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Correspondence

Dr P.V.L.N. Srinivasa Rao
Executive Editor-in-Chief
Journal of Clinical and Scientific Research
Editorial office
II Floor, New OPD Block
Sri Venkateswara Institute of Medical Sciences
Tirupati 517 507
Phone: +91-877-2287777; Ext. 2465
e-mail: jcsr@svims.gov.in; editorjcsr@gmail.com

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5th National Seminar on Bioinformatics (NSBI 2014)

Poster Presentations

5th National Seminar on Bioinformatics (NSBI 2014)

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Editors' Message

Bioinformatics is attributed to have profound impact in research on human health, agriculture and environment. Acknowledging the growing importance, the Department of Biotechnology (DBT), Ministry of Science and Technology, has approved a centre for Bioinformatics Infrastructure Facility (BIF) in the Department of Bioinformatics, Sri Venkateswara Institute of Medical Sciences (SVIMS), Tirupati, for the promotion of Biology Teaching through Bioinformatics. The BIF organizes National level seminar/workshop annually to foster bioinformatics skills of researchers. The 5th National Seminar on Bioinformatics was organized from 14th to 15th February 2014 at Sri Venkateswara Institute of Medical Sciences, Tirupati. This seminar mainly focussed on drug designing also covering relevant areas of genomics and proteomics.

The *Journal of Clinical and Scientific Research,* in its endeavour to publish and highlight research has provided the scientific abstracts of the research papers (Invited lectures, oral presentations and poster presentations) presented at the 5th National Seminar on Bioinformatics to its readers as a Supplement to Vol. 3(2) of the journal.

P.V.L.N. SrinivasaRao
Executive Editor-in-Chief

B. Vengamma
Honorary Editor-in-Chief

Scientific Programme

5th National Seminar on Bioinformatics (NSBI 2014)

Friday 14th, February 2014

09:30 AM – 10:00 AM	Registration	
10:00 AM - 10:45 AM	**Inauguration**	**B. Vengamma,** Director-cum-VC, SVIMS, Tirupati
		B.C.M. Prasad, Dean, SVIMS, Tirupati
10:45 AM - 11:00 AM	Tea Break	

SESSION – I

Chairpersons: P.V.L.N. Srinivasa Rao, P.V.G.K. Sarma

11:00 AM - 12:00 noon	**A disorder induced domino-like destabilization mechanism governs the folding and functional dynamics of the repeat protein IKBα** **Athi Narayanan,** IIT Madras, Chennai
12:00 noon - 01:00 PM	**Structural Bioinformatics and protein folding** **N. Gautam,** University of Madras, Chennai
1:00 PM - 2:00 PM	Lunch Break

SESSION – II

Chairpersons: V. Jayaram, D.V.R. Sai Gopal

2:00 PM - 3:00 PM	**Accelerating drug discovery using computational drug design** **R. Raghu,** Vice-President, Schrodinger LLC
3:00 PM - 4:00 PM	**Oral Presentations**
4:00 PM - 4:15 PM	Tea Break
4:15 PM - 5:00 PM	**Poster Presentations**

Saturday 15th, February 2014

SESSION – III

Chairpersons: Alladi Mohan, P. Uma Maheswari Devi

09:30 AM - 10:30 AM	**Viral proteomics: a novel approach for human therapeutics** **D.V.R. Sai Gopal,** Head, Dept. of Virology, S.V. University, Tirupati
10:30 AM - 11:30 AM	**Proteomic approaches in combination with systems biology to reveal cancer relevant biomarkers and proteins from intracellular signaling pathways** **U. Ramesh,** IICT, Hyderabad
11:30 AM - 11:45 AM	Tea Break
11:45 AM – 1:00 PM	**Oral presentations**
1:00 PM - 2:00 PM	Lunch Break

SESSION – IV

Chairpersons: M.M. Suchitra, G. Rajitha

2:00 PM – 3:00 PM	**A computational and experimental approach for design of Inhibitors for cell division protein** **Mukesh Doble,** IIT Madras, Chennai
3:00 PM - 3:20 PM	**Antibiotic resistance challenges and recent approaches** **V.V.Lakshmi**, Dept. of Applied Microbiology, SPMVV, Tirupati
3:20 PM - 3:40 PM	**Identifying targets for common inhibitor design against strains of bacterial leaf blight and bacterial leaf streak pathogens of rice** **M. Hemanthkumar,** RARS, ANGRA University, Tirupati
3.40 PM – 4.00 PM	**Down Regulation of NF-KB by α-Mangostin: autodock analysis** **P. Uma Maheswari Devi**, Dept. of Applied Microbiology, SPMVV, Tirupati
4:00 PM – 5:00 PM	**Valedictory Session & Certificate Distribution**

A disorder induced domino-like destabilization mechanism governs the folding and functional dynamics of the repeat protein IκBα

Srinivasan Sivanandan,[1] Athi N. Naganathan[2]

[1]Department of Biotechnology, Indian Institute of Technology Kharagpur 721302, Kharagpur and

[2]Department of Biotechnology, Indian Institute of Technology Madras, Chennai

The stability of IκBα, a transcription inhibitor, is critical for the functioning of the NF-κB signaling module implicated in an array of cellular processes including disease, immunity and apoptosis. Here, we provide a quantitative picture of the folding and dynamic behavior of IκBα repeat protein employing an structure-based Ising-like statistical mechanical model that is in agreement with experimental ensemble thermodynamics and kinetics, and single-molecule measurements. We identify a unique mechanism at work in IκBα folding wherein disorder in one domain initiates a domino effect partially destabilizing neighboring domains thus resulting in a multi-- state and dynamic conformational landscape that is populated by increasingly partially folded ensembles upon destabilization. Our results provide a rationale to the promiscuous binding of IκBα, expands the functional repertoire of disordered regions in proteins and introduces a simple procedure to model disorder in systems that undergo binding-induced-folding guided by equilibrium experimental observables.

Srinivasan S, Naganathan AN. A disorder induced domino-like destabilization mechanism governs the folding and functional dynamics of the repeat protein IκBα. J Clin Sci Res 2014;3(Suppl 1):S1.

Structural bioinformatics and protein folding

N. Gautham
CAS in Crystallography and Biophysics, University of Madras, Chennai

The central paradigm of biophysics, indeed of physics in general, is 'Structure implies Function'. Thus, in order to understand and perhaps modify the behaviour of biomolecules, it is necessary to know and understand their structure. One of the most dramatic illustrations of this principle came with the discovery of the double-helical structure of DNA. It was immediately clear how DNA could function as the storage and carrier of genetic information. Protein structure and virus structures also illustrate the truth of this principle.

Proteins are an important class of biological polymers. They range in size from a few kilodaltons to hundreds of kilodaltons. All proteins are built up from 20 amino acids, which constitute the monomers. The sequence in which these amino acids are arranged differs from protein to protein and is referred to as the primary structure of the protein. Some sequences of amino acids are known to arrange themselves into regular three-dimensional structures that are referred to as the secondary structure of the proteins. At the next level of structural organisation, the secondary structural units arrange themselves into globular shapes. This is called the tertiary structure and is stabilised mainly by interactions between the amino acid side chains. Also discernible at this level are domains corresponding to compactly arranged groups of secondary structural features. In the next higher level of structure, globular folded polypeptide chains come together in specific arrangements called the quartenary structure.

