A curcuminoid is a curcumin or its derivative with different chemical groups. During the last few decades, curcuminoid have been utilized in biological and pharmaceutical fields, because of its remarkable anti-tumor, anti-oxidant, anti-arthritic, anti-amyloid, anti-ischemic and anti-inflammatory properties. Curcumin is a hydrophobic compound and shows lipid solubility. Being hydrophobic, curcumin needs a carrier system to transport to different parts of the body. Although curcumin has potential for extensive use in disease treatment, there are two major challenges that limit this target. First, curcumin has low solubility in aqueous solution, which poses a severe limitation on the achievable concentration in biological systems. Second, the soluble portion undergoes rapid degradation at physiological pH. Several methods have been proposed to address the issues of low solubility and stability. Recently, the use of serum albumin as a carrier for curcumin has been reported. Results by Wang et al., indicate that degradation of curcumin in buffer solutions is suppressed in the presence of serum, of which the major components are water (92%) and proteins (6-8%).The principal aim of this work is to perform a computational study of the structural and electronic properties of different conformations of curcumin and four other Curcuminoids by DFT Method to find the most stable equilibrium structure and to define the nature of the molecular orbitals, HOMO and LUMO that are important to explain binding characteristic. Then interaction of curcuminoids with albumin protein was studied by using molecular docking and molecular dynamics simulation. By computational methods, we can recognize that group of residues which participate in bonding with curcuminoids and binding energy and kind of interactions. Lys276 and Gln268 amino acids are in suitable position to be involved in making H-bonds with the carbonyl oxygen functions at the center and phenolic ring of curcumin, respectively.

Keywords: Curcumin, Molecular Docking, DFT, Molecular Dynamics, Human Serum Albumin.

Abstract No.105

Investigating the Role of the Salt Bridige Between Asp100 and Arg80 in TMGS Allosteric Behavior

Mona Atabakhshi[1], *Khosro Khajeh*[1], *Reza Hassan Sajedi*[1], *Malihe Mohamadi*[1], *Mahdieh Hadi*[2], *Reihaneh sadat Mirhassani*[2]

1. Dept. of Biochemistry, faculity of Biological Sciences, Tarbiat Modares University, Tehran, IR
2. Dept. of Biotechnology, College of Science, University of Tehran, IR
(E-mail: m.atabakhshi@modares.ac.ir)

The Allosterically regulated enzyme methylglyoxal synthase (MGS, EC 4.2.3.3) is a homohexameric enzyme that catalyzes the conversion of dihydroxyacetone phosphate (DHAP) to methylglyoxal and phosphate in the first step of the methylglyoxal bypass of glycolysis pathway. Thermophilic type of MGS was first isolated and expressed from Thermus sp.GH5 (TMGS). Phosphate was found to be a strong inhibitor and negative allosteric effector of the enzyme. According to the crystallographic structure of phosphate bound MGS, conformational changes in the conserved regiones of the protein closes the entry of the channel leading to the active site and affects the interresidual interaction at the monomer-monomer interface. New interaction between residues Arg80 and Asp100 occur upon phosphate binding to the enzyme and may provide a pathway by which allosteric inhibitory signal is transmitted through the intersubunit interface. To test this hypothesis, this two residues were mutated with Quik change site directed mutagenesis and allosteric behavior of mutated variants were investigated.

Keywords: TMGS, Allosteric Inhibitor, Methylglyoxal.

Abstract No.106

Targeting Undifferentiated hBM-MSCs with Polymeric Nanocurcumin

*Mohamad Javidi**, *Majid Sadeghizadeh*

Department of Genetics, Faculty of Biological sciences, Tarbiat Modares University, Tehran, IR
(E-mail: maj136@gmail.com)

The prevalence of diabetes for all age-groups worldwide was estimated to be 2.8% in 2000 and 4.4% in 2030. The main reason for diabetes type I is that pancreatic beta cells do not produce insulin sufficiently. Organ/islet transplantation and daily insulin injection are conventional methods have been utilized until now. The search for alternatives have started several years ago and methods based on stem cells differentiation is an ongoing task have suggested, significant goals having been achieved in most experimental settings (e.g. insulin production and euglycaemia restoration). Mesenchymal stem cells (MSCs) are uniquely capable of crossing germinative layers borders and are considered as promising cells for regenerative medicine approaches in several diseases. Type I diabetes therapy should potentially benefit from such differentiated cells. MSCs are obtainable in high numbers via ex vivo culture and can be differentiated towards insulin producing cells (IPCs). An important obstacle on the way of this kind of cell-based therapy, is the risk of tumorigenecity in the patients.

