



Offer Description:

We are seeking a computational chemist with solid background on molecular simulations eager to pursue/consolidate a career in structure-based drug discovery. The work involves target assessment (druggability analysis), hit identification (virtual screening), establishing structure-activity relationships and supporting a multidisciplinary team in the identification of clinical candidates.

Essential Requirements:

The ideal candidate holds a PhD, optionally with 2-3 years of post-doc experience, has a solid theoretical understanding of molecular recognition (protein-ligand association, protein folding), demonstrated experience in the use of molecular dynamics and is skilled in programming/scripting tools that ensure reproducibility and efficiency. Advanced analytical and critical problem-solving skills are essential.

The ability to deal with multiple tasks and deliver results in a timely manner is essential. Equally important, the selected candidate will be able to work effectively in a multidisciplinary team, will be proactive in the identification of tasks to support the project and will communicate the results in a clear and effective manner.

The following specific computational chemistry skills are considered essential. The candidate should be proficient on most of them, and will be able to master the rest in a short amount of time.

- Molecular dynamics
- Molecular docking (protein-ligand)
- MD-based free energy calculations
- Advanced method for analysis of MD trajectories (e.g. MSM, clustering)
- Experience in the use of X-ray crystallographic or cryo-EM data
- As someone familiar in the use of computers, the candidate will have excellent command of shell scripting, python programming and the use of high-performance computing environments.

Essential Requirements:

Knowledge on one or more of these specific areas is an important advantage:

- Chemoinformatics
- Machine learning
- Homology modelling
- Bioinformatics

Knowledge of adjacent scientific areas, such as structural biology, medicinal chemistry, molecular biology, pharmacology, etcetera, will facilitate the integration in multidisciplinary teams and will be considered as a plus.

We Offer:

- Full time contract. Salary will be commensurate with academic level and experience.
- Stimulating, interdisciplinary research and high-quality international scientific environment.
- Measures to reconcile work and family life.
- Eligible for Employee Referral Bonus.

To apply:

Interested candidates should send a letter of motivation, CV and two contacts that can provide references to hres@gaintherapeutics.com