Thermodynamic experiments by Anfinsen have shown that the functional three-dimensional structure of the protein is encoded in its primary amino acid sequence. Thus a polypeptide chain in solution will automatically fold into its three dimensional structure given only that the conditions of temperature, ionic strength, pH, etc., are within a fairly wide range. The nature of the forces and natural algorithm involved in this process areas yet not completely understood. This makes the task of understanding protein structure and of predicting its structure from knowledge of only the sequence a demanding one.

Gautham N. Structural bioinformatics and protein folding. J Clin Sci Res 2014;3(Suppl 1):S2.

Abstracts of Invited Lectures (NSBI 2014)

Accelerating drug discovery using computational drug design

R. Raghu
Vice-President, Schrodinger LLC

Today computational techniques play a critical role in pharmaceutical research and development. Thanks to recent advancements in understanding the biology, growth in vast amount of biological data which led to the need to analyse these data and fetch out the valuable information. Computational techniques are widely adopted in understanding the structure function relationship, screening millions of molecules and in lead identification and optimization. My talk would highlight on how these computational techniques helped in screening and designing molecules for few tough targets in shorter span of time to the file IND and clinical trials. Talk will also highlight the importance and role of water molecules CADD.

Raghu R. Accelerating drug discovery using computational drug design. J Clin Sci Res 2014;3(Suppl 1):S3.

Viral proteomics: A novel approach for human therapeutics

D.V.R. Sai Gopal
Department of Virology, Sri Venkateswara University, Tirupati

Viruses are an obligate parasites have classified as non-enveloped and enveloped viruses and also have unique features of Genome diversity as dsDNA, ssDNA, dsRNA, ss RNA viruses, segmented genomes, partite characters. Viruses have been studied not only for their pathology and associated disease but also as model systems for molecular processes and as tools for identifying important cellular regulatory proteins and pathways. Recently the mass spectrometry approaches revealed the development of proteomic have greatly facilitated the detection of virion components. Viral protein interactions in infected cells and virally induced changes in the cellular proteome, resulting in a more comprehensive understanding of viral infection. The high-resolution structures for viral proteins have explained the mechanism of action of these viral proteins as well as aided in the design and understanding of specific inhibitors that could be used in antiviral therapies. The viral proteomic studies conducted on all eukaryotic viruses and bacteriophages, covering virion composition, viral protein structures, virus-virus and virus-host protein interactions, and changes in the cellular proteome upon viral infection. Many approaches have successfully analyzed the composition of a variety of virions and those have proven to be complementary and together have led to a more complete picture of the viral particle and the data sets obtained by different methods and can result in missed or additional protein identifications in viral coded proteins in the host system. Enveloped DNA viruses – pox, herpes, in general are composed of a large number of viral proteins, including many that are not strictly structural but are known or predicted to function once released into the host cell. In herpesviruses, the tegument is the major site of packaging of these proteins and several host proteins are also packed in HIV, vaccinia virus and herpesvirus particles. There is some overlap in the nature of the host proteins packaged in all of these virions, several highly abundant host proteins have been reported for many types of virions eg. actin, β-tubulin, elongation factor 1α, elongation factor 2, hsp70, and hsp90 have been found in HIV, vaccinia virus and two or more types of herpesvirus virions. It is not yet known whether these cellular proteins play a conserved functional role in these virions, are passenger proteins that are accidentally packed due to their location and high abundance or are contaminants that copurify with the virions. The latter possibility seems unlikely, since the different types of virions analyzed were prepared using different methods and, in each case, checked for purity prior to analysis. Whether or not the above-described host proteins are purposefully packaged in the virions will require more extensive investigation. However, it is not hard to imagine that host chaperone proteins like hsp70 and hsp90 may be required to chaperone various viral proteins during packaging and/or release from the virions and hence are packaged along with their viral partners. This will be thoroughly discussed at the time of presentation.

Sai Gopal DVR. Viral proteomics: a novel approach for human therapeutics. J Clin Sci Res 2014;3(Suppl 1):S4.

Proteomic approaches in combination with systems biology to reveal cancer relevant biomarkers and proteins from intracellular signaling pathways

Ramesh Ummanni

Center Chemical Biology, CSIR-Indian Institute of Chemical Technology Tarnaka, Hyderabad

Cancer is the leading problem causing most of the deaths in western countries. Especially lung and prostate cancers are standing first in row in cancers affecting men. High accurate diagnostic procedures as well as better treatment strategies enable to treat cancer patients early and effectively save their life. Deficient sensitivity and specificity of current diagnostic methods for prostate diseases demand further investigations. Proteomic analysis of tissue samples is a promising approach for molecular characterization and is usually performed on surgical material. Using 2DE in combination with mass spectrometryapproach we identified a panel of differentially expressed proteins. However, analysis of large-scale proteomes with biological context is very difficult. Further, we have implemented various bioinformatics tools for validating proteomic data and characterized interesting proteins using *invitr*o cellular models. As aforementioned, lung cancer is also major problem and due to heterogeneous types of lung cancer often patients will develop resistance to treatment. We applied proteomics approach especially Reverse phase protein arrays (RPPA) to address cancer initiating signaling pathways associated with molecular subtypes of lung cancer further to stratify patients for personalized medicine.

Ramesh U. Proteomic approaches in combination with systems biology to reveal cancer relevant biomarkers and proteins from intracellular signaling pathways. J Clin Sci Res 2014;3(Suppl 1):S5.

A computational and experimental approach for design of inhibitors for cell division protein

Mukesh Doble

Department of Biotechnology, Indian Institute of Technology Madras, Chennai

Antimicrobial resistance is a global concern and the emergence of resistant bacteria has necessitated the need to discover new drugs as well identifying new targets. FtsZ (Filamenting Temperature Sensitive mutant Z) is a bacterial cytoskeleton protein which assembles into a protofilament. In the cell division in bacteria assembly of FtsZ takes place at the assembly site. FtsZ has GTPase activity as well as polymerisation. FtsZ has become an attractive target, due to its evolutionary distance from eukaryotic tubulin. The structures of tubulin and FtsZ show striking similarity; together with the functional similarities, provides a strong indication that it is a true homolog of tubulin. FtsZ displays a Mg^{2+} dependent GTPase activity. A substituted benzamide and thiazolopyridine moieties linked with an ether bond is known to kill methicillin-resistant Staphylococcus aureus, Staphylococcus, and Bacillus subtilis by targeting the FtsZ. This talk will focus on design of phytochemicals based inhibitors for this protein using computational and experimental techniques. These natural products inhibit both the GTPase as well as the polymerisation ability of the protein. Quantitative structure activity relationship is developed to determine the structural feature necessary in the small molecule for the observed activity.

Doble M. A computational and experimental approach for design of inhibitors for cell division protein. J Clin Sci Res 2014;3(Suppl 1):S6.

