

recognized by plant RNA polymerase so we measured 14,000 RLU/sec after 5 days of transfection.

Keywords: Cytomegalovirus Promoter, Luciferase, Cloning, In vivo assay.

Abstract No.217

QSAR Study of Neuraminidase Enzyme by Molecular Mechanic Method, for Nano Drug Design

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Nowadays drug design is made by two methods namely QSAR & Docking. QSAR reveals a quantitative relation between structure & function based on Hammett & Hansch equations. Statistical analysis, molecular mechanics & molecular graphics have done a great assistance in drug designing. For the purpose of understanding of drug designing methods we should have a complete knowledge of Receptor, Ligand, Binding site & Target site. Since H1N1 influenza A infection is highly contagious, its spread as epidemics & pandemics has made it a horrible disease. The WHO has many concerns in this issue & expends millions of dollars to produce drugs to suppress or treat this disease. For treatment of this disease a thorough knowledge of neuraminidase protein is essential in order to produce potent drugs to suppress this enzyme. Due to virus's genomic inconstancy & point mutations, drugs that are no longer useful against this virus should not be used & new more potent & suppressing drugs must be designed. We studied the drug binding sites in dielectrics (32, 63 & 78, 39) in various temperatures (310, 315, 329 & 333 K), using Bioinformatics, molecular mechanics & MM+ Monte Carlo methods. We measured the potential energy of amino acids binding to the drug. Drug binding sites are more dependant to dielectric constants rather to temperature and the optimum dielectric constant is 39/78.

Keywords: Molecular mechanic, Influenza A, Dielectric, Neuraminidase enzyme.

Abstract No.218

Nano Theoretical Studies of Testis-Specific Protein/gene 10 structure of Homo Sapiens and its Comparison with the TSGA10 protein/gene of Rattus Norvegicus

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The isolation of a novel gene, TSGA10, is described by differential mRNA display which is expressed solely in adult human testis. It seems likely that the gene is expressed during spermatogenesis possibly in spermatocytes. The gene is composed of 19 exons extending over more than 80 kb. The complete cDNA contains an open reading frame of 2094 nucleotides, which appears to encode a novel protein. It was predominantly expressed in the testis in adult normal tissues. Cancer-testis genes are a group of genes expressed in testicular germinal cells and a range of human cancers. Testis-specific gene A10 (TSGA10) is expressed in testis and actively dividing and fetal differentiating tissues. Testis-specific gene antigen (TSGA10) is expressed in fetus, testis and frequently in human solid cancers and acute leukemias, making it a candidate for immunotherapy. There is also evidence for potential TSGA10 involvement in cell proliferation. It was reported its expression TSGA10 in human monocyte-derived dendritic cells (DC) and macrophages in vitro and in murine spleen CD11c(+) cells ex vivo. It is proposed that TSGA10 could influence the function of antigen presenting cells (APC) via its interaction with cytoskeletal proteins such as vimentin. Autoimmune polyendocrine syndrome type 1 (APS1) is a rare monogenic autosomal recessive disorder. We used the methods geometry optimization, Molecular Dynamics, Langevin Dynamics and Monte Carlo and The force fields are MM, AMBER, BIO(Charmm) and OPLS and temperatures are 295, 300, 305, 310, 315. By these methods were evaluated and significant results were obtained.

Keywords: TSGA10 protein, TSGA10 gene, Molecular Dynamics, Geometry Optimization, Charmm.