Curcumin, the main compound of spice turmeric- as one of the natural products- was demonstrated to possess effective anti-cancer properties, with no significant effect on normal cells. Also many studies have been accomplished using curcumin for diabetes treatment. Therefore we based the main aim of this study on improving the efficiency of differentiating human MSCs into IPCs utilizing polymeric nanocurcumin. The absorption efficacy of curcumin is too low to make dramatic results in therapy. Curcumin bioavailability could be improved using nanoparticle carriers. Our data indicates that polymeric nanocurcumin -in specific dose and time- reduces the expression of nestin (protein coding gene, expressed in IPC progenitors) with no significant effect on insulin expression in mRNA and protein level.

Keywords: Diabetes type I, Regenerative Medicine, MSCs, IPCs, Polymeric Nanocurcumin.

Abstract No.107

Electrochemical Investigation of Hemoglobin via Gold-Coated Magnetic Nanoparticles

*Aghdas Banaei** [1,2]

1. Research Institute of Applied Science, Academic Center of Education, Culture and Research (ACECR), Shahid Beheshti University, Tehran, IR
2. Institute of Biochemistry and Biophysics, Tehran University, Tehran, IR
(E-mail: abanaei@ibb.ut.ac.ir)

Using direct electrochemistry of redox proteins it is possible to establish a foundation for fabricating the mediator-free biosensors. In the last few years, by development of nanotechnology, magnetic gold nanoparticles as especial carrier for immobilizing biomolecules have aroused great interest. Among the various protein immobilization approaches, the technique based on electrostatic interactions has much attention due to their facility and wide availability of materials.The direct electron-transfer of hemoglobin (Hb) immobilized on magnetic gold nanoparticles was achieved. Magnetic gold nanoparticles were dropped on the surface of Au electrode and hold on it by using magnet behind electrode. The cyclic voltammograms (CVs) of Hb, heme and globin on gold nanoparticles were obtained in phosphate buffer solution (pH 6.8) and air saturated conditions. Hb showed a quasi-reversible CV corresponding to the Fe3+/ Fe2+ redox couple with a formal potential of about −0.33 V (vs. Ag/AgCl). The immobilized Hb exhibited good electrocatalytic activity toward hydrogen peroxide (H2O2). The gold nanoparticles provided a biocompatible micro-environment for protein and could promote the direct electron transferring of Hb. This method may also be examined to other proteins too.

Keywords: Gold Magnetic Nanoparticles, Hemoglobin, Globin, Heme, Direct Electron Transfer.

Abstract No.108

Cloning and Sequencing of Endoglucanase Gene from a Native Strain of Bacillus spp.

Saber Zahri, *Zahra Hamidzade Moghadam**, *Saeid Latifi Navid*

Department of Biology, Faculty of Sciences, University of Mohaghegh Ardabili, Ardabil, IR
(E-mail: zahrahamid39@yahoo.com)

An endoglucanase producing strain of Bacillus spp. was isolated from the forest soils of Ardabil province. The 16S rDNA was amplified using universal primers and the sequencing results were analyzed by nucleotide Basic Local Alignment Search Tool. The data showed that the strain was Bacillus pumilus. A pair of primers was designed according to upstream and downstream sequence of the gene using bacteria genome (NCBI ACCESSION: AY339624) as template, and the gene was amplified using standard three-step PCR reaction. A specific 2200 bp DNA band was amplified and purified from agarose gel. The DNA was cloned into pTG19 vector using T/A cloning method and transformed into E. coli DH5α. The recombinant vector was extracted and sequenced. The results confirmed the endoglucanse gene with two distinct domains of glycosil hydrolase family and cellulose binding domain which was followed a signal peptide in the 5′ end.

Keywords: Bacillus spp., Endoglucanase Gene, PCR Amplification, Cloning.

Abstract No.109

Lung Cancer Tumors Classification by Using Data Mining Tools on Important Protein attributes Derived from Structural and Physicochemical Descriptors Of Involved Proteins

Faezeh Hosseinzadeh [1], *Mansour Ebrahimi** [2], *Narges Shmabadi* [3], *Bahram Goliaei* [4]

1. Laboratory of Biophysics and Molecular Biology, Institute of Biophysics and Biochemistry, University of Tehran, Tehran, IR