Antibiotic resistance-challenges and recent approaches

V.V. Lakshmi

Department of Applied Microbiology, S.P. Mahila Visvavidyalayam, Tirupati

Bacterial resistance to antibiotics is an increasingly serious threat to the ability to routinely treat microbial infections. The emergence of bacteria resistant to several important classes of antibiotics has become a major clinical problem in the last decade. This is resulting in increased hospitalization and mortality. While it is well recognized that there is an urgent need to develop new antibiotics, attempts to identify novel classes of compounds have been remarkably less productive. There has been an almost a 30 year gap before the clinical introduction of two new types of systemic antibiotics in 2000 (the oxazolidinones, linezolid FDA approved 2000) and 2003 (the lipopeptides, daptomycin FDA approved 2003). Furthermore, structural or mechanistic novelty does not guarantee immunity from resistance, with strains resistant to linezolid identified prior to FDA approval. Two Gram positive bacteria, *Enterococcus faecium and Staphylococcus aureus*, are members of the 'ESKAPE' family of pathogen 'superbugs' that have developed partial or complete resistance to multiple antibiotics. The synergistic use of either ampicillin or vancomycin with an aminoglycoside, such as kanamycin or gentamicin, has long been the optimal therapy for serious Enterococcal infections. However, many previously susceptible Enterococcal strains have since acquired resistance to the aminoglycosides. Resistance to the aminoglycosides through enzymatic deactivation, although seemingly straightforward, is in reality a complex problem involving three different classes of enzyme namely ATP dependent phosphotransferases (APH) and adenyltransferases (ANT), and the acetyl coenzyme A-dependent *N*-acetyltransferases (AAC). Thus it is imperative that new antibiotics need to be developed to tackle global public-health problem. Bioprospecting natural antimicrobials, host defense peptides or antimicrobial peptidesusing genomic approaches are being actively pursued from the largely underexplored marine environment, that holds promise as a source of unusual bioactive metabolites. Structural biology is another important approach presently utilized to counter antibiotic resistance. This includes modifying existing antibiotics to overcome resistance mechanisms. The structures of enzymes mediating resistance present opportunity to rationally develop effective new drugs more rapidly than screening for new structures. The crystal structure of several antibiotic modifying enzymes and their preferred substrate complexes and the competitive inhibitors are determined to identify the specific interaction and mechanisms of antibiotic inactivation. The analysis of structure in association with bioinformatics analysis is revealing possible way to circumvent the activity. The example of how crystal structure of APH(2") family phosphotransferases determined can be used to develop modified aminoglycoside that still binds to the recognition site at the "base" of the APH(2")-IIa binding cleft, but have restricted interaction between potential sites of phosphorylation on the substrate and the phosphate of ATP is elucidated.

Lakshmi VV. Antibiotic resistance-challenges and recent approaches. J Clin Sci Res 2014;3(Suppl 1):S7.

Identifying drug targets for common inhibitor design against strains of bacterial leaf blight and bacterial leaf streak pathogens of rice

Marisetti Hemanthkumar

Principal Scientist, Bioinformatics Lab, Institute of Frontier Technologies, RARS, ANGRA University, Tirupati

Rice (*Oryza sativa (L.*)) is one of the important staple food crops in India fulfilling 43% of the caloric requirement of Indian population. An improvement in the production from 105.3 mt to 140 mt strengthens the country's food grains security by 2025. This target is challenged by various abiotic and biotic factors. Of the many causes for low productivity, biotic factors contribute more and make rice cultivation difficult. Among the biotic factors bacterial diseases are difficult to control. The two most important bacterial diseases are bacterial leaf blight and bacterial streak caused by *Xanthomonas oryzae* pathovar *oryzae* (Xoo) and *Xanthomonas oryzae* pathovar *oryzicola* (Xoc), respectively. Xoo and Xoc collectively cause crop losses up to 50%. Control methods that are in vogue are not effective and are not practiced. Many researchers have focused on a single strain of one pathogen to develop control measures. Presence of different strains of the pathogens makes the control complicated. However availability of genomes of the pathogens and host along with bioinformatics tools opens a possibility of developing a common bactericide to combat the devastating effects of many strains of more than one related pathogens. Genome sequences of nine strains of Xoo and Xoc were retrieved from NCBI. Among them the genomes of four strains were completely sequenced. Pv. *oryzae* KACC 10331 is prevalent in Asiatic countries and was used as reference organism. The strains; KACC 10331, MAFF 311018, PXO 99 A and BLS 256 genomes were compared to find 4115 common genes. Analysis of 4115 common proteins using Database of Essential Genes revealed that 1622 genes were essential for survival of *Xanthomonas oryzae*. 965 essential genes were non-homologous to *Oryza sativa* therefore could be considered as common potential drug targets. Twenty one common drug targets were very unique to the pathogens with no hits against host genome. These drug targets would be intriguing starting point for rational drug design against bacterial leaf blight and bacterial streak diseases in rice.

Hemanthkumar M. Identifying drug targets for common inhibitor design against strains of bacterial leaf blight and bacterial leaf streak pathogens of rice. J Clin Sci Res 2014;3(Suppl 1):S8.

Down regulation of NF-κB by α-Mangostin: Autodock analysis

Palempalli Uma Maheswari Devi

Department of Applied Microbiology, Sri Padmavati Mahila Visvavidyalayam, Tirupati

α-Mangostin, a bioactive natural product derived from the pericarp of Mangosteen fruit belongs to *Garcinia mangostana*. In this study, the concept of docking was utilized to understand the interaction between inflammatory mediators and α-Mangostin. By using Auto Dock 3.0, the molecular interaction mechanisms of α-Mangostin and Indomethacin with the two pro-inflammatory genes namely COX-2 and iNOS, which are involved in chronic inflammation was investigated. Comparative docking of Indomethacin and α-Mangostin with COX-2 suggested a similar hydrogen bond interaction with Ser353. In addition, Indomethacin showed hydrogen bonds with Arg120 and Trp387, and these residues lie at the junction of the anchoring site of the COX-2 active site. The lack of selectivity towards Arg120 may be a significant component of α-Mangostin selectivity towards COX-2. The docking energies of α-Mangostin and Indomethacin with iNOS were found to be -12.20 kcal/mol and -2.75 kcal/mol respectively. The elevated levels of mPGES-1 are often observed concomitantly with COX-2 over-expression. In fact, *in vitro* studies have demonstrated that mPGES-1 is localized at the perinuclear membrane and endoplasmic reticulum and is in general functionally coupled with COX-2, thereby enabling efficient generation of PGE_2 during inflammation. The present docking analysis of α-Mangostin into the active site of mPGES-1(PDB_ID:3DWW) showed a hydrogen bond interaction with Arg180 of bond length 1.965AU.The transcription factor NF-κB is a very interesting target molecule for designing anti-inflammatory, anti-tumoral and pro-apoptotic drugs . Proper function of the NF-κB network is therefore critical for human health. The docking of α-mangostin into the active site of NF-κB showed two strong hydrogen bond interactions with Arg30, Leu280 residues and the obtained docking energy was –7.81kcal/mol.

