# Integrative, information-driven modelling of biomolecular complexes

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**Abstract**

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://haddock.science.uu.nl) [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 with as most recent addition cryo-EM maps [4]. In my talk, I will illustrate HADDOCK's capabilities of integrating different types of experimental data with various examples and describe some recent developments around the modelling of membrane protein complexes and large assemblies. I will also introduce the concept of explorative modelling in which the interaction space defined by a limited number of restraints is systematically mapped [5].

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