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Protein structure prediction and protein design

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Abstract:

Protein structure prediction aims to determine spatial location of every atom in protein molecules from the amino acid sequence by computational simulations, while protein design is a reverse procedure of protein structure prediction that aims to engineer novel protein sequences with desirable structure and function. In this talk, I first review recent progress in computer-based protein structure prediction, and show that a new approach combining template-based modeling and *ab initio* folding can break though the barrier of physics-based protein folding and resulted in folding of proteins larger than 150 residues in the community-wide blind CASP experiments. Next, we introduce an evolutionary based approach to engineer new functional XIAP (X-linked Inhibitor of Apoptosis Protein) BIR3 domains that bind Smac peptide but not inhibit caspase-9 activity, representing a new therapeutic potential to change the caspase-9 initiated apoptosis pathway through computational protein design.

Biography:

Dr. Yang Zhang is a professor in the Department of Computational Medicine and Bioinformatics and the Department of Biological Chemistry, University of Michigan. He serves as the Associate Chair for Research in the Department of Computational Medicine and Bioinformatics. The research interest of Dr. Zhang's Lab is in protein structure prediction and protein design. The I-TASSER algorithm developed in his lab was ranked as the No 1 method for automated protein structure prediction in the worldwide CASP competitions in 2006, 2008, 2010, and 2012. He is the recipient of the US National Science Foundation (NSF) Career Award in 2008, the Alfred P Sloan Award in 2008, and the Dean's Basic Science Research Award in 2013.