CAPRI – a versatile and community-wide blind experiment in atomic-detail protein docking

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Most cellular functions are performed by physically interacting proteins. The atomic-detail characterization of these interactions is of prime importance to biological understanding and the topic of computational protein docking. The CAPRI experiment is a community-wide effort aimed at the improvement of protein-protein docking algorithms and has proven to act as a catalyst therein since the early 2000's, through the organization of blind prediction trials.

With the increase in computing power, recent years have seen a rise in the use of physics-based methodologies, and this with encouraging results. Few docking algorithms however, account for the presence of water molecules. Nevertheless individual soluble proteins are surrounded by a first shell of water molecules that show different behavior from bulk water. These water molecules influence protein motion and therefore the process of binding.

In CAPRI, models are assessed using measures that account for the quality of the predicted protein-protein interface and global ligand positioning. Two additional quantities have recently been added, to account for side-chain positioning and interfacial water molecules.

I will give an overview of the CAPRI experiment, and discuss these issues.