Research Programmes

Structural and Computational Biology

Patrick Aloy: Structural bioinformatics and network biology group

Group Members

Group Leader
Patrick Aloy. ICREA Research Professor

Research Associates
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Highlights

• We have developed a computational approach that integrates various types of biological information to generate a list of 90 potential Aurora substrates, with a prediction accuracy of about 80%. We have demonstrated the specific phosphorylation of NUSAP (nucleolar and spindle-associated protein) by Aurora A in vivo.

• Our analyses of the structural features of known protein-interaction motifs reveal that they tend to have a particular stretched and elongated structure, unlike most other peptides of the same length. We have used these features to identify unnoticed peptide-mediated interactions and to provide molecular details for the binding of over 6,000 protein interactions.

• Through network and systems biology strategies, we have proposed a novel way to approach complex human diseases and new therapeutics. We have revealed a molecular relationship between type II diabetes and the metabolic changes induced by very-low carbohydrate diets.

Publications


• Panjkovich A and Aloy P. Predicting protein-protein interaction specificity through the integration of three-dimensional structural information and the evolutionary record of protein domains. Mol Biosyst, 6 (4), 741-9 (2010)


• Stein A and Aloy P. Novel peptide-mediated interactions derived from high-resolution 3-dimensional structures. PLOS Comput Biol, 6 (5), e1000789 (2010)

Collaborations
• Novel strategy for network-based therapeutics. José Manuel Mas, Infosciencia & Anaxomics Biotech (Barcelona, Spain)
• Novel ways of assessing protein-DNA interactions. Anastassiss Perrakis, Nederlands Kanker Instituut (Amsterdam, Netherlands)
• Structural systems biology. Juan Fernández-Recio, Barcelona Supercomputing Center (BSC) (Barcelona, Spain); Baldo Oliva, Pompeu Fabra University (Barcelona, Spain); Mohan Madan Babu, LMB-MRC (Cambridge, United Kingdom); Miquel Pons, IRB Barcelona (Barcelona, Spain)

Research projects

PhD theses

Patents
• Methods and Systems for identifying molecules or processes of biological interest by using knowledge discovery in biological data. Mas JM, Pujol A, Farrés J and Aloy P. Publication number/date: WO2011051805 (18/08/2010). Status: Pre-grant publication