

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](mailto: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>