

Applications are invited for a **Postdoc position available on 1.7.2022** in the Computational Pharmaceutical Chemistry & Molecular Bioinformatics group (Prof. Dr. Holger Gohlke; <http://cplab.uni-duesseldorf.de>) at the Heinrich-Heine-University, Düsseldorf, Germany.

TOPIC: Continuous, stable processes for the sustainable enzymatic production of chiral amino alcohols integrating downstream processing

Background: In MetaProcess, we will use a multidisciplinary approach to generate stable carboligase and transaminase variants, able to withstand repetitive batch/continuous production of amino alcohols, such as metaraminol and methoxamine, on a longer time scale. Rational design and directed evolution will be used to identify optimized variants, which will be integrated into a comprehensive industrial workflow for chiral amino alcohol production. The developed platform will be evaluated through techno-economic analysis and a life cycle assessment (LCA), identifying parameter sensitivities and evaluating sustainability and economic feasibility.

This project addresses this demand within the realm of the Bioeconomy Science Center (BioSC, <https://www.biosc.de/>), which integrates highly diverse research disciplines and bundles high-level scientific expertise into a single integrative approach.

The Postdoc will engage in rational design to improve the molecular stability of the involved biocatalysts, assessing intramolecular and solvent effects and applying state-of-the-art computational biophysical chemistry approaches such as rigidity theory to identify structural weak spots within the proteins. From the obtained molecular knowledge, new variants will be proposed and integrated into the continuous reaction mode.

Requirements: Ideal candidates will have a record of excellence (PhD in chemistry, biochemistry, biophysics, (structural) biology) and a strong background in computational biochemistry/chemistry or structural bioinformatics, a high interest in working in 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>