



Possible roles of S...O and S...N interactions in the functions and evolution of phospholipase A2

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To investigate possible roles of S...X (X=O, N, S) interactions in the functions and evolution of a protein, two types of database analyses were carried out for a vertebrate phospholipase A2 (PLA2) family. A comprehensive search for close S...X contacts in the structures retrieved from protein data bank (PDB) revealed that there are four common S...O interactions and one common S...N interaction for the PLA2 domain group (PLA2-DG), while an additional three S...O interactions were found for the snake PLA2 domain group (sPLA2-DG). On the other hand, a phylogenetic analysis on the conservation of the observed S...O and S...N interactions over various amino acid sequences of sPLA2-DG demonstrated probable clustering of the interactions on the dendrogram. Most of the interactions characterized for PLA2 were found to reside in the vicinity of the active site and to be able to tolerate the conformational changes due to the substrate binding. These observations suggested that the S...X interactions play some role in the functions and evolution of the PLA2 family.

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