



Bioinformatics Seminar

Speaker: Jerome Waldispuhl, Ecole Polytechnique & BC

Title: Modeling and predicting the structure of transmembrane proteins

Date: Monday, 7 March 2005

Time & Location:

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:

Modeling and predicting the structure of proteins is an important challenge of computational biology. Exact physical models are too complex to be used without approximations as prediction tools and most ab-initio methods only use local information to fold a given sequence.

We show that transmembrane protein structure can be modeled with a multi-tape S-attributed grammar. An efficient structure prediction algorithm using both local and global constraints is designed, compiled by our system and evaluated. Comparison with existing methods shows that the prediction rates as well as the definition level are increased or equivalent on 124 known structures of 80 to 600 residues. The accuracy of distinguishing globular from membrane proteins has been evaluated with success on a dataset of 567 sequences. We are able to deal with both alpha-bundles and beta-barrels for the first time. Furthermore, the model we propose is very versatile and can be easily augmented with new features. It should be emphasized that the global structure prediction in its principles does not depend on machine learning methods.

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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