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

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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

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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

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