

Class 18: Structure Prediction (1)

Held: Tuesday, 3 November 2009

Summary: We begin to consider computational approaches to predicting the structure of proteins.

Related Pages:

- EBoard.
- Reading: Chapter 7.

Notes:

- Fun event Saturday a.m.: Grinnell Destination ImagiNation Fun Run/Walk. More info outside my office.
- If you are registered in Powesheik county, don't forget to vote.
- Don't forget Thursday's "Thursday Extra": The Ontological domain model of medical imaging informatics. (Yes, it will be more interesting than it sounds.)

Overview:

- Protein structure: What is it and why care?
- The Chou-Fasman Algorithm
- Web exploration

Structure Prediction

- Lots of kinds of structures:
 - Primary, secondary, tertiary, quaternary
- Proteins have structure.
- RNA has structure.
- Even DNA sometimes has non-obvious structure
- Why do we care?
- Can we write programs that predict structures?
- Not perfectly (at least not yet)
- But can get some potentially useful info

The Chou-Fasman Algorithm

- Chou and Fasman provided an algorithm (well, perhaps more of a heuristic) for predicting some secondary structure:
 - alpha helices
 - beta sheets (aka beta strands)

- hairpin turns (aka beta turns)
- The algorithm is mostly statistical
 - We look at the likelihood that each amino acid participates in each structure
- Basic algorithm: We pass a “sliding window” along the sequence
 - The window selects a small number of amino acids (e.g., six)
 - When some heuristic is met (e.g., at least four amino acids out of six have a high probability of participating in an alpha helix), we expand out
 - We then apply a second heuristic to the expanded sequence

Web Exploration

- Do the Web exploration for Chapter 7.
- You can find the PSIPRED stuff at
<http://www.cs.grinnell.edu/~rebelsky/Courses/CS295/2009F/Examples/>.
- You can run Cn3D with
`/home/rebelsky/bin/cn3d`

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