years relevant commercial experience including some hands on protein modelling and/or ligand design; a drug discovery background gained within a pharmaceutical company or a CRO is preferred, however an academic only background with strong credentials in development and application of novel methods will also be considered, as long as you can demonstrate the ability to design/optimise either proteins or ligands.

- You will be able to apply protein homology modelling procedures and understand applicability of relevant techniques and approaches, especially for sequences of low identity to structural template
- Use and proficiency of a programming language such as Python and libraries such as RDkit an advantage
- Excellent time management skills
- Excellent communication (both verbal and written) and organisational skills
- Proven ability to work as part of a team of people with diverse skills and scientific backgrounds

and

- Use of MOE program and SVL language a significant advantage.
- Use of molecular dynamics using AMBER, GROMACS or NAMD and critical analysis of outputs and methodologies an advantage.
- Experience of alchemical methods an advantage
- Familiarity with HPC and GPU implementations a distinct advantage
- Experience of modelling membrane bound systems an advantage

or

- You will have hands-on experience of antibody modelling and understand what features of antibodies can be optimised using in silico techniques
- Use of Rosetta program a significant advantage

This is a challenging and rewarding role for which all applicants with an appropriate scientific background are encouraged to apply.

RxCelerate offers a competitive salary with an annual bonus scheme and company benefit package.

Application process

When applying for this role, please include a cover letter outlining how you meet the competencies described above. Interested applicants should send a cover letter and curriculum vitae in PDF format to careers@rxcelerate.com by Friday 28th May.

Informal enquires can also be directed to this email address. Applicants must be eligible to work in the UK. No agencies please.