

CRELUX, part of WuXi AppTec HitS, is a global provider of structure based drug discovery solutions.

We have been delivering customized and integrated services in drug discovery, X-ray crystallography, protein supply, biophysical analysis, fragment and DNA-encoded library screenings, to support small and large molecule, as well as biopharmaceutical drug discovery, for more than a decade. Our mission is to enable our clients to perform their work faster, more efficiently and more successfully. Integrating the comprehensive portfolio of services offered by our parent company WuXi AppTec, CRELUX offers a unique opportunity for our collaborators to accelerate discovery activities.



Scientist / Senior Scientist Computational Chemistry

Role

WuXi AppTec HitS has three locations – Shanghai, Boston and Munich. Our site in Munich is looking to strengthen and expanding the medicinal chemistry team with a **PhD in computational chemistry** for a **full-time** position and **immediate entry**. The HitS team is offering hit identification services, specifically fragment screening and DEL-screening. DNA-Encoded Library (DEL) screening is a technology that enables fast screening of billions of small molecule compounds for drug discovery in a single tube.

You will play a key role in communicating screening results to project teams. You will become an expert in analyzing DEL screening data. You will support the design of compounds in our fragment based drug discovery projects together with experts in medicinal chemistry and crystallography. You will collaborate with a range of departments around the world, including biophysics, crystallography, and screening groups. You will help to develop protocols and best practices for data analysis.

Responsibilities

You will

- collaborate with colleagues around the world
- perform data analysis of screening results, perform cleaning and curation of data sets and do visualizations
- communicate data analysis with our partners (in English)
- support medicinal chemistry with cheminformatics and structure based activities
- play a key role in project teams to help ensure successful hit identification and lead optimization campaigns in drug discovery projects

Required Skills

You

- have a PhD (or equivalent) in organic chemistry with a focus in medicinal chemistry or computational chemistry
- have knowledge of the principles of medicinal chemistry
- are familiar with methods and software to perform modern structure based and ligand based modelling techniques
- can perform cheminformatic analysis tasks and you are familiar with the calculation of physchem properties
- have hands-on experience with Python and RDKit
- have the ability to analyze large data sets (including the cleaning and curation of data as needed)
- can easily communicate orally and in writing in English

We offer

A permanent contract of employment as well as an exciting and wide-ranging job in an international, innovative environment of pharmaceutical contract research.

Are you interested?

We look forward to receiving your detailed application by email, with a cover letter and a current CV, stating your desired salary and the earliest possible starting date, to our human resources department, Ms Evelyn Frey-Royston, Email: crelux_office@wuxiapptec.com.