degradation process. Knowing the answer of these questions made us to investigate the probable ROS accumulation by chemiluminescence method and detecting heme degradation products by fluorescence spectroscopy (ex: 321 nm and ex: 460 nm) at the same time intervals. Our results (obtained from in vitro diabetic conditions at 37 °C and pH 7.4) demonstrated on noticeable accumulation of ROS in the fructose solution even at the beginning of its solution. The amounts of detected ROS in the presence of proteins were less than fructose solution by an increasing pattern in the first week of incubation. On the other hand, after passing the increasing phase of accumulated ROS, heme degradation products started to accumulate. Little by little amounts of heme degradation arises and made a plateau where detected ROS was at the plateau line too. Such studies indicate that diabetic patients should pay more attentions to use enough antioxidant agents in their diets.

Keywords: Hemoglobin, ROS, Glycation, Heme Degradation, Diabetes.

Abstract No.170

The Role of Bir1 in Caspase Inhibition

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Apoptosis is a controlled process of cellular destruction through which a group of proteases named caspases (Cysteinyl aspartate-specific proteases) are activated. The activity of these enzymes is brought under control through Inhibitor of Apoptosis Proteins (IAPs). Each IAP protein contains at least one BIR (Baculoviral IAP Repeat) domain, which contains ~70 amino acids folded around a zinc atom. The BIR domains alone or in combination with other domains of IAPs are responsible for directly and specifically inhibiting the caspases. The different BIR domains exhibit distinct functions. The second BIR domain (BIR2) inhibits the activity of caspase-3 and -7 whereas the third BIR domain (BIR3) targets the caspase-9. Previous studies failed to demonstrate any role for the BIR1 domain of IAPs in inhibition of executioner caspases. Therefore in this study, recombinant proteins containing BIR1 were produced to investigation their effect on caspase-7. Enzyme kinetics assays showed that BIR1 domain is essential for caspase inhibition by cIAP1 protein whereas in the case of XIAP, presence of BIR1 causes concentration dependent caspase-7 inhibition by this IAP.

Keywords: Apoptosis, IAP, BIR1, Inhibition Mechanism, Caspase-7.

Abstract No.171

In Silico Modeling of Receptor Binding Mode for two Novel Peptides Developed as EGFR Antagonists

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Epidermal growth factor receptor (EGFR) is one of the most common targets for developing anticancer drugs. It is a cell-surface receptor which plays a key role in many of human epithelial cancers. Recently we identified two novel peptides (P1 and P2) for EGFR. From drug discovery and design point of view introducing short peptides which could inhibit the protein-protein interaction is of great importance.Our aim in the current investigation was to study their mode of interactions to the receptor using computational methods. Computational approaches have become increasingly important in drug design processes. Modern computational approaches such as structure-based drug design have efficiently speeded up the drug discovery process based on some proven theoretical bases at different levels of approximation which can provide useful tools for studying the structural and dynamics behavior of biomolecules. Furthermore, such computational methods can be used to predict the possible interactions in ligand-receptor complexes and to get an estimate of binding free energies for the complexes.In order to predict the mode of interactions of the peptides initially, P1 and P2 were docked onto the active site of the receptor using GOLD program and interactions in the complex of ligand- receptor were analyzed using Ligplot program. Then the docked peptides were subjected to different MD simulation with the time lengths ranging from 0.4 to 6 ns using AMBER program and then the binding free energy were evaluated by applying the MM-PBSA/GBSA methods. The result of this study can be used in identifiying pharmacophore responsible for molecular interaction which can be useful in drug design processes.

Keywords: EGFR, Binding free energy, Amber, Docking, MMPBSA/GBSA.
