Introduction: 
Integrative modeling of molecular complexes

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Ron Dror
Molecular complexes

• Proteins (and other biomolecules such as RNA) often come together to form large complexes
• Determining structures for these complexes is difficult
  – Getting a crystal is very hard
  – Electron microscopy is more feasible but often leads to low-resolution structures, where it’s not clear which blob is which protein

Nuclear Pore Complex
Alber et al., *Nature* 2007
Idea: supplement traditional structure determination methods with other forms of data

- Example: using techniques such as affinity purification or cross-linking + mass spectrometry, one can determine small sets of proteins that are in direct physical contact
- One can combine all of this information computationally to deduce structure (and in some cases, even multiple conformations) of these large complexes
Integrative modeling: combining diverse experimental data to deduce structures of large complexes
Background information

• Review article

• Software article
    • [http://dx.doi.org/10.1371/journal.pbio.1001244](http://dx.doi.org/10.1371/journal.pbio.1001244)