Funded by: DST-SERC programme

Uma Maheswari Devi P. Down regulation of NF-κB by α-mangostin: Autodock analysis. J Clin Sci Res 2014;3(Suppl 1):S9.

Temperature dependent extracellular synthesis and characterization of nanoscale calcium pyrophosphate crystals using marine thermophilic bacteria

N. Supraja

Department of Biotechnology, Thiruvalluvar University, Vellore

We report for the first time on temperature dependent extracellular synthesis of nanoscale calcium pyrophosphate (α Dicalcium phosphate and β Dicalcium phosphate) crystals using thermophilic *Bacillus* sp. which is isolated from marine environment rocks. This calcium precipitating bacterium was identified by biochemical test and microbiological aspects of calcium pyrophosphate crystals and their role on corrosion and these biogenic calcium crystals were analyzed using XRD, FT-IR techniques. The corrosion behavior of Calcium precipitating bacteria (CPB) on mild steel was studied by the electrochemical method (Polarization and Impedence). The calcium pyrophosphate crystals formations by bacteria reduces the cathodic corrosion current in CPB-1, 2, 3 and CPB-4 reduces anodic corrosion current, where resistance was lower in the prescence of bacteria. It is claimed that the temperature is one of the causative factor for calcium carbonate crystals formation and corrosion in marine water system.

Supraja N. Temperature dependent extracellular synthesis and characterization of nanoscale calcium pyrophosphate crystals using marine thermophilic bacteria. J Clin Sci Res 2014;3(Suppl 1):S10.

Molecular modelling strategies of drug design

G. Tulasi

Deparment of Sericulture (Division of Zoology), Sri Padmavathi Mahila Visva Vidyalayam, Tirupati

The action of a drug on the organism implicates the physico-chemical binding of a drug molecule to the target protein, which induces pharmacological and toxicological effects. The biological reactions are beneficial or adverse, manifestation of the drug molecule and determined by the interactive binding between definitive atoms or groups of the drug molecule and the macromolecular target in three-dimension. The interaction of a drug with the organism involves both the disposition of a drug by the organism and the action of a drug on the organism. Such critical atoms, groups, or fragments responsible for the interaction reflect the microscopic structures of drug molecules and are called pharmacophore. In this context, a drug molecule is presumed as an assembly of macroscopic property and microscopic structure, with the macroscopic properties determining the absorption, distribution, metabolism and elimination of drugs and the microscopic structure coining pharmacological action. The goal of molecular drug design is to integrate the macroscopic and microscopic factors in optimized manner.

Tulasi G. Molecular modelling strategies of drug design. J Clin Sci Res2014;3(Suppl 1):S11.

In silico modelling and drug designing of epidermal growth factor receptor (EGFR) involved in cancer

Jayasimha Rayalu Daddam,[1] CH. Bhargavi,[2] Venkata Swamy Tangeti,[3] Ramesh Konka[4]

[1]Department of Biotechnology, JNTUA, Anantapur and
[2]Department of Biotechnology, DR.Rayalu's Biotech PVT LTD, Himayat nagar, Hyderabad and
[3]Department of Chemistry, Pondicherry Central University, Pondicherr. and
[4]Department of Biotechnology, Akshaya Biological Corporation, Himayat nagar, Hyderabad

The epidermal growth factor receptor (EGFR), cell-surface receptor for epidermal growth factor family exists on the cell surface and is activated by binding to epidermal growth factor. Mutations that lead to EGFR over expression have been associated with a number of cancers. In this work we have identified a better inhibitor for mutated EGFR to reduce the Cancer risk. In order to understand the mechanisms of interactions between the drug derivatives and the EGFR, a three-dimensional (3D) model of the EGFR was generated based on the crystal structure of the Template by using Modeller. After BLAST search sequence that showed maximum identity with EGFR was aligned and used as a reference template to build a 3D model for EGFR. The final model obtained was further assessed by ERRAT and Ramachandran plot, which shows that the model is reliable. With this model, a flexible docking study is performed with Gefitinib derivatives. After the docking studies, important determined residues in binding were identified. The hydrogen bonds play an important role for the stability of the complex. These results may be helpful for further experimental investigations.

Daddam JR, Bhargavi CH, Tangeti VS, Konka R. *In silico* modelling and drug designing of epidermal growth factor receptor (EGFR) involved in cancer. J Clin Sci Res 2014;3(Suppl 1):S12.

Role of glycolysis enzymes in cancer development

B. Ravi babu and M. Jagadish Naik
Departments of Biotechnology and Zoology and Aquaculture, Acharya Nagarjuna University, Guntur

Glycolysis is the process for preparing, and breaking down, glucose to make pyruvic acid, which is used in anaerobic respiration or as one of the starting reactants in the citric acid cycle. Three points in the process of glycolysis occur with a large negative free energy and are therefore, irreversible. These three points are hexokinase, phosphofructokinase, and pyruvate kinase.Cells can obtain energy through the oxygen-dependent pathway of oxidative phosphorylation (OXPHOS) and through the oxygen-independent pathway of glycolysis. Since OXPHOS is more efficient in generating ATP than glycolysis, it is recognized that the presence of oxygen results in the activation of OXPHOS and the inhibition of glycolysis (Pasteur effect). However, it has been known for many years that cancer cells and non-malignant proliferating cells can activate glycolysis in the presence of adequate oxygen levels (aerobic glycolysis or Warburg effect). Accumulating evidence suggests that the persistent activation of aerobic glycolysis in tumor cells plays a crucial role in cancer development; the inhibition of the increased glycolytic capacity of malignant cells may therefore represent a key anticancer strategy.glycolysis generates pyruvate from glucose,which is further metabolise to produce ATP,and various intermediate precursors which are utilized for the biosynthesis of cellular components.The first step of glycolysis,which is catalyzed by an evolutionary conserved enzyme.These enzymes show various concentration changes results in the development of cancers in humans.

Ravi Babu B, Naik MJ. Role of glycolysis enzymes in cancer development. J Clin Sci Res 2014;3(Suppl 1):S13.

Structure based pharmacophore modelling and virtual screening of potent inhibitors for ADAMTS1

Anushree Majumdar, Puja, Rathi Suganya
SRM University, Chennai

ADAMTS1 [Disintegrin and metalloproteinase with thrombospondin motif-1] is a secreted protein which belongs to ADAM protein family. It is an enzyme that in humans is encoded by the *ADAMTS1* gene. The expression of this gene may be associated with various inflammatory processes as well as development of cancer cachexia. This gene is likely to be necessary for normal growth, fertility, organ morphology and function. Aggrecanases from the ADAMTS family are important therapeutic targets due to their essential role in aggrecan depletion in arthritic diseases. The structure of the protein ADAMTS1 (2V4B) was retrieved from protein data bank (PDB). In Maestro (Schrodinger product), the structure was imported and the protein preparation wizard was used to optimize and minimise the structure. The ligands binding to ADAMTS1 were retrieved from Binding DB. The ligand preparation was done doing Ligprep option in Schrodinger. The ligand in the protein was selected and grid was generated for the chosen ligand using receptor grid generation option in Maestro. After protein and ligand preparation, they were taken for docking studies. Ligand with CID 10160968 was found to be the best ligand with XP GScore -10.723, kcal/mol. Schrödinger module of energy based pharmacophore (EPharmacophore) was used for the structure based screening of unknown ligands. The result of Epharmacophore contains the functional groups which are involved in their bioactivity towards target protein. From the 7 features generated, 3 features (1 donor, 1 acceptor, 1 ring) were selected based on hydrogen and hydrophobic interactions. The above result was then used to screen the zinc database for natural and synthetic compound containing 3,55,467 and 2,31,029 unique structure records respectively and then using find matches to hypotheses option in the 'Phase' tab, 535 and 2478 compounds with matching pharmacophoric features were found for zinc natural and synthetic compounds . The matched compounds were screened. 5 and 4 unique compounds were obtained for zinc natural and synthetic compounds respectively. From the five zinc natural compounds, ZINC00652090 compound had the maximum docking score of -9.24 kcal/mol. From the four synthetic compounds, Pub Chem cid 54352406 had the maximum docking score of -10.95 kcal/mol.

