

COMPUTATIONAL REDESIGN OF FUNCTIONAL ENZYMES

Bian Wu, Institute of Microbiology, Chinese Academy of Sciences
wub@im.ac.cn

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Rising demands for enzymes in biotechnological applications have fueled efforts to tailor their properties towards desired functions, such as activity, selectivity, and stability. Computational methods are increasingly used in this task, providing designs that efficiently navigate large regions of sequence space with a greatly reduced experimental burden. With the improvement of enzyme redesign algorithms, model-based methods have achieved significant success in recent decades. Meanwhile, the rapid growth in protein databases has also promoted the development of data-driven approaches. In this talk, we provide a brief overview of the field of computational enzyme redesign and present the latest examples of using computational methods to create enzymes for real-world applications. We anticipate a marriage between model-based and data-based approaches which may offer opportunities to achieve more ambitious enzyme engineering goals in the coming years.