



## **Chemoinformatics Scientist**

### **Responsibilities:**

Construct new compound libraries for the company's screens  
Assist in ligand-based optimization approaches by using ADME predictors and SAR rationales  
Determine the binding modes of leading compound/s to the biological target of interest  
Conduct target-based optimization cycles of Hits, Advanced Hits and Leads in the company's pipeline  
Bring-in or help to develop/test new tools & technologies aimed to improve the computational capabilities of the chemistry team

### **Requirements:**

MSc or PhD degrees in Computational Chemistry/ Chemoinformatic (mandatory)  
Deep knowledge about Chemoinformatic and SAR tools Computational ADME-Tox profiling knowledge  
Experience in optimizing compounds within Hit development campaigns  
Knowledge about Structural biology/biophysics (advantage)  
Knowledge about protein modelling & MD simulations (advantage)  
Knowledge about protein-ligand interactions (advantage)  
Industrial experience of 3+ years or alternatively a postdoctoral experience (advantage)

CV TO: [jobs1@stepup-hr.com](mailto:jobs1@stepup-hr.com)