Computational design of protein/peptide self-assembly

Ingemar André
Biochemistry & Structural Biology, Lund University, Lund

Large protein complexes carry out some of the most complex functions in biology. Such structures are often assembled spontaneously from individual components through the process of self-assembly. By coupling the powerful design template of self-assembly with computational protein design we can engineer new protein assemblies with custom-made structure and function. I will describe three denovo-designed protein/peptide assemblies created using this approach: A Leucine Rich Repeat Protein with predefined geometrical shape, a peptide fiber with a unique subunit fold and a higher order coiled-coil with a pH dependent oligomerization switch. I will also describe how this design approach can be applied to the engineering of more complex assemblies and touch upon some of the challenges involved in the design of self-assembling systems.