## Research Investigator, Computational Chemistry

**Job Summary (Primary Function)**

The Research Investigator, Chemistry is responsible for structure-based drug design and cheminformatics to support ongoing medicinal chemistry projects.

**Essential Functions of The Job (Key Responsibilities)**

- Apply structure/ligand-based design, molecular docking and pharmacophore models to evaluate and improve potency of the lead compounds.
- Apply computational methods for in-silico evaluation of potential new targets.
- Implement cheminformatics solutions to support the Discovery Chemistry projects.
- Collaborate with project team members to analyze scientific data.

Qualifications (Minimal acceptable level of education, work experience, and competency)

- PhD in Computational Chemistry or related fields. Post-doctoral experience is preferred.
- Strong track record of external publications and presentations demonstrating scientific innovation in structure-based drug discovery and protein modelling is essential.
- Expertise in common computer programming and scripting languages (i.e. Python, C#, Java, etc.) is essential.
- Expertise in several computational methods, and familiarity with others is essential (docking, molecular dynamics simulations, free energy simulations, homology modeling, large scale data analysis and visualization, multi-parameter optimization, QSAR).
- Excellent communication skills and the ability to work well within a multi-disciplinary team are required.

Disclaimer: The above statements are intended to describe the general nature and level of work performed by employees assigned to this job. They are not intended to be an exhaustive list of all duties, responsibilities, and qualifications. Management reserves the right to change or modify such duties as required.