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Challenges in modelling of biocatalytic reactions

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Enzymes are promising catalysts for a wide range of biocatalytic processes. Because protein engineers still lack a deep molecular understanding of biocatalytic systems, finding the optimal biocatalyst is time consuming, and trial-and-error strategies are widely used.

A more directed rational design strategy responds to three challenges. Although enzyme-substrate interactions are successfully modelled by molecular simulation and experimental data are successfully modelled by macroscopic ODE based models of enzyme kinetics, both modelling methods are separated by many orders of length and time scales. Therefore, the major challenge is to bridge the gap between molecular and kinetic modelling. The second challenge is a holistic model, which includes reaction conditions. Kinetic models describe the reaction medium by adjustable parameters and can therefore become complex. In contrast, molecular simulation allows for the reliable prediction of thermophysical properties of mixtures from first principles. The third challenge is data management. Due to high-throughput experimentation techniques for biocatalytic experiments, enzyme data is rapidly growing, complex, and unstructured. Making big biodata accessible to data mining and modelling is widely seen as a major bottleneck to the digitalization of industrial biotechnology, and rules for data management such as the FAIR data principles or the STRENDA recommendations are increasingly accepted by the scientific community.