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S E M I N A I R E

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«High-resolution, integrative modelling of biomolecular complexes from fuzzy data»

The prediction of the quaternary structure of biomolecular macromolecules is of paramount importance for fundamental understanding of cellular processes and drug design. In the era of integrative structural biology, one way of increasing the accuracy of modelling methods used to predict the structure of biomolecular complexes is to include as much experimental or predictive information as possible in the process.

We have developed for this purpose a versatile information-driven docking approach HADDOCK (http://www.bonvinlab.org/software/haddock2.2) [1,2]. HADDOCK can integrate information derived from biochemical, biophysical or bioinformatics methods to enhance sampling, scoring, or both [3]. The information that can be integrated is quite diverse: interface restraints from NMR, mutagenesis experiments, or bioinformatics predictions; shape data from small-angle X-ray scattering [4] and, recently, cryo-electron microscopy experiments [5,6].

In my talk, I will illustrate HADDOCK's capabilities with various examples. I will also introduce the concept of explorative modelling in which the interaction space defined by a limited number of restraints is systematically mapped [7], which allows, for example, to identify false positive restraints from MS cross-link experiments. We have developed for this purpose the DisVis web server available from: http://milou.science.uu.nl/services/DISVIS
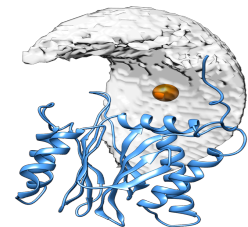
DISVIS visualization of the accessible interaction space consistent with at least 7 restraints

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