

Seminar title: IntEnzyDB: An Integrated Structure-Kinetics Database for Enzymes

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Abstract:

Identification of efficiency-enhancing enzyme mutations is significant for biocatalysis and biomedicine research but remains as a holy-grail challenge in computational chemistry and biology. Data-driven modeling presents a promising strategy to map sequence-structure-function relationships for enzyme catalysis and to inform catalyst-optimization strategies. However, collecting and cleaning structure and kinetics enzymology data are still very difficult. In this talk, I will introduce our ongoing efforts to construct an integrated structure-kinetics database, IntEnzyDB, which contains experimentally characterized enzyme structure and kinetics data. I will discuss the architecture of the database that enables efficient data processing. I will also talk about the use of the database for statistical profiling of rate/efficiency-enhancing mutant hydrolases with single amino acid substitution.