to HRP efficiency and also that is more efficient in comparing with the catalytic efficiency of SDS – Imidazole – heme system.

Keywords: Nano Artificial Enzyme, SDS Micelle, Heme, Imidazole-Tosyl Group, Enzymatic Efficiency, Biomimetic.

Abstract No.113

Semi-empirical Analysis of Interaction Between Bisphosphonates and Farnesyl Pyrophosphate Synthase

Mohammad Hossein Karimi-Jafari [1], *Rohouhollah Firouzi** [2]

1. Institute of Biochemistry and Biophysics, University of Tehran, Tehran, IR
2. Chemistry and Chemical Engineering Research Center of Iran (CCERCI), Tehran, IR
(E-mail: Firouzi.chemist@yahoo.com)

Nitrogen-containing bisphosphonates (N-BPs) are important pharmaceuticals in treatment of various bone related diseases. Major molecular target of N-BPs is the enzyme farnesyl pyrophosphate synthase (FPP_S). Here, we conducted quantum mechanical calculations for several N-BPs and their surrounding residues in the active site of FPPS.

X-ray structures of all complexes were obtained from PDB and were saturated for missing hydrogen atoms and a computationally tractable model was built by cutting all residues within 4.5 Å of the ligand. Dangling bonds in the N and C terminals of selected residues were capped by CH_3-CO- and –NH-CH_3 fragments, respectively. PM6 semiempirical Hamiltonian was used for optimization of added hydrogen atoms and calculation of interaction energies. Different computational tasks in this work were performed by VMD-1.9, MATHEMATICA-8, REDUCE-3.14 and MOPAC-2009 programs.

Optimized structures show that the phosphonate groups interact mainly with an aspartate-rich region in the active site of FPPS via bridges of divalent metal ions. In addition, the hydroxyl group of N-BPs show direct interaction with proximally located, positively charged lysine residues. This study also reveals a strong dependence of number of hydrogen bonding interactions of the phosphonate groups with FPPS and the side chain of N-BPs. The heterocyclic N-BPs (such as Minodronate) make more hydrogen bonding.

Keywords: Bisphosphonates, FPPS, Computational, Osteoporosis.

Abstract No.114

Mammalian Intestinal Alpha Glucosidase Inihibitory Activity of Novel Pyrimidine Fused Heterocycles

*Mohamad Mehraban** [1], *Reza Yousefi* [1], *Farhad Panahi* [2], *Ali Khalafi-Nezhad* [2]

1. Protein Chemistry Laboratory (PCL), Dept. of Biology, College of Sciences, Shiraz University, Shiraz, IR
2. Dept. of Chemistry, College of Sciences, Shiraz University, Shiraz, IR
(E-mail: saido666@gmail.com)

The prevalence of diabetes which is partly associated to the amount of carbohydrates in the diet has risen at alarming rate. Mammalian starch digestion primarily occurs in lumen of the small intestine by α-amylase to yield both linear and branched chain oligosaccharides, neither of which can be absorbed into the blood-stream without further hydrolysis by α-glucosidases (EC 3.2.1.20) to release glucose. In this regard, intestinal α-glucosidases plays a critical role in carbohydrate digestion and absorption, and therefore, the inhibition of this enzyme provides an effective anti-diabetic option by targeting postprandial hyperglycaemia. In this study a novel class of pyrimidine fused heterocyclic compounds were synthesized and their inhibitory effect against mouse alpha-glucosidase examined spectroscopically. Both kinetic- and pharmacologic parameters including mode of inhibition, inhibition constant (Ki) and half maximal inhibitory concentration (IC50) were calculated for the synthetic compounds, presenting promising inhibitory effect against the mammalian enzyme. This study suggests a novel molecular scaffold as template for synthesis of anti-diabetic compounds with promising inhibitory activity against alpha-glucosidase.

Keywords: Alpha-glucosidase, Inhibition, Diabetes, Pyrimidine-Fused Heterocycles.

