



## Bioinformatics Seminar

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Speaker: Dr. Fabrizio Ferrè, Boston College

Title: Functional annotation by identification of local surface similarities: a novel tool for structural genomics

Date: Monday, 20 October 2003

Time & Location

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

Talk: 11:30 am to 1 pm in the Applied Mathematics Conference Room Building 2, Room 338

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

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Abstract:

One of the major and more difficult tasks of the next years will be the function prediction of the several structures of protein without significant similarity with any other known protein, which will be solved by structural genomics projects in order to expand our knowledge of the protein world. In this work we describe a systematic large-scale approach aimed at the identification and annotation of protein surface patches of functional interest. A new procedure was developed able to highlight local surface similarities associated to functional relationships even when they cannot be revealed via standard sequence or structure alignment methods. We validate this procedure on a training set of structures and then use the defined conditions to annotate a dataset composed of protein chains of known structure and not yet clearly identified function. We obtained at least one annotation for 228 protein chains, 70% of which are confirmed in the literature, 30% are new. Since the number of uncharacterized proteins whose structure is and will be solved in the structural genomics era is growing at high speed, this procedure will probably prove to become more and more useful as a predictive tool to infer functional abilities of novel solved structures in the? difficult cases?, where standard sequence or structure comparison methods fail in the identification of functional sites out of the already known context.

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