Majumdar A, Puja, Suganya R. Structure based pharmacophore modelling and virtual screening of potent inhibitors for ADAMTS1. J Clin Sci Res 2014;3(Suppl 1):S14.

Validation of Bhageerath and Bhageerath-H Software Tools

A. Ranganadha Reddy, K. Bhanu Prakash
School of Biotechnology, Vignan University Vadlamud, Guntur

Generally, to know the structure of a protein X-ray crystallography or NMR techniques are followed but in some cases such as family B GPCRs these techniques are always not successful. So, we opted for the homology modeling techniques. There are many softwares available in the market which is both free for access and to be paid for their usage; two of those free softwares available in the market are Bhageerath and Bhageerath-H. Study of these two softwares was presented in the paper. Computational tools of SCHRÖDINGER software were used for molecular dynamics studies.

Ranganadha Reddy A, Bhanu Prakash K. Validation of Bhageerath and Bhageerath-H Software Tools. J Clin Sci Res 2014;3(Suppl 1):S15.

New anti-inflammatory p-acetamido phenol derivatives: molecular docking and synthesis

B. Kiruthiga, P. Valentina

SRM college of pharmacy, Kattangulathur, Kancheepuram Dist., Tamil Nadu

Objective: In an attempt to discover potent anti-inflammatory agents with minimum adverse effects, a series of p- acetamido phenol derivatives with a wide range of heterocyclic substitutions viz, thiazine, oxazine, isoxazine, Isoxazole and pyrazole were hypothetically designed by ligand based virtual screening methods.

Method: The molecular docking studies was carried out with Argus Lab-12 software. The crystal structure of the enzymes 5-lipoxygenase (PDB code:3V92) and thromboxane synthetase (PDB code: 1TQN) were obtained from protein data bank. The ligands were sketched using ACD Chemsketch and the length of the hydrogen bond was measured by PyMOL software.

Result and interpretation: The ligand pose energy of the designed entities is in the range of -7.565 kcal/mol to -10.541 kcal/mol for both the enzymes. The target compounds were synthesized by Claisen-Schmidt condensation and characterized by IR, ^{1}HNMR and Mass spectral studies. The *in vitro* anti-inflammatory activity of the synthesized compounds was evaluated by HRBC membrane stabilization method. The compounds showed noticeable activity with percentage inhibition of 59.87% to 68.59%. The derivatives were subjected to Lipinski's rule of five and were in compliance with standard drug likeness parameters.

Conclusion: From the above findings it is evident that the *in vitro* studies corroborate with the binding interactions of the synthesized compounds through docking studies.

Kiruthiga B, Valentina P. New anti-inflammatory p-acetamido phenol derivatives: molecular docking and synthesis. J Clin Sci Res 2014;3(Suppl 1):S16.

Docking studies on the anti-diabetic potency and efficacy of the glycosides jamboline and chrysanthemin

K. Anita Priyadharshini, P. Valentina

SRM College of pharmacy, Kattangulathur, Kanchipuram dist.

Objective: Diabetes mellitus (DM), is one of the diseases for which innumerable synthetic drugs have been discovered and put into use. In traditional Indian medicine, two plants *Syzygium cumini* commonly called Jamun and *Chrysanthemum cinnerarifolium* known as Crown daisy are well-known for their anti-diabetic claims. In the present study, Jamboline and Chrysanthemin, the main glycosides present in the above two plants respectively, have been selected for docking studies.

Method: These two ligands were sketched with ACD Chemsketch 12 and the enzymes aldolase, α-amylase, dipeptidyl peptidase and N-acetyl β-glucosaminidase, which are involved in mediating DM was accessed from the Protein data bank.(PDB codes:1WA3,1HVX,1Z68,1ZHO). Molecular docking studies were done using Argus Lab-12 and visualized with a PyMOL viewer.

Results: Effective docking of the two ligands with the enzymes was observed. Jamboline and Chrysanthemin showed docking scores of -6.2685 kcal/mol and -10.7938 kcal/mol respectively with dipeptidyl peptidase and scores of -6.7703 kcal/mol and -10.0643 kcal/mol respectively, with enzyme α-amylase. In addition, Jamboline showed a docking score of -5.3618 kcal/mol with N-acetyl β-glucos aminidase and Chrysanthemin gave a score of -9.6323 kcal/mol with the enzyme aldolase.

Conclusions: Both ligands effectively bind with the enzymes and thus the mechanism of anti-diabetic action can be hypothetically traced. Comparison between the two ligands reveals that chrysanthemin is a much better anti-diabetic entity than jamboline hypothetically, and these findings can help in further ligand –based virtual screening.

Priyadharshini A, Valentina P. Docking studies on the anti-diabetic potency and efficacy of the glycosides jamboline and chrysanthemin. J Clin Sci Res 2014;3(Suppl 1):S17.

Prediction and analysis of novel inhibitors against oestrogen-related receptor alpha

Y. Suneetha, C. Kumaraswamy Naidu

Department of Zoology, Sri Venkateswara University, Tirupati

Estrogen-related receptor alpha (ERRalpha) is a nuclear receptor involved in the control of energy metabolism. Protein encoded by ERRalpha act as a site-specific transcription regulator known to interact with estrogen and is closely related to the estrogen receptor. ERRalpha is one of the most studied one in the context of breast cancer i.e., as a negative prognostic marker in ER (–) tumors it induces VEGF mRNA expression and contributes to the malignant phenotype of a breast cancer cell line. Being a key receptor in the malignancy of breast cancer, predicting the novel inhibitors against ERR alpha is an important area of research. In the present study we use the bioinformatics tools to predict novel inhibitors against ERRalpha.

Suneetha Y, Naidu CK. Prediction and analysis of novel inhibitors against oestrogen-related receptor alpha. J Clin Sci Res 2014;3(Suppl 1):S18.

