

Séminaire externe



Vendredi 27 octobre 2017 à 11h00 Salle de conférence du CBM

Protein domains as units of communication

Parallels are often drawn between protein regulation on hand and information one and communicaprocessing tion on the other hand. This metaphor can be made concrete as Shannon's information theory can be used to quantify exchange information the through the structure of proteins. The difficulty is to identify which residues and dynamics processes are involved in the information exchange. I'll present a computational biology method allows one to identify from NMR structural data the set of residues implicated in transducing a signal through the structures of simple protein domains. I will explain this method using the SH2 domain of Fyn as example. This computational biology research generates novel insights into dynamic and structuaspects of regulation of ral proteins by their domains.

Capturing the ambiguous behaviour of proteins from sequence-based predictions

Protein conformations are not fixed in time, and conformational transitions are often essential for protein functionality. In addition, many of the as yet uncharacterised proteins in the 'dark proteome' likely exhibit behaviour that conformational cannot be captured by discrete conformational states. With our work, we aim to create a more probabilistic picture of protein behaviour that requires only their sequence. We predict per-amino acid residue biophysical characteristics such as dynamics, conformation and capacity for early folding, as influenced by the local sequence environment. The approach is applicable to any protein, and can be further combined with evolutionary information in an attempt to better understand the capacity proteins have for ambiguous and complex behaviour.

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