

The core competence of the research group of Prof. Schwaneberg (<http://www.biotec.rwth-aachen.de/>) is the evolutionary and rational design of proteins. Our projects range from basic research to elucidate structure-function relationships and their modeling, methodological developments for Directed Evolution and optimization of biocatalysts for industrial production and peptides as materials for medical applications.

Master Thesis: Computer simulations of biocatalysts in non-aqueous solvents

Description:

Understanding the influence of nonaqueous solvents on biocatalytic reactions is important for the engineering of enzymes to efficiently operate in such media. Gaining molecular insights into the protein interaction on nonaqueous solvents will provide information to guide computer assisted rational protein engineering. Molecular modeling methods are effective tools to address the atomistic detail of solvation mechanism that would be difficult to study experimentally. The main aim of this project is to use a range of tools from computer simulations techniques including computational protein engineering, molecular simulations, to big data and statistical analysis to shed light on the nature of non-aqueous solvent effects on biocatalysts. This work is carried out in a close collaboration within experimental researchers in the group.

Qualifications

- Master student (m/f) in the field of biotechnology, biology, chemistry, physics, computer science, etc.
- Confident in using the usual MS Office-programs
- Good knowledge in English (spoken and written)
- High motivation, flexibility, creativity, team-, organizational- and communicational skills
- Previous experience with molecular modeling will be an advantage, but is not a prerequisite
- Programming experience is welcome, but is not essential
- The candidate with special interest in computer simulations of molecular systems (computational or theoretical biology and chemistry)

What we offer /Techniques you will learn:

In this project, the theoretical and computational knowledge in the field of computational and structural biotechnology methods and tools including protein structure design and modeling, molecular dynamics simulations, bio- and chemo-informatics analysis, statistical data analysis, protein biochemistry and enzymology will be gained. The candidate will enjoy working in an open and dynamic environment and cooperate actively with experimental collaborators.

Estimated time: According to "Studienordnung"

Deadline: applications will be considered until the position is filled

Contact person:

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