achieved by these methods. Statistical analysis has been revealed at least six fine individual structures for HSA. Each structures present individual and exclusive function. It can be concluded that, albumin unique features and functions are due to its switching capability to different possible fine structures with the lowest energy exchange.

Keywords: Human Serum Albumin, Fine Structures, Structural And Functional Alteration.

Abstract No.287

Mixed Quantum Mechanical/ Molecular Mechanical (QM/MM) Study of the S-nitrosylation Reaction 4-phenyl-3-Furoxancarbonitrile as Inhibition of Thioredoxin Glutathione Reductase (TGR)

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Combined quantum mechanics/molecular mechanics (QM/MM) methods allow computations on chemical events in large molecular systems. We present a theoretical study of a mechanism for the S-nitrosylation Reaction4-phenyl-3-furoxancarbonitrile or furoxan belongs to an oxadiazole-2-oxide class whose therapeutic effects are largely due to their inhibition of thioredoxin glutathione reductase (TGR)for thecontrol of schistosomiasis bases in QM/MM calculations at the DFT RB3LYP/6-31G+(d)//SCC-DFTB AMBER level. The activity of the oxadiazole 2-oxides was associated with a donation of nitric oxide. We first attempted to dock inhibitor in the active site of enzyme available in the Protein Data Bank, (PDB codes: 3H4K), to see how intact inhibitor would bind. Since our interest was focused on the region were reaction should take place, all molecules that might potentially be involved in the mechanism of nucleophilic attack, namely furoxan, residues Cys159, and nearby water molecules, were treated by QM, while the rest of the protein, as well as the bulk water, were treated by traditional molecular mechanics. As soon as a preliminary minimization of complex was carried out on TGR using the hybrid QM/MM potential, migration of the Cys159 to the carbon 3 furoxan was observed. We were quite surprised by this outcome, while the formation of the tetrahedral intermediate might be a reasonable explanation for location of the initial nucleophilic attack shows this mechanism: The potential energy of the system with respect to the initial state (ΔU) along the minimum energy reaction path (MERP) is also reported with the 3D structures of relevant intermediates. The results are consistent with the available experimental data and provide new insight into the detailed mechanism of this important reaction.

Keywords: Quantum Mechanic, Molecular Mechanical, Thioredoxin, Glutathione Reductase.

Abstract No.288

Effect of Glycine, as Chemical Chaperone, on Catalase Glycation by Glucose

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Oxidative mechanisms are thought to have a major role in several biological phenomena, including cataract formation and diabetic complications. Glycation of catalase, as a powerful antioxidant enzyme, by glucose alters its structure and function and increases the risk of cataract formation in diabetic patients. Glycine is a chemical chaperones that inhibit protein glycation and stabilize them against thermal and chemical denaturation. Therefore, we investigated the effects of this chemical chaperone on catalase glycation.Catalase solution, pH 7.4, was incubated separately with glucose in the presence or absence of glycine at 37ºC in a shaker incubator. The aliquots were collected every week and stored at -80ºC. Then, they were analyzed by fluorescence spectroscopy, circular dichroism spectroscopy (CD) and polyacrylamide gel electrophoresis (PAGE). The activity of catalase in each sample was also determined.Structure and activity of catalase were changed due to the glycation with glucose. Glycation caused an increase in the fluorescence emission and electrophoretic mobility and a decrease in the alpha helix content and catalase activity. Glycine inhibited this phenomenon and the fluorescence emission, alpha helix content, electrophoretic mobility and activity of catalase were closed to the normal values.Our results indicated a decrease in the catalase glycation by glucose in the