



Innovative medicines for people and animals have for more than 130 years been what the research-driven pharmaceutical company Boehringer Ingelheim stands for. Boehringer Ingelheim is one of the pharmaceutical industry's top 20 companies and to this day remains family-owned. Day by day, some 50,000 employees create value through innovation for the three business areas human pharmaceuticals, animal health and biopharmaceutical contract manufacturing. In 2016, Boehringer Ingelheim achieved net sales of around 15.9 billion euros. With more than three billion euros, R&D expenditure corresponds to 19.6 per cent of net sales.

Post Doc in Computational Chemistry

Note: To make it easy to find our job postings we use the customary title "post doc". Of course, this posting is not only addressed to applicants directly after completing their doctorate but to all qualified candidates. A postdoctoral research position is available in the Computational Chemistry group at our research site in Biberach. The Computational Chemistry group is part of the Medicinal Chemistry Department interacting closely with colleagues in Medicinal Chemistry, Structural Research, Screening and Profiling, Screening Logistics as well as Pharmacology and Computational Biology. We want to advance our method portfolio for investigating and predicting protein-ligand complex formation with respect to covalent binders. This vacancy is limited for 2 years.

<https://tas-boehringer.taleo.net/careersection/global+template+career+section+28external29/jobdetail.ftl?job=178952>

Tasks & Responsibilities

- As a postdoctoral scientist you develop and apply computational protocols for predicting protein-ligand complex formation, focussing on covalent binders.
- You will work closely with computational chemists, medicinal chemists and colleagues from structural biology by applying novel protocols predicting protein-ligand interactions. These protocols include the analysis of protein binding pockets, estimation of binding pocket drugability for covalent binders, and calculation of reactivity of ligand functional groups.

Requirements

- PhD in computational chemistry or related field (chemistry, pharmacy, theoretical chemistry, chemoinformatics, biophysics)
- Strong programming skills (preferably python)
- Familiarity with Unix/Linux and HPC environments
- Familiarity with the basic concepts of covalent binders
- Experience with the analysis of protein-ligand interactions, docking, binding mode prediction of ligands
- Experience with molecular dynamics simulations and/or quantum mechanics. Skills in reactivity assessments and reaction mechanism elucidation will be a plus
- Fluency in written and spoken English

Contact

For further information please contact Recruiting Services: Agnes Woyke, Tel: +49 (7351) 54-141 408

Boehringer Ingelheim is an equal opportunity employer who takes pride in maintaining a diverse and inclusive workplace. We embrace all aspects of diversity and inclusion which benefit our employees, patients and communities. We look forward to receiving your online application. **Job ID: 178952**
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