Abstract No.115

Antibacterial Activity and Conformational Study of Brevinin-2R

*Robab Hasanvand** [1], *Asadollah Asadi* [1], *Hashem Yaghoubi* [2], *Saber Zahri* [1]

1. Department of Biology, Faculty of Science, Mohaghegh Ardabili University, Ardabil, IR
2. Department of Biology, Faculty of Science, Islamic Azad University of Ardabil, Ardabil, IR

(E-mail: Robab.hasanvand@yahoo.com)

Brevinin-2R belongs to amphibian peptides family and could be synthesized via solid phase method. Our results showed strong antimicrobial activity of brevinin-2R, a 25-amino acid synthetic cationic peptide, due to probable interaction with lipid membrane. Furthermore it has an N-terminal hydrophilic region and a C-terminal loop that is delineated by an intra-disulfide bridge.The minimum inhibitory concentrations (MIC) of brevinin-2R against reference strains of Staphylococcus aureus and Staphylococcus epidermidis by broth micro dilution (BMD) method, based on current National Committee for Clinical Laboratory Standards (NCCLS) susceptibility guidelines, respectively were 1.56 and 0.39 microgram/ml. Circular Dichroism (CD) Spectroscopy was conducted to investigate the structure-activity relationship. The CD analysis revealed that amphipathic α-helical conformation of the synthesized peptides is involved in antimicrobial effects.

Keywords: Amphibian Peptides, Antimicrobial Activity, Brevinin-2R, Circular Dichroism, Broth Micro Dilution.

Abstract No.116

The Mechanism of Superb Antioxidant Activity of Curcumin

*Abolfazl Barzegar**

Research Institute for Fundamental Sciences (RIFS), University of Tabriz, Tabriz, IR
(E-mail: barzegar@tabrizu.ac.ir)

Reactive oxygen species (ROS) namely superoxide radical ($O_2\bullet^-$), hydroperoxyl radical ($HO_2\bullet$), hydroxyl radical (HO●), peroxyl radical (ROO●), alkoxyl radical (RO●) and hydrogen peroxide (H_2O_2) are thought to be the causative agents of various diseases. A growing body of research suggests that curcumin, the yellow pigment of turmeric and curry (Curcuma longa Linn), has potential for the prevention of ROS in the biological systems. But its mechanism of action is still unclear. So far conflicting findings about both of the site of curcumin reactivity with radicals and the reaction mechanisms in ROS scavenging (H-atom transfer, HAT, or electron transfer, ET, mechanisms), have been drawn by several groups. In this research, we aimed to declare the unknown antioxidant mechanism and active sites of curcumin in polar aqueous medium (inside the cells), using different experimental methods and range of quantum computations. We found that two phenolic OH play a major role in the antioxidant activity of curcumin. Results suggest that enol and keto tautomers of curcumin reduce free radicals via ET and HAT mechanism respectively. Also, enol is more active than keto tautomer of curcumin. While, ET mechanism dominates for ROS scavenging but keto/enol tautomerism of curcumin exist at pH 7.4 and both of HAT and ET mechanism is conceivable at physiological conditions.

Keywords: B3LYP, Reducing Power, DFT, Intracellular ROS, BDE.

Abstract No.117

Effect of some Dendritic Nanocarriers on Anticancer Properties of Cucumin from Turmeric (Curcuma longa)

Vahid Erfani Moghadam [1], Alireza Nomani [2], Maryam Tahmasebi Mirgani [3], Majid Sadeghizadeh [3]*

1. Department of Nanobiotechnology, School of Biological Sciences, Tarbiat Modares University, Tehran, IR
2. Department of Pharmaceutics, Zanjan University of Medical Sciences, Tehran, IR
3. Department of Genetics, School of Biological Sciences, Tarbiat Modares University, Tehran, IR
(E-mail: v_erfani@yahoo.com)

Nanotechnology enables us to design novel drugs with new properties such as enhanced bioavailability, targeting specific tissues, controlled released, biocompatibility and biodegradability. Curcumin from Turmeric (Curcuma longa) has been used extensively as food additive and drug historically in eastern countries. In recent decades, anticancer effect of Curcumin has been proved by several researches. Curcumin has influence on multiple cell signaling pathways and prevent cell proliferation, invasion, metastasis and angiogenesis. But solubility of Curcumin in water and therefore its bioavailability is very low and it restricts the anticancer properties of Curcumin. In this research we tried to find appropriate nanobiotechnology tools such as dendritic nanocariers to improve solubility of Curcumin. We determined in vitro solubility and drug release of these nanocarriers and localization study by florescence quenching by acrylamide and iodide has been performed to prove that Curcumin is encapsulated inside of the dendritic nanocarriers or on the sufaces of them. Measured quantitative cellular uptake and cell toxicity of nanocurumins by MTT test in tumor cells shows that these new nano formolations have ability to increase efficiency of anticancer properties of curcumin.

Keywords: Nanocurcumin, Dendritic Nanocarrier, Curcumin, Florimetry, Anticancer.
