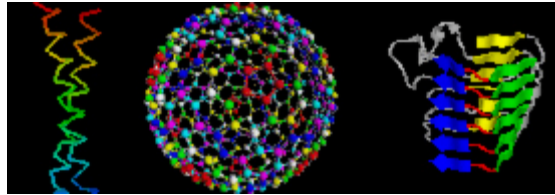


MIT
Department of Mathematics
& The Theory of
Computation Group
At CSAIL



Bioinformatics Seminar

Speaker: Matt Menke , EECS/ CSAIL, MIT

Title: Wrap-and-Pack: A New Paradigm for Beta Structural Motif
Recognition with Application to Recognizing Beta Trefoils

Date: WEDNESDAY, 10 March 2004 * *note special day*

Time & Location:

Refreshments: 11:00 am in the Applied Mathematics Common Room
at MIT's Building 2, Room 349

Talk: 11:30 am The Applied Mathematics Conference Room Building 2,
Room 338

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

Abstract:

A method is presented that uses beta-strand interactions at both the sequence and the atomic level, to predict the beta-structural motifs in protein sequences. A program called Wrap-and-Pack implements this method, and is shown to recognize beta-trefoils, an important class of globular beta-structures, in the Protein Data Bank with 92% specificity and 92.3% sensitivity in cross-validation. It is demonstrated that Wrap-and-Pack learns each of the ten known SCOP beta-trefoil families, when trained primarily on beta-structures that are not beta-trefoils, together with 3D structures of known beta-trefoils from outside the family. Wrap-and-Pack also predicts many proteins of unknown structure to be beta-trefoils. The computational method used here may generalize to other beta-structures for which strand topology and profiles of residue accessibility are well conserved.

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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