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## Integrative structural biology with atomic force microscopy data

*Wednesday, 14 February 2024 11:05 (25 minutes)*

Understanding the molecular and cellular function of biological molecules requires an accurate perception of their functional assemblies. The term “functional” refers to the actual structure of the bioactive molecule: it includes, but is not limited to, oligomerization, molecular partners, and their multiscale dynamics. Achieving such a functional goal requires a combination of techniques that provide details from atomic to macromolecular assembly resolution. Atomic force microscopy (AFM) provides information at nanoscale resolution (10-20 angstroms) with an exceptional signal-to-noise ratio. The output of AFM is, in the best cases, an isolated single molecular topography with nanometer resolution. We have developed tools to use AFM topographic data to assemble macromolecular systems from their constituent units. In addition, the reconstruction of flexible macromolecular systems under the experimental constraints of AFM topography allows us to study molecular dynamics at the structural unit level. Tools and applications will be presented.

### Submitting to:

Integrative Computational Biology workshop

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**Session Classification:** Protein conformational flexibility and solution experiments