Prediction and analysis of inhibitors for phosphoprotein phosphatase-2A

B. Uma Devi, C. Kumaraswamy Naidu, Y. Suneetha

Department of Zoology, Sri Venkateswara University, Tirupati

Lung cancer is one of the significant cancers faced by the people around the world. Target based cancer therapy plays a prominent role in lung cancer and control Non-Small cell lung carcinoma (NSCLC). Phosphoprotein phosphatase-2A (PP2A) is considered as a marker protein for lung cancer and is expressed ubiquitously in cells and is known to interact with cancer causing factors leading to lung cancer risk. Therefore, inhibiting PP2A may play a key in regulating the tumor growth. In the present study, we designed relational molecules for PP2A through computational approach.

Uma Devi B, Naidu CK, Suneetha.Y. Prediction and analysis of inhibitors for phosphoprotein phosphatase-2A. J Clin Sci Res 2014;3(Suppl 1):S19.

Analysis of structural impact of CHEK2 variations in breast cancer

C. Kumaraswamy Naidu,[1], Y. Suneetha,[2] K. S. N. M. Megana[2]

Department of Zoology, Sri Venkateswara University, Tirupati

Breast Cancer is one of the common cancers faced by women around the world. Several factors that may confer susceptibility include genetic and non genetic. Some of the non genetic factors include lifestyle, environmental factors whereas genetic factors include variations in the low, medium and high penetrance genes. One such genetic factors conferring susceptibility to breast cancer are variations in *CHEK2* gene. In the present study, we analyze the structural impact of such variations in CHEK2 using *in silico* approach.

Naidu CK, Suneetha Y, Megana KSNM. Analysis of structural impact of CHEK2 variations in breast cancer. J Clin Sci Res 2014;3(Suppl 1):S20.

Drug designing of hypothetical protein (HSP) 90

T. Madhuri, B. Lakshmi kalyani and P. Suvarnalatha Devi

Department of Applied Microbiology, Sri Padmavathi Mahila Visvavidyalam, Tirupati

The complete human genome sequence in the public database available, which provides a way to understandthe blue print of life. The human genome may be limited to about 30,000 genes where as the human proteome may be estimated of one million proteins. Legions of protein have been described and information about these structures is readily available in databanks. There remains a large series of unknown or hypothetical proteins (HPS) might be involved in the pathomechanisms of brains abnormality in Down syndrome. Hypothetical proteins may provide biochemical or biophysical /molecular experimental methods can assign accurate function for genes in these genomes,however the process is time consuming and costly.several computational algorithms have been developed for predicting protein function using the information derived from sequence similarity, phylogenetic profiles, protein-protein interactions, protein complex and gene expression profiles. Importance of context information the database STRING was developed which is a precomputed global resource for the exploration and analysis of these associations. STRING is updated continuously and currently it contains 261,033 orthologs in 89 fully sequenced genomes. The database predicts functional interactions at an expected level of accuracy of at least 805% for more than half of the genes. The aim of our present study was to identify function of hypothetical protein >gi/6807647 by sequence similarity searching tools PSI-BLAST. Our hypothetical protein shares 63% homologous to Hsp 90-Sba 1 closed chaperone. Which shows asemerging target for rationalchemotherapy of many cancers. Further, we have identified its domains, family and signal etc. Due to lack of crystal structure of our hypothetical protein we have modeled by taking template as HSP90-SBA1.further we have performed docking studies with anticancer drugs.

Madhuri T, Lakshmi Kalyani B, Suvarnalatha Devi P. Drug designing of hypothetical protein (HSP) 90. J Clin Sci Res 2014;3(Suppl 1):S21.

Preliminary analysis of data on prevailing breast cancer in the district of Guntur

P. Priyadarshini, J. Rajeswari

Department of Biochemistry, Acharya Nagarjuna University, Guntur

Breast cancer is the third most common cancer in the world. In India, it is the second leading cancer in females. It can spread to nearby lymph glands, pleura, bone, pelvis and liver. It can also spread to other parts of the body without invading the auxiliary nodes even when the primary breast tumor is small.

The mammographic, histopathological studies and FNCA reports of the women showed rich cellularity consisting of ductal epithelial cells arranged in sheets, loose clusters and discretely. The cells reveal mild to moderate nuclear pleomorphism and inconspicuous nucleoli. Smears from nodule of left anterior axillary fold also show similar picture along with occasional macrophages and lymphocyte which is suggestive of duct cell carcinoma. Data collected from case history of 100 women in Guntur district, showed with one or more different types of high risk histopathologic lesions (80%), tubular hyperplasia (37%) and ductal carcinoma in situ (43%). We further demonstrated the familiar predisposition to the breast cancer in a population prevailing to the hereditary, age of the individual at risk with their food habits. The data showed the higher risk with 65% of women under the age of 55 years may be due to change in the hormonal levels and 35% in above 55-75 years aged persons with a positive family history as well with age related factors. When considered the food habits, it reveals that 100% of the women with risk are consumers of rich protein and fat diet in the form of non vegetative food.

Priyadarshini P, Rajeswari J. Preliminary analysis of data on prevailing breast cancer in the district of Guntur. J Clin Sci Res 2014;3(Suppl 1):S22.

Identification and docking studies of phyto constituents as competitive antagonists against metabotropic glutamate receptor 5, towards a better drug lead for epilepsy

S.Vijayasri,[1] Soumendu Sanyal, Waheeta Hopper[2]

Department of Bioinformatics, Faculty of E& T, SRM University, Kattankulathur

Background: Metabotropic glutamate receptors (mGluRs) are G protein-coupled receptors involved in the regulation of glutamergic transmission. There are eight types of mGluRs which is divided into three sub-groups (I-III) according to their sequence similarity, transduction mechanism and pharmacological profile. Epilepsy is a long-term neurological disorder characterized by epileptic seizures. Recent studies indicate that excitatory group I mGluRs (mGluR1 and mGluR5) contribute to neurotoxicity and hyperexcitability during epileptogenesis. Due to anxiolytic, antidepressant and anti-addictive effect mGlu5 has always been in the list of interest for pharmacological studies. We propose that the epilepsy can be controlled by targeting and inhibiting these excitatory glutamate receptors.

Methods: To our knowledge, none of the approved anti-epileptic drugs functions by inhibiting these receptors. A dataset of approved anti epileptic drugs and the phytochemicals form the plants that are being used traditionally for treating epilepsy was docked against this receptor using extra precision docking.

Results: The phytochemicals were found to interact with the glutamate active site residues. They also showed favourable bonded and non-bonded interactions with satisfactory docking scores comparable to that of the drugs. The ADMET properties have also been studied.

Conclusions: Based on the study, the phytochemicals with the competitive antagonistic activity against mGluR5 have been identified using computational approaches. These can be verified for their activity using wet lab techniques. Hence in future, these can well be considered as drug lead for the treatment of epilepsy.

Vijayasri S, Sanyal S, Waheeta Hopper. Identification and docking studies of phyto constituents as competitive antagonists against metabotropic glutamate receptor 5, towards a better drug lead for epilepsy. J Clin Sci Res 2014;3(Suppl 1):S23.

