



Bioinformatics Seminar

Speaker: Daniel R. Caffrey, Pfizer

Title: Are protein-protein interfaces more conserved in sequence than the rest of the protein surface?

Date: Monday, 27 September 2004

Time & Location: ***PLEASE NOTE TIME & PLACE

Refreshments: 11 am in the Theory of Computation Lab at MIT's Building 32, Stata Center Room G-575

Talk: 11:30 am the Theory of Computation Lab at MIT's Building 32, Stata Center, Room G-575

URL: <http://www-math.mit.edu/compbiosem/>

Abstract:

Protein interfaces are thought to be distinguishable from the rest of the protein surface by their greater degree of residue conservation. We test the validity of this approach on an expanded set of 64 protein-protein interfaces using conservation scores derived from two multiple sequence alignment types, one of close homologs/orthologs and one of diverse homologs/paralogs. Overall, we find that the interface is slightly more conserved than the rest of the protein surface when using either alignment type, with alignments of diverse homologs showing marginally better discrimination. However, using a novel surface-patch definition, we find that the interface is rarely significantly more conserved than other surface patches when using either alignment type. When an interface is among the most conserved surface patches, it tends to be part of an enzyme active site. The most conserved surface patch overlaps with 39% (+/- 28%) and 36% (+/- 28%) of the actual interface for diverse and close homologs, respectively. Contrary to results obtained from smaller data sets, this work indicates that residue conservation is rarely sufficient for complete and accurate prediction of protein interfaces. Finally, we find that obligate interfaces differ from transient interfaces in that the former have significantly fewer alignment gaps at the interface than the rest of the protein surface, as well as having buried interface residues that are more conserved than partially buried interface residues.

The seminar is co-hosted by Professor Peter Clote of Boston College's Biology and Computer Science Departments and MIT Professor of Applied Math Bonnie Berger. Professor Berger is also affiliated with CSAIL & HST.

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