

**Speaker:**

Andrey Sali

**Title:**

Integrating Diverse Data for Structure Determination of Macromolecular Assemblies

**Abstract:**

To understand the workings of the living cell, we need a detailed description of the architectures of its macromolecular assemblies. We show here how proteomic data can provide a rich source of structural information that can be integrated into realistic representations of such assemblies. The process involves collection of sufficient and diverse high-quality proteomic data, translation of this data into spatial restraints, and an optimization that uses these restraints to generate an ensemble of structures consistent with the data. Analysis of the ensemble produces a detailed architectural map of the assembly. We developed our approach using the nuclear pore complex (NPC), which acts as a dynamic barrier to control access to and from the nucleus. The NPC is a large (~50 MDa) and flexible proteinaceous assembly, thus presenting a challenging model system. Our resulting structure reveals the configuration of the proteins in the NPC, and provides insights into the evolution and architectural principles of this assembly. The present approach should be applicable to many other macromolecular assemblies.