Energy based pharmacophore modelling and virtual screening for identification of potential inhibitors for GSK3β

J.B. Sheema, Sivaranjani, Anshika Srivastava, Waheeta Hopper

Department of Bioinformatics, School of Bioengineering, SRM University, Kattankulathur

Background: Wound healing is a highly ordered and well-coordinated process that involves inflammation, cell proliferation, matrix deposition, tissue modeling, collagenation and epithelialization. It has been proven that Wnt/b-catenin pathway can enhance wound healing through the inhibition of GSK3β protein which is an important regulatory enzyme. Several plant compounds have been used experimentally to treat skin disorders, including wound injuries in traditional Indian medicine.

Objectives: Energy based pharmacophore modeling and virtual screening for identification of potential Inhibitors for GSK3β.

Methods: The Molecular docking of ligand molecules nitrofurazone, sulphathiazole (standard drugs) and entagenic acid, lupeol, oleanolic acid (phytoconstituents) with GSK3β was performed. After docking the best inhibitor was selected and the docking result was then imported to find the pharmacophoric features. The constructed e-pharmacophore model was screened with more than 70 active phytoconstituents to find out novel compounds with similar pharmacophore features that can act as potentially active compound against GSK3β. Docking simulation of GSK3 β and the novel compounds was performed using the Glide docking program in Schrödinger software. The highest scoring phytoconstituents were selected for further evaluation.

Conclusions: After visual inspection, the most favorable compounds with the best binding modes (High glide score,Glide energy and length of the hydrogen bond) were selected. The active inhibitor would be further evaluated for wound healing using animal models to find the most effective inhibitor against GSK 3β.

Sheema JB, Sivaranjani, Srivastava A, Hopper W. Energy based pharmacophore modelling and virtual screening for identification of potential inhibitors for GSK3β. J Clin Sci Res 2014;3(Suppl 1):S24.

Phylogeny of estuarial prawn on Alikuppam coast, Tamilnadu

M. Muthukumaran,[2] Nagalakshmama, [1]A.Vijaya Baskara Rao
[1]Department of Ecology and Environmental Sciences, Pondicherry University, Puducherry and
[2]Department of Sericulture, Sri PadmavathyWomens University, Tirupati

It is well known that a phylogenetic tree contribute a vital idea of the inferred evolutionary relationship among living organism. The present study is aimed to analyse the origin and maintenance of prawn biodiversity in Alikuppam estuary coast. The genus of Fenneropenaeus, Penaeus, Metapenaeus are estuarial and marine living prawns in order of Decapod crustaceans that was found in estuarial region of Alikuppam. In our study the phylogenic tree of prawn were constructed, which are based on cytochrome oxidase. The cytochrome oxidase encountered in 6 prawns. Among the prawns, the phylogenic evolutionary relationships obtained from the ecological adaptation by different forms of migration. The phylogenic tree of prawn was analyzed by using the cytochromes oxidase and it was claded into two groups. The results suggest that protein level of unpaired rooted phylogeny relationships among the prawns due to ecological adaptations of corresponding protein.

Muthukumaran M, Nagalakshmama, Vijaya Baskara Rao A. Phylogeny of estuarial prawn on Alikuppam coast, Tamilnadu. J Clin Sci Res 2014;3(Suppl 1):S25.

Development of a new rating scale as a need to make improvements to an existing measure in the qualification process for drug development tools

Swaroopa Maralla
Academic Consultant, Department of Sericulture, Division of Zoology,
Sri Padmavathi Mahila VisvaVidyalayam, Tirupati

Recent advances in biomedical science as might be possible have not as strongly affected the process of drug development and the availability of new therapies. The nature of drug development has become increasingly challenging and resource intensive. One of the key areas enabling advances in drug development is the application of scientific advances as new tools to aid drug development. Developing well-defined and reliable tools that assess important aspects of patient health status and integrating them into clinical trials can make certain trials more informative concerning the benefits and risks of treatment. These tools may, in part, address some of these difficulties and speed the availability of new products that might also be more effective or safer with clinical characteristics that are better understood. Often there are no existing tools specific to the disease/condition and the clinical trial population to serve as well-defined and reliable assessments of clinical benefit. Qualification is a conclusion that within the stated context of use, the results of assessment with a DDT can be relied upon to have a specific interpretation and application in drug development and regulatory decision-making. The qualification process for drug development tools (DDTs) is intended for potential use, over time, in multiple drug development programs. DDTs include, but are not limited to, biomarkers and patient reported outcome (PRO) instruments. The rationale for the proposed DDT and its context of use, newly acquired data, open questions regarding the context of use that require further data collection, potential studies to obtain that data, and identification of other gaps in the existing information that should be addressed before proceeding to the review stage of the qualification process. The goal of this process is to reach a conclusion regarding the adequacy of the submitted data to support the DDT's qualification and context of use.

Maralla S. Development of a new rating scale as a need to make improvements to an existing measure in the qualification process for drug development tools. J Clin Sci Res 2014;3(Suppl 1):S26.

Molecular modelling and docking studies on histamine 4 receptor (H4R) for histamine mediated allergic diseases

S. Shobana,[1] S. Gopinath[2]

[1,2]SRM University, Department of Bioinformatics, School of Bioengineering, Kattankulathur

Background: H4R is the novel member of the histamine receptor family which belongs to class 'A' of the GPCR super family. It is mainly distributed on hematopoietic cells and plays a key role in allergic conditions, inflammation and etc. It mediates histamine induced chemotaxis in mast cells and eosinophil cells. The expression pattern and the biological function suggest the role of H4 receptor in allergy and inflammation, thus being an attractive and potential target for drug designing.

Objectives: Developing 3D structure for H4 receptor by homology modeling to study the interactions of target with the ligands and to identify potential natural inhibitors for the H4 receptor.

Methods: Having H1 receptor as template, Easy modeler tool was used to prepare a model of Histamine H4 receptor. Later the model was energy minimized and verified by SAVES server and then Schrodinger's Maestro tool was utilized for docking studies. Natural ligands were collected from phytochemical databases which are then screened and docked.

Interpretation: Initially the 3D model of H4 receptor was developed then H4 antagonist was docked and active site interactions are analyzed. In order to overcome certain side effects, docking studies are done with various natural antihistamines, and the compounds are screened based on the pharmacophore and the resulting compounds are docked against the target H4 receptors.

Results: The 3D structure of the H4 receptor is modeled, and then interacting amino acids are identified by docking of H4 antagonist. Potential natural ligands are identified by pharmacophore screening and docking analysis.

Shobana S, Gopinath S. Molecular modelling and docking studies on histamine 4 receptor (H4R) for histamine mediated allergic diseases. J Clin Sci Res 2014;3(Suppl 1):S27.

