

S006 Information-driven modelling of biomolecular complexes **Alexandre M.J.J. Bonvin**

*Bijvoet Center for Biomolecular Research,
Faculty of Science, Utrecht University*

With the presently available amount of genetic information, a lot of attention focuses on systems biology and in particular on biomolecular interactions. Considering the huge number of such interactions, and their often weak and transient nature, conventional experimental methods such as X-ray crystallography and NMR spectroscopy will not be sufficient to gain structural insight into those. A wealth of biochemical and/or biophysical data can however easily be obtained for biomolecular complexes. Combining these data with docking, the process of modeling the 3D structure of a complex from its known constituents, should provide valuable structural information and complement the classical structural methods.

We have developed for this purpose a data-driven docking approach called HADDOCK (High Ambiguity Driven protein–protein DOCKing) (<http://www.nmr.chem.uu.nl/haddock>) which is now also available as web server (<http://www.haddocking.org/>). HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. Flexibility is accounted for in different ways during the docking which allows to model (small) conformational changes taking place during complex formation. In my talk I will discuss the various sources of data that can be used to map interactions and illustrate their use in HADDOCK with examples from our laboratory together with results from our participation to the blind docking experiment CAPRI (Critical Assessment of PRedicted Interactions) (<http://capri.ebi.ac.uk>).