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Prof. David Baker

Institute for Protein Design (IPD) University of Washington, Seattle, USA



Protein Design Using Deep Learning

Proteins mediate the critical processes of life and beautifully solve the challenges faced during the evolution of modern organisms. Our goal is to design a new generation of proteins that address current-day problems not faced during evolution. In contrast to traditional protein engineering efforts, which have focused on modifying naturally occurring proteins, we design new proteins from scratch to optimally solve the problem at hand. We now use two approaches. First, guided by Anfinsen's principle that proteins fold to their global free energy minimum, we use the physically based Rosetta method to compute sequences for which the desired target structure has the lowest energy. Second, we use deep learning methods to design sequences predicted to fold to the desired structures. In both cases, following the computation of amino acid sequences predicted to fold into proteins with new structures and functions, we produce synthetic genes encoding these sequences, and characterize them experimentally. In this talk, I will describe recent advances in protein design using both approaches.

Zoom link: https://desy.zoom.us/j/66630756955

Meeting ID: 666 3075 6955 Password: 138110



Host: Paul L Xavier and Henry N Chapman / FS-CFEL-1 Coherent Imaging Division