Docking Predictions of Protein-Protein Interaction

EMBO Practical Course

Barcelona Supercomputing Center, Barcelona, Spain, October 14-17, 2008

SPONSORS
The European Molecular Biology Organisation
The 3D-Repertoire Integrated Project (European Commission FP6)
The SPINE2-Complexes Integrated Project (European Commission FP6)

ORGANIZERS
Joël Janin, Université Paris-Sud, Orsay, France
Juan Fernandez-Recio, Barcelona Supercomputing Center, Barcelona, Spain
Alexandre Bonvin, Utrecht University, The Nethelands
Michael Sternberg, Imperial College London, UK
Shoshana Wodak, Hospital of Sick Children, Toronto, Canada
Haim Wolfson, Tel Aviv University, Israel
Martin Zacharias, Jacobs University Bremen, Germany

MAJOR OBJECTIVES

The prediction and analysis in silico of protein-protein interaction plays an increasing role in functional genomics. The course will present methods based on docking that predict how two proteins interact when their three-dimensional structure is known. Classes will cover the major algorithms for rigid-body docking, methods to predict and simulate conformation changes, scoring functions and refinement procedures, the use of non-structural information in docking, the assessment of the methods on benchmarks and in blind predictions. Half of the course will be practicals in which actual calculations will be performed on biological problems of interest to the students.

We aim to have a mix of Ph.D. students and junior research fellows in bioinformatics, and of molecular biologists and structural biologists who study protein-protein interaction by experiment. To both publics, we will convey the same message: the in silico analysis of protein-protein interaction is not a substitute, but a useful complement to biochemical and structural studies. We will introduce state-of-the-art procedures for this analysis, and explicit the conditions under which it can be done efficiently and reliably.

Classes and practicals will be on the same site. Lecturers and students will be housed together. The pauses between classes and the poster session with drinks will offer the opportunity for discussion. Lecturers will participate in the final summing-up.

The practicals will allow students to do actual large-scale calculations, either locally or on remote computer sites. Students will be encouraged to set up procedures and perform calculations on biological systems of their own choice, especially on those they do experimental work on. They will run several established docking procedures under the supervision of instructors who are experts in these procedures, and have access to at least three Web servers performing protein-protein docking. We will contact the managers of the servers, whether in Europe or in the US, and arrange that they interact by e-mail with the students. The last day will be devoted to a detailed analysis of the results of the calculations, a comparison of the procedures' performances, and an evaluation of the predictions against experimental results.

PRELIMINAY PROGRAM

Tuesday Oct. 14
10:30-12:00 Protein-protein interaction in Structural Biology (J. Janin, Orsay)
14:00-14:45 Seminar (M. Coll, Barcelona)
15:00-18:30 Practicals
Wednesday Oct. 15
9:00-10:30 Docking algorithms 1 (M. Sternberg or V. Lesk, London)
10:45-12:15 Modeling conformation changes (M. Zacharias, Bremen)
14:00-14:45 Seminar
15:00-18:30 Practicals
Thursday Oct. 16
9:00-10:30 Docking algorithms 2 (H. Wolfson, Tel Aviv)
10:45-12:15 Scoring and refining prediction models (J. Fernandez-Recio, Barcelona)
14:00-17:30 Practicals
18:00-20:00 Poster session and drinks
Friday Oct. 17
9:00-10:30 Using external information in docking (A. Bonvin, Utrecht)
10:45-12:15 Assessing predictions: the CAPRI experiment (S. Wodak, Toronto)
14:00-17:00 Practicals - evaluation and summing up

APPLICATIONS
The Course will be limited to 28 students.

Applicants should be registered as students in a Master's or Ph. D. program of a European University in structural biology, molecular biology, biochemistry, biophysics, bioinformatics, computational biology or computational chemistry. They will be selected based on a letter of application and their tutor's recommendation. Applicants with a Ph. D. will be asked for a CV and list of publications. Non-European applications will be considered if recommended by scientists actively engaged in the analysis of protein-protein interaction.

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