

SEMINAR ANNOUNCEMENT: Wed, Oct 26 at 3:30 pm

OH 123

Dr. Yang Zhang, University of Michigan

Protein structure prediction and protein design

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



Yang Zhang
Department of Biological
Chemistry
Department of
Computational Medicine
and Bioinformatics
University of Michigan