Abstract No.291

Lys Therapy of Diabetes: from in vitro Studies to the Animal Models of Diabetes and Type 2 Diabetic Patients

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Hyperglycemia is one of the most important reasons of diabetic complications. It causes the biomacromolecules, especially protein glycation which in order result in protein conformational change. Here the effect of glycation on the structure and function of several important proteins from various comportments e.g. plasma, extracellular medium, cytosol and nuclei is presented. Then, the effect of Lys, as a chemical chaperone from amino acid family, on the non-enzymatic glycation of many proteins and its inhibitory effect on this process that was investigated in our Lab. will be discussed. In addition, our in vivo results showed that Lys administration in the animal model of diabetes of both types 1 and 2, as well as the type 2 diabetic patients result in the decrease in serum glucose, increase in insulin secretion and decrease insulin resistance, increase serum antioxidant capacity, improve the lipid profile and HDL functionality, induce HSP70 production, reduce fibrin activity due to correction of its folding, stop the progression of cataract, etc. In conclusion, the obtained data by our team in the in vitro and in vivo studies indicate the beneficial effects of Lys therapy on reduction of diabetic complications thus it is suggested as a complement therapy for diabetes.

Keywords: Diabetes, Animal Model, Hyperglycemia, Antioxidant.

Abstract No.292

Molecular Dynamics Simulation on the Protein Structure

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The protein structure changes in the presence of different denaturants such as temperature and chemicals. These variations can be followed by different techniques such as X-ray, NMR, CD, IR and so on. There are some complementary methods same as molecular dynamics (MD) simulation and homology modeling that used in the structure determination so that some of PDB codes in protein data bank were exclusively obtained by MD. On the other hand X-ray crystallography only obtains the crystal structure of macromolecules but not solution. NMR spectroscopy investigates both liquid and crystal structures while CD and IR determine secondary structure in solution phase. The first two methods are precise and rigorous but very expensive. On the other hand MD is a powerful method in determination of tertiary structure of macromolecules specially in homologues proteins. MD methods use the classical and statistical mechanics theorem for movement and interaction of molecules. So it is an approximation method that dose not consider electron interaction in its calculations. It makes atoms to move in different direction based on Newtonian laws subsequently thermodynamic parameters. In this study, I report some applications of molecular dynamics in biology. Structural parameters such as solvent accessible surface area, hydrogen bond, CD222nm, radius of gyration and radial distribution function were obtained for enzyme by molecular dynamics and compared with experimental data.

Keywords: Molecular Dynamics Simulation, Tertiary Structure, Accessible Surface Area, Hydrogen Bond.

Abstract No.293

New Strategies in Structure-function Relationship Study of Peptides

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Peptides play significant roles in biological world especially in human life. There are a great number of peptides and proteins which are used as therapeutics and more are under development as pharmaceutical targets. However, design and prediction of their activity remain one the most challenging area in life sciences due to large amount of arrangement possibilities. Quantitative sequence-activity model (QSAM), employs quantitative structure-activity relationship (QSAR) strategies to quantify biosequence-activity/function relationship for the peptides, proteins and nucleic acids, becomes an attractive and active area in peptide researches. Therefore, a lot of efforts were done in the past to model the relation between the peptide structure/sequence with its biological activity. On the basis of QSAR concept, functions and structures of peptides or proteins are resolved by the information enclosed in the amino acid arrangements. In this methodology, a set of