

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-arthritis, 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 Bridge Between Asp100 and Arg80 in TMGS Allosteric Behavior

Mona Atabakhshi¹, Khosro Khajeh¹, Reza Hassan Sajedi¹, Malihe Mohamadi¹, Mahdieh Hadi², Reihaneh sadat Mirhassani²

1. Dept. of Biochemistry, faculty 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 regions 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 Javid, Majid Sadeghzadeh*

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 tumorigenicity in the patients.