

Applications are invited for a **PhD student position** in the Computational Pharmaceutical Chemistry & Molecular Bioinformatics group (Prof. Dr. Holger Gohlke; <http://cpclab.uni-duesseldorf.de>) at the Heinrich-Heine-University, Düsseldorf, Germany.

PhD student position (available 1.10.2019): Development of novel modulators for the nicotinic acetylcholine receptor for the treatment of nerve agent poisoning

Nicotinic acetylcholine receptors play an important role in cholinergic neurotransmission. Thus, a malfunction of these receptors can quickly reach life-threatening proportions by paralysis of the respiration. Such a malfunction can be caused by nerve agent poisoning, leading to accumulation of acetylcholine, thereby desensitizing the receptor and causing a non-functional state. Active ingredients for elimination of desensitization of nicotinic acetylcholine receptors therefore are of great importance for the treatment of nerve agent poisoning.

As shown in *in vivo* and *in vitro* experiments, there are some substances from the group of bispyridinium salts capable of desensitizing nicotinic acetylcholine receptors, or if it occurred already, to bring back receptors to a functional state (i.e., "resensitize"). However, because of their low potency, such substances are currently not suitable for therapy.

The goal of the project is to develop active ingredients that have a sufficiently high potency and, in addition, drug-like properties, such that they can be used as antidotes for the treatment of nerve agent poisoning.

The project will be performed in close collaboration with experimentalists at LMU Munich.

Requirements: Ideal candidates will have a record of excellence and a strong background in computational (bio)chemistry, molecular informatics, and computational structural biology as well as a high interest in working in an interdisciplinary research field, and profound knowledge in state-of-the-art molecular dynamics simulations (Amber) software and molecular modeling.

How to apply: Applicants should submit applications (a one-page letter of motivation *why* they are interested in the respective project and *how* they can contribute to the project's success, a current CV, and contact data of three references) by email to gohlke@uni-duesseldorf.de . **Please provide all documents as one PDF file and specify for which position you are applying.**

Detailed **information about living and studying in Düsseldorf** is provided here: <http://www.uni-duesseldorf.de/home/leben-in-duesseldorf.html>