

Invited Talk

**Docking protein domains using a contact map representation**

Stefano Lise and David Jones

University College London, UK

In this talk I will discuss the possibility of predicting protein-protein interactions (docking) using a contact map representation. Rather than providing a full three dimensional model of the predicted complex, the method predicts contacting residues across the interface. A scoring function is used that combines structural, physicochemical and evolutionary information, where each potential residue contact is assigned a value according to the scoring function and the hypothesis is that the real configuration of contacts is the one that maximizes the score. The search is performed with a simulated annealing algorithm. The method has been tested on interacting domain pairs with encouraging results. Lastly, we find that predicted contacts can often discriminate the best model (or the native structure, if present) among a set of optimal solutions generated by a standard 3-D docking procedure.