# Postdoctoral Fellow in structure-based drug design by NMR





Location: Heidelberg, Germany Staff Category: Postdoctoral Fellow

Contract Duration: 2 years Grading: N/A

Closing Date: 19 February 2012 Reference number: HD\_00183

## Job Description

The European Molecular Biology Laboratory (EMBL) is one of the highest ranked scientific research organisations in the world. The Headquarters Laboratory is located in Heidelberg (Germany) and the outstations are in Grenoble (France), Hamburg (Germany), Hinxton (UK) and Monterotondo (Italy).

We welcome applications for one post-doc position in the group of Biomolecular NMR Spectroscopy in the Structural and Computational Biology Unit at the EMBL in Heidelberg in collaboration with AstraZeneca. The aim of the research is to develop and validate new approaches to describe the binding mode of organic ligands to a macromolecular target protein without the use of crystallographic data. The post-doctoral fellow will work at the development of a novel strategy to determine the pharmacophore superimposition of multiple competitive ligands from NMR experiments that use the ligands' signals as reporters. The methodology is based on high-throughput modeling guided by NMR data and does not require structural information for the receptor protein.

Travelling between the EMBL site in Heidelberg and the AstraZeneca sites in Sweden and in the United Kingdom, as well as exchange of the results between the academic and industrial partners will be an integral part of the job. The post-doctoral fellow will be based at the EMBL in Heidelberg and will visit the AstraZeneca sites for about 20% of the time.

## **Qualifications and Experience**

Applicants should hold a Ph.D degree and should have received outstanding training in NMR spectroscopy including a solid theoretical background. Experience in modeling of intermolecular interactions will be considered as a bonus. A solid publication record, strong motivation and excellent scientific skills are essential, as well as willingness to work in a team. Due to the collaborative nature of this project outstanding communication skills and open mindedness are central to the job.

# **Application Instructions**

Please apply online through www.embl.org/jobs

### **Additional Information**

EMBL is an inclusive, equal opportunity employer offering attractive conditions and benefits appropriate to an international research organisation.

Please note that appointments on fixed term contracts can be renewed, depending on circumstances at the time of the review.

### Facts:

The NMR facility at the EMBL features a 800 MHz and a 600 MHz spectrometer, both equipped with

cryoprobes, and a 700 MHz spectrometer equipped for solid-state NMR. In the Structural and Computational Biology Unit a broad range of techniques, such as X-ray crystallography, single particle electron microscopy, EM tomography, single molecule light microscopy and molecular modeling, are used to describe biological systems at various levels of spatial and temporal resolution. Excellent resources (2000 core cluster) and extensive expertise are available in the area of computation. The EMBL offers excellent opportunities for training in a multicultural and interdisciplinary environment.

AstraZeneca is a major international healthcare business engaged in the research, development, manufacture and marketing of prescription pharmaceuticals and the supply of healthcare services. AstraZeneca has a unique workplace culture that inspires innovation and collaboration. The biomolecular NMR facilities at AstraZeneca features several high field spectrometers (600 and 800MHz) equipped with cryoprobes. The spectrometers are fully automated with sample preparation robots. Biomolecular NMR is highly integrated with other biophysical techniques such as X-ray crystallography, ITC and SPR as well as groups working with computational chemistry and protein expression and purification. The main hubs for Structural Chemistry at AstraZeneca are located in Mölndal, Gothenburg, Sweden and Alderley Park, Manchester, UK.