Analysis of phosphorylation sites in 3D protein structures

ID - 200

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Motivation

Protein phosphorylation plays a central role in signal transduction in all cells. The mechanisms that allow a kinase or a phosphatase to recognize its substrate are not well-understood yet. Despite the great importance of phosphorylation sites and the fair number of annotated phosphoresidues in the Protein Data Bank, an accurate and exhaustive analysis of such sites in 3D does not exist in the literature.

Methods

We present an analysis of the substrate residues directly involved in phosphorylation (serine, threonine and tyrosine) and of the region surrounding phospho residues both in sequence and in structure. The analysis is carried out in terms of relevant properties of amino acids in 3D: solvent accessibility, secondary structure, temperature factor, hydrogen bonding, quaternary structure, cavities, evolutionary conservation.

Results

Preliminary results indicate that properties distinctive of phosphorylation sites exist. Based on this, we obtain a picture of the general phophorylation site environment, which will hopefully provide a better understanding of the mechanisms involved in phosphorylation. This information will be collected in a resource for 3D phospho sites and used to train new predictors for the inference of not yet characterized phosphorylation sites.

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