Computational programs used to predict the composition of protein complexes

The results presented in this paper open new possibilities for the modeling of protein complexes as a step towards the interpretation of cancer related mutations.

Barcelona, 23rd February 2011 – The prestigious journal *Molecular Systems Biology* published the first extensive study demonstrating the ability to use computational docking programs to predict protein-protein interactions. This research was carried out by Mark Wass and Gloria Fuentes, from the Spanish National Cancer Research Centre (CNIO), Carles Pons from the Barcelona Supercomputer Center (BSC) and Florencio Pazos, from the Spanish National Centre for Biotechnology (CNB-CSIC), under the direction of Prof. Alfonso Valencia, Head of the CNIO's Structural Biology and Biocomputing Programme.

"In this study, we showed for the first time that a docking method can be used to differentiate between interacting and non-interacting proteins. We observed that the score distribution of interacting proteins can be distinguished from that of non-interacting proteins. This finding was possible after running more than 100,000 docking experiments using the MareNostrum supercomputer" says Carles Pons, from BSC.

The authors use protein docking programs, which are normally used to model the details of the structure of complexes between proteins already known to interact, to detect the components of protein complexes scanning large collections of protein structures. These calculations are extremely demanding and were possible thanks to the intensive use of the facilities of the Barcelona Supercomputing Center.

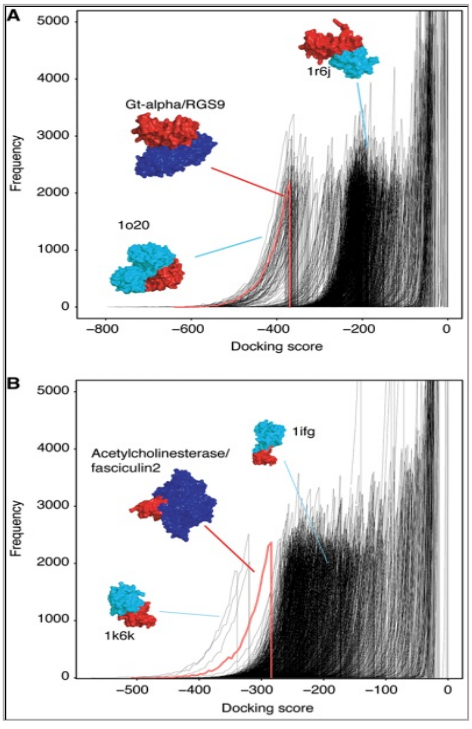

Fig.1 Docking score distributions for benchmark complexes

Protein complexes are central to all the processes occurring in our cells but to date only for a small fraction of them the composition and molecular details of their interaction have been characterized. This knowledge is essential for the understanding of the consequences of mutations and for the development of potential inhibitors. The results presented in this paper open new possibilities for the modeling of protein complexes as a step towards the interpretation of cancer related mutations.

Reference article:

Towards the prediction of protein interaction partners using physical docking

Mark N Wass, Gloria Fuentes, Carles Pons, Florencio Pazos and Alfonso Valencia. *Mol Syst Biol* 7:469, doi:10.1038/msb.2011.3 Available for download at http://www.nature.com/doifinder/10.1038/msb.2011.3