Using protein design to dissect the form and function of biological networks

I will discuss recent applications of the Rosetta protein structure prediction and design platform to understanding genomes. There are two main ways we can use structural bioinformatics to aid in the building of genome wide models: 1) providing predictions about the structure, function and interaction of proteins, and 2) designing new molecules that can be used as tools to specifically perturb individual functions and interactions. In this talk I will primarily focus on the design of new tools. I will describe our recent efforts to accurately predict temperature sensitive mutations that can be used to investigate the effects of essential genes. I will also describe our efforts to include non-cannonical amino acids and non-canonical backbone structures (such as N-branched side chains, peptoids) in the design of peptidomimetics that target specific protein-interactions. All protocols for prediction and design are seamlessly integrated into the Rosetta package and available at the Rosetta-commons: http://www.rosettacommons.org/