

Expert Scientist, Computational Chemistry

Experience

- PhD in computational chemistry, structural biology or a related field with a minimum of 3 years of post-doctoral experience with cheminformatics, molecular modeling and medicinal chemistry concepts applied to Protein-Protein Interaction inhibition and Protein Degradation.
- Extensive working knowledge in small molecule and protein docking, structure-based design and deep understanding of protein-ligand interactions (Schrodinger, Rosetta, Discovery Studio).
- Experience in molecular dynamics simulations (AMBER, DESMOND, GROMACS) with small molecule ligands
- Experience in library design, virtual screening, hit expansion, scaffold hopping and predictive modelling.
- Experience in scientific workflow systems (Pipeline Pilot, KNIME)
- Experience with Fragment Based Drug Design or similar technologies.
- Experience in Structural Biology (X-Ray crystallography, Cryo-EM).
- Skills in managing multiple projects in different therapeutic targets with clear understanding of project needs and ensuring delivery of high-quality data with clear communication of timeline.
- Effective communication skills for working in interdisciplinary teams that include chemists, biologists and DMPK scientists.
- Experience leading research scientists as well as managing interactions with external partners, collaborators and CROs.
- Good knowledge of the drug discovery process with a proven track record of delivery to progress drug discovery projects.
- Previous experience in the pharmaceutical industry as well as bioinformatics knowledge will be highly valued.

Tasks and Responsibilities

- Take a lead role in Almirall's structural biology and computational methodologies applied to Protein-Protein Interaction modulation and Protein Degradation.
- Work closely with the drug discovery teams applying molecular modelling and cheminformatics tools in the design and optimization of bioactive compounds.
- Contribute to the development of novel methods for the design of protein degraders.
- Support hit and target identification and validation.
- Application of visualization and predictive analytical tools to help to identify next steps in the



drug discovery projects.

- Communicate research work and project deliverables to the team and management committees
- Interact with internal and external experts, academic groups and CROs to establish, manage and follow-up project and collaborations