

UniCat Colloquium

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Lecturer: **Prof. Uwe T. Bornscheuer**, Ernst-Moritz-Arndt-University, Dept. of Biotechnology & Enzyme Catalysis, Institute of Biochemistry, Greifswald, Germany

Title: Protein Engineering on the Move from Directed Evolution to in Silico Approaches

Abstract: Protein engineering has developed in the past decade to a highly important technology as it is a useful tool to create enzymes with desired properties (with respect to e.g., substrate specificity, stereoselectivity or thermostability), but also helps to understand how proteins evolved and how they function.

Whereas initially rational protein design based on detailed analysis of three-dimensional structures was the method of choice, directed evolution – in essence a random mutagenesis followed by screening or selection of desired mutants – became an important alternative. More recently, researchers used combinations of both methods. In this lecture, the principle strategies and current challenges in protein engineering will be highlighted. Examples will include the creation of an epoxide hydrolase from an esterase scaffold within the α/β -hydrolase fold enzyme family and the inversion of enantioselectivity of an esterase active towards sterically demanding tertiary alcohols. In addition, we developed a method for in vivo selection and cell sorting to identify enantioselective enzymes.

The vast number of protein sequences available from databases substantially facilitates protein engineering. We used this plethora of information to develop a method for an "*in silico* neutral drift" based on the analysis of >2.800 sequences of enzymes from the α/β -hydrolase fold family using the 3DM database. This resulted in 'small, but smart' focused protein libraries, from which enzyme variants with substantially enhanced thermostability, enantioselectivity and altered substrate range could be identified Finally, a detailed *in silico* analysis enabled the identification of a toolbox of novel (*R*)-selective transaminases.

 Date:
 Wednesday, 13 June 2012

 Time:
 5:15 pm - around 6:45 pm

Location: TU Berlin, Department of Chemistry Straße des 17. Juni 115, 10623 Berlin Building C, Lecture Hall C 264

Organiser: Prof. Nediljko Budisa (TUB) and Prof. Roderich Süßmuth (TUB)

Coffee and tea will be served thirty minutes prior to the lecture start. Guests are cordially invited to attend!

Prof. Dr. Matthias Driess, Chair of the Cluster of Excellence UniCat