New DBP Ideas

CIBC EAB Meeting 2013

Possible DBP in Protein Modeling
Collaborators at Northeastern:

- Lee Makowski, Professor of ECE and Chemistry
- Jay Bardhan, Research Asst. Prof. in ECE
- Both have strong background in experimental and computational analysis of protein structure
- Perform regular SAXS and WAXS experiments at Argonne NL
- Particular interest in solution scattering
- Existing NIGMS support (R01, R21)
- Existing NSF grant (Makowski, Brooks, Erdogmus)
New DBP Ideas

Idea and innovation:

Simple shape-based models of protein structures:

- Can be found using fast solution scattering experiments (SAXS/WAXS)
- Identify biologically critical protein behaviors
  - Changes of shape on binding (ions, drugs, substrates, etc)
  - Flexibility and ranges of motion
  - Assembly into complex “molecular machines”
- 100X fewer unknowns than atomistic models!
- Can leverage CIBC’s rigorous, extensible computational analysis and visualization tools
Discussions started 2 weeks ago so all very preliminary

- Use meshing, shape statistics, and dynamics to characterize protein behavior
DBP Ideas

Use X-ray scattering data (SAXS/WAXS) data to capture protein / buffer behavior.

Chacon et al. ‘00
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- Match models (MD, coarse-grained) and predict/invert scattering data (crystallography, NMR, S/WAXS)
- Exploring protein fold possibilities
- Identify small shape changes during protein function
- Resolve folding dynamics with solution scattering and time-resolved measurements