

20.320, notes for 10/30

Tuesday, October 30, 2012

9:31 AM

A PDB file contains x, y, & z coordinates for all the atoms in the model. PyRosetta can convert between those and the bond rotation angles for every residue in the protein. This is a much more powerful representation, because changing a single angle can move the entire protein downstream from there.

Proteins with similar structure or sequence within the same organism are called paralogues. Between different organisms, they're called orthologues. Which parts are or aren't conserved among related proteins are related to functionality. There's conservation pressure on the hydrophobic interior because that dictates folding. There are also functional constraints on any region that interacts with other proteins, due to the need to conserve that interaction.

There's plenty of diseases where we'd like to use proteins as drugs. Protein therapeutics, though are troublesome because the proteins must be injected (lest they be digested in the GI tract), they are unstable (due to proteases), and they are hard to synthesize. Regardless of these problems, though, there are plenty of reasons to try anyway. HIV, for example, is a virus whose life cycle (and getting into new cells, specifically) depends on a protein-protein interaction.

[Some parts of this lecture missing]

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