Applications are invited for a **PhD student position available 1.12.2019** in the Computational Pharmaceutical Chemistry & Molecular Bioinformatics group (Prof. Dr. Holger Gohlke; http://cpclab.uni-duesseldorf.de) at the Heinrich-Heine-University, Düsseldorf, Germany.

TOPIC: Enzymatic halogenation: enzyme identification, characterization, application

Background: Organohalogen moieties occur frequently in pharmaceuticals and agrochemical products as halogen insertion can improve compound properties, including bioactivity. However, traditional synthetic halogenation methods are complicated by a lack of specificity and regioselectivity and/or require toxic and environmental-harmful halogen sources. Therefore, methods for the facile, selective, and environmental-friendly installation of halogen-substituents are required.
This project addresses this demand within the realm of the Bioeconomy Science Center (BioSC, https://www.biosc.de/): It aims at identifying, characterizing, and utilizing novel halogenase enzymes from secondary metabolism of algae, that way introducing a novel strategy for exploiting natural resources towards halogenating enzymes and leading to the development of novel synthetic methods for the creation of new compounds with enhanced functions.
The PhD student will engage in structure prediction, active site characterization, halogenase classification, prediction of substrate scope and selectivity, and identification of suitable halogenases for a halogenase toolbox as well as in the prediction of halogenated, pyrazolidine-dione-based C4 plant-specific herbicides as an application.

Requirements: Ideal candidates will have a record of excellence (Master degree in chemistry, biochemistry, biophysics, (structural) biology) and a strong background in computational biochemistry/chemistry or structural bioinformatics, a high interest in working in an interdisciplinary collaboration, and profound knowledge in state-of-the-art molecular modeling (OpenEye, Schrödinger) and molecular dynamics simulations (Amber) software.

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