Abstract No.219

Nano Study and Simulation of the Na⁺/K⁺ Channels Proteins Membrane, Using MD/MM Methods

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Sodium channels are integral membrane proteins that form ion channels conducting sodium ions through a cell's plasma membrane. The voltage sensitivity of this channel is due to positive amino acids located at every third position. Voltage-gated sodium channels have

three types of states. channels are classified according to the type of ion for which the channel is selective, e.g. K⁺ channels, Na⁺ channels, Cl⁻ channels. Voltage gated cation (Na⁺, K⁺) channels are responsible for the generation and propagation of action potential in neurological signal transmission. K1 selective channels are widely spread in all organisms and have the ability to conduct K1 ions at near diffusion limit. The KcsA channel shares sequence and structure similarities with all members of the K1 channel family. We have used geometry optimization, molecular mechanics simulations to calculate the relative binding energies of Na and K in the KcsA ion channel. We investigated the complex of Na and K ions with ion channels in different temperature (300, 305, 310, 315) and calculated potential energy of these molecule in force fields MM, AMBER, BIO (charmm) and OPLS. Maximum potential energy of complex of Na⁺ ion channels with MONTE CARLO and OPLS method at T=300 K is 3614.84 kcal/mol.

Keywords: Molecular mechanic, KcsA ion channel, OPLS, AMBER, Hyperchem.

Abstract No.220

The Study of Glucose Interference on Interaction of Doxorubicin and Hemoglobin

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Hemoglobin (Hb) is the iron containing oxygen transport metalloprotein in the red blood cells. Quaternary structure and the associated subunit interaction property of tetrameric Hb confers it the regulatory property when small ligands such as metabolites or drugs bind to it and modulate the functional activity of this important protein. Protein-Drug interactions play an important role in a variety of biological processes and disease treatment. Doxorubicin (DOX) is a very effective anti-tumor drug that is effective in the treatment of solid tumors. It has been suggested that on reduction DOX reacts directly with oxyHb. It seems the role that Hb plays in disposition of DOX or its interaction with the drug is important. The direct interaction of this protein with drugs may also affect its functionally important structural conformation. Binding of some ligands to Hb induce alterations in the structure and function of this protein. However, competitive binding displayed by different ligands may result from allosteric effects. Hemoglobin exposure to plasma glucose causes glycation of hemoglobin in a non-enzymatic glycation pathway. Normal levels of glucose produce a normal amount of glycated hemoglobin. As the

average amount of plasma glucose increases, the fraction of glycated hemoglobin increases in a predictable way. In this study, hemoglobin was incubated with doxorubicin and with different concentrations of glucose and was studied by uv-visible spectroscopy technique. Observations showed a hyperchromic effect upon Hb treatment by doxorubicin, however this effect was relieved through glycation in elevated concentrations of glucose.

Keywords: Hemoglobin, Doxorubicin, Glycation, Ultraviolet Spectroscopy.

Abstract No.221

Purification and Biochemical Characterization of Acidic Metalloprotease from *Serratia* sp. HR-1

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Proteases are used in a great variety of commercial sectors. An acidic extracellular protease produced by an isolate from soil samples was purified to homogeneity in three steps including ammonium sulfate precipitation, SP-Sepharose cation-exchange and Sephacryl S-200 size exclusion chromatography. The purified protease exhibited an apparent molecular mass of 50 kDa either by SDS-PAGE or gel filtration chromatography. It was found as a cold-adapted acidic protease with optimum temperature and pH of 30-35 °C and 4.0, respectively. The protease showed 24% of its initial activity after incubation at 50 °C for 60 min, which indicates a relatively low thermostability. The enzyme was classified as a metalloprotease according to its unaffected function in the presence of inhibitors: Aprotinin, E-64, Chymostatin, Pefabloc SC, Pepstatin, Leupeptin, Bestatin and Antipain-dihydrochloride and its complete inhibition by 10 mM of EDTA. Although the enzyme was identified as a metalloprotease, no significant effect of 1,10-phenanthroline on caseinolytic activity showed Zn²⁺ dependency of the protein. No inhibitory function of Phosphoramidon, as a thermolysin-like metalloprotease inhibitor, revealed that the purified protease is not a member of M4 family of metalloproteases. In overall, regarding to the acidic properties and low temperature stability of the protease, it proposed that the purified acidic metalloprotease can be an ideal choice for applications in food industry especially in cheese making.

Keywords: Metalloprotease, *Serratia* sp. HR-1, Acidic Protease, Protease Inhibitors.