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Molecular Dynamics Simulation Study of Lipase B from Candida Antarctica

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Candida antarctica lipase B (CalB) belongs to the α/β hydrolase family which is act on the ester bonds of tri-acyl glycerol. CalB is a psychrophilic lipase that is able to perform lypolytic activity at low temperatures. Cold-active lipases have several applications in industry, production of pharmaceuticals, food, and fine chemical. To understand the mechanisms involving in the psychrophily of CalB, molecular dynamics (MD) simulation has been undertaken to explain its dynamics at atomic level. Crystal structure of CalB was obtained from Protein Data Bank (1TCA) as the initial structure for MD simulations. MD simulations were performed by AMBER 10.0 with all-atom force filed ff99SB. The structure was hydrated in a 10 Å layer of TIP3P water model. In this study, several MD simulations have been performed for 30 ns at three different temperatures (5, 35 and 60 °C). A highly flexible alpha helix (α5 helix) was identified in which act as a lid for the active site clef of CalB. According to the results obtained from RMSF graphs, the extent of flexibility is much higher at low temperature rather than higher temperatures. Further investigation of the active site revealed that the starting open conformation of the enzyme become close immediately at 35 and 60 °C while it remains open for a considerable time. Radial distribution function of water molecule in the activeite also verifies the movement of the lid. The presence of water molecules at open conformation is higher than that of closed state. It is suggested that the cold-activity of Calb is tightly related to the movement of the lid at low temperatures. As it observed in the current study, open state is more stable at 5 °C rather that 35 and 60 °C.

Keywords: Candida Antarctica Lipase B, Psychrophilic Enzymes, Molecular Dynamics Simulation, Open-Closed Conformations.

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Molecular Dynamics Study of two Mechanistic Mutations in Mnemiopsin from Mnemiopsis leidy

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Mnemiopsin from Mnemiopsis leidy emits light in the presence of Ca^{2+} decomposing into apomnemiopsin, coelenteramide and CO_2. To understand mechanism of the reaction, a comparative structure-function study was undertaken with respect to two single mutants, Leu36His and Phe186His located in the substrate binding cavity. Our experimental results showed that these mutations stop bioluminescent reaction. Molecular dynamic simulation studies indicated an increase in overall flexibility of Ca^{2+}-binding loops and substrate binding cavity residues in mutants compared to the wild type. Further analyses on Phe186His mutant revealed that mobility of coelenterazine in some regions and substrate-protein interaction energy is decreased, while these structural properties are not changed in Leu36His mutant. Finally these findings revealed that these two substitutions prevent disruption of peroxide group of coelentrazine and consequently bioluminescent reaction by altering the dynamic and energetic properties in this region.

Keywords: Mnemiopsin, Structure-function, Molecular Dynamics Study.

Abstract No.255

Artificial Superoxide Dismutase Activity of Copper-Cysteine to Electrochemical Detection of Superoxide

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Superoxide dismutase (SOD) represents an essential defense system against oxygen-derived free radicals, specifically superoxide radical anion. Superoxide can initiate a series of free radical reactions, which causes a vast number of diseases. So, quantitative analysis of in vivo is very important. In most of the analysis methods, SOD was immobilized through cysteine self assembled monolayer on gold (Cys/Au) electrode. Here, we design and compare three approaches of superoxide