Enzyme function - much to understand, optimize, and discover

Enzymes are powerful biocatalysts. However, there is still a large gap between the number of enzyme-based practical applications and that of naturally occurring enzymes. An increasing number of computational methods have been developed in the fields of structural bioinformatics and computational biophysical chemistry that assist in a structure-based manner in the analysis and modification of enzymes towards better properties.

Here, we introduce such methods from our own work, covering areas of protein structure prediction, analysis of substrate specificity and promiscuity, solvent stability, as well as improvement of enantioselectivity and thermostability.

Chair: Prof. Matthias Rarey

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