

Integrative modeling based on electron microscopy data

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Determining the atomic structure of macromolecular complexes is crucial for understanding their function and mechanism of action. Recently, revolutions in electron microscopy (EM) brought structures of numerous complexes at near-atomic resolution. However, many complexes do not achieve high resolution due to intrinsic structural flexibility. Moreover, technological advances in in situ electron tomography now enable generating EM maps of large complexes or even organelles in the cell, but at low resolution. Integrative structural modelling allows determining the structure of such complexes by integrating low-resolution EM data with data from other experiments, such as X-ray crystallography, NMR, SAXS or cross-linking mass spectrometry. During my talk, I will present an introduction to fitting atomic structures into EM maps and basics of integrative modelling of protein complexes. I will use examples from our own research on human nuclear pore complex and Elongator complex.