Computational approaches to modeling receptor flexibility upon ligand binding: Application to interfacially activated enzymes - DTU Orbit (08/11/2017)

Computational approaches to modeling receptor flexibility upon ligand binding: Application to interfacially activated enzymes

Receptors generally undergo conformational change upon ligand binding. We describe how fairly simple techniques may be used in docking and design studies to account for some of the changes in the conformations of proteins on ligand binding. Simulations of protein-ligand interactions that give a more complete description of the dynamics important for ligand binding are then discussed. These methods are illustrated for phospholipase A(2) and lipase, enzymes that both undergo interfacial activation.

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