COMPUTATIONAL DESIGN OF REPROGRAMMED AND NEW PROTEIN FUNCTIONS

Tanja Kortemme, University of California San Francisco (UCSF), CA, USA
kortemme@cgl.ucsf.edu

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There has been exciting progress in the computational design of proteins with new structures and functions, highlighting the potential to advance many applications in biological engineering, as well as to provide insights into the design principles of function. Many significant challenges remain, both in the accuracy of current computational approaches, and in the complexity of functions that can be designed at present. I will discuss our recent progress with computational methods and describe new approaches and their applications, including reshaping of protein active sites for new functions. Most recently, we utilized computational design to engineer new small-molecule binding sites into protein-protein interfaces. The designed proteins function as sensor/actuators that detect and respond to new small molecule signals in living cells.