Computational approaches for aflatoxin and their analogs bind to *Cyprinuscarpio* (common carp) liver x receptor

J.A. Pradeepkiran,[1] E.Madhuri,[2] M.Bhaskar[1]

[1]Division of Animal Biotechnology, Department of Zoology, Sri Venkateswara University, Tirupati and [2]Yogivemana University, Department of Zoology, Kadapa

Heterodimerization of the liver x receptor (LXR) occurs on binding of oxysterols (agonist) and 9-cis retinoic acid receptor (RXR). In common carp *Cyprinuscarpio*mycotoxins are interact with this receptor and causing cellular signaling through the contaminated feed. In general fungal species produce numerous toxins, and secondary metabolites among those the aflatoxin B1 are play a pivotal role and act as agonist for LXR and leads to over expression in liver carcinoma. These mechanisms of aflatoxins interactions were little known, Herein, the present study we aimed to revels the binding mode of aflatoxins to *Cyprinuscarpio* LXR, using homology modeling with human LXR (3IPQ) as a template and optimized in Modeller through VTFM (variable target function method) with conjugate gradients (CG), and then refined the protein restraints using molecular dynamics (MD) with simulated annealing (SA) and validate the protein by stereo chemical quality checking and Verify_3D. Docking affinity was calculated for aflatoxin and related analogs from pubchem bioassay database through AutoDockVina in PyRx. The predicted binding models were better understood to design a novel inhibitors, for instance structure based drug design, virtual screening and QSAR studies.

Pradeepkiran JA, Madhuri E, Bhaskar M. Computational approaches for aflatoxin and their analogs bind to Cyprinuscarpio (common carp) liver x receptor. J Clin Sci Res 2014;3(Suppl 1):S28.

In silico approach of drug discovery process

P. Naga Jyothi*, K. Praveenkumar

Department of Fishery Science & Aquaculture S. V. University, India

Production of new drug potentials and enlarge the scope of diseases through drug discovery process is a very cost effective method in pharmaceutical industry. Induction of drug target identification leads to a time consuming process and it may causes failures in conventional approaches like *in vivo* and *in vitro* methods. Advent of sophisticated Insilico approaches developed to identify new drug targets which prevents time factor during clinical trials. Present work provides appropriate approaches to characterize the targets of bioactive compounds through the genes or proteins associated with the diseases.

Naga Jyothi P, Praveenkumar K. *In silico* approach of drug discovery process. J Clin Sci Res 2014;3(Suppl 1):S29.

In silico gene prediction for autosomal recessive essential fructosuria

M. Sreekanth, P. Jacob Doss

Division of Toxicology, Department of Zoology, S.V. University, Tirupati

Essential fructosuria caused by a deficiency of the enzyme hepatic fructokinase. Incomplete metabolism of fructose in the liver, leading to its excretion in urine. KHK (ketohexokinase (fructokinase)) is a protein-coding gene. Diseases associated with KHK include fructosuria, and obstructive jaundice, and among its related super-pathways are Fructose catabolism and Metabolic pathways. GO annotations related to this gene include ketohexokinase activity and ATP binding. Mutations in the *KHK* gene, located on chromosome 2p23.3-23.2 responsible for Autosomal recessive. The chromosomal markers were determined by using FGENESH, GeneMark, HMM, GenScan (eukaryotes) and Augustus. The analysis suggests that DNA contigs not yet mapped in 2p23.3-23.2, may be involved in Essential fructosuria. These potential genes could assist in understanding the pathogenesis of Essential Fructosuria.

Sreekanth M, Jacob Doss P. *In silico* gene prediction for autosomal recessive essential fructosuria. J Clin Sci Res 2014;3(Suppl 1):S30.

Terminalia tomentosa crude extract regulates adipogenesis and body weights in HFD-fed obese rats

G. Muniswamy, M. Ramgopal, T.K.Padmaja and Balaji Meriga
Department of Biochemistry,Tissue Culture and Molecular Biology Laboratory, Sri Venkateswara University, Tirupati

Obesity is a lifestyle associated disorder leading to several health complications such as cardiovascular diseases, arthritis, hypertension, diabetes etc. Our study investigates the possible anti-hyperlipidemic and anti-obesity activity of *T. tomentosa* bark crude extract (TTCE) at 100 and 200mg/kg b.wt doses on high fat diet (HFD)-induced obese rats. Body weights and lipid profiles were increased in HFD fed groups where as oral administration of TTCE at 200mg/kg by weight has significantly reduced the body weights and fat percentage. Also, TTCE supplementation has substantially normalized the altered lipid profiles of HFD-fed rats. These results were also supported by the histopathology examination of adipose tissue. Microphotographs of adipose tissue sections clearly showed enlarged adipocytes with fat-laden droplets in HFD-fed rats, however reduced size of adipocytes and fat droplets were noticed in HFD+ TTCE treated rats demonstrating the anti-adipogenic and anti-obesity activity of TTCE.

Muniswamy G, Ramgopal M, Padmaja TK, Balaji Meriga. Terminalia tomentosa crude extract regulates adipogenesis and body weights in HFD-fed obese rats. J Clin Sci Res 2014;3(Suppl 1):S31.

Green synthesis of zinc oxide nanoparticles for cell proliferation synthesized through *Adhatoda vasica* Nees

G. Bhumi, P. Yugandhar and N.Savithramma

Department of Botany, Sri Venkateswara University, Tirupati

Biologically synthesized nanoparticles have been widely using in the field of medicine. Research in nanotechnology highlights the possibility of green chemistry pathways to produce technologically important nanomaterials. *Adhatoda vasica* is an important medicinal belongs to the Family Acanthacece. It is used as an expectorant, abortifacient, antimicrobial, antitussive and anti cancer. The synthesized ZnO-NPs were characterized with FT- Raman spectroscopy, scanning electron microscopy, energy dispersive X-ray diffraction and XRD. Phytochemicals present in the plant were responsible for the quick reduction of Zn+ ion to metallic zinc oxide nanoparticles. The synthesized ZnO-NPs had the potential to mitigate the bacterial cell proliferation particularly *Escherichia coli*, *Bacillus thuringiensis*, *Pseudomonas aeurogonisa* and *Staphylococcus areus*. The objective of the present study is to test the green synthesized zinc oxide nanoparticles (ZnO-NPs) against the bacterial cell proliferation. This results leads to formation of novel Drug development.

Bhumi G, Yugandhar P, Savithramma N. Green synthesis of zinc oxide nanoparticles for cell proliferation synthesized through Adhatoda vasica Nees. J Clin Sci Res 2014;3(Suppl 1):S32.

E-Pharmacophore based virtual screening to identify lead molecules for GSK-3β induced Alzheimer's disease

Natarajan Pradeep, Swargam Sandeep, Kanipakam Hema, Amineni Umamaheswari

Department of Bioinformatics, Bioinformatics Centre, SVIMS University, Tirupati

Background: Glycogen synthase kinase-3β (GSK-3β) is a serine/threonine kinase that has attracted significant attention during recent years in drug design studies. Increased activity of GSK-3β results in hyper phosphorylation of tau and leading to microtubule destabilization and oligomerization of the tau protein within the cell. Oligomerization of tau contributes to form neurofibrillary tangles (NFT) which leads to apoptosis of the neuron and alleviates memory deficits in Alzheimer's disease. Given its role in the formation of NFT leading to AD, it has been a major therapeutic target for intervention in AD.

Methods: Twenty co-crystal structures of GSK-3β were retrieved andligands were clustered using Canvas.Ligands were optimizedfor the pharmacophore design requirements based on the energy involved in binding for mapping five e-pharmacophoremodels.Shape based screening for the e-pharmacophore models against nine established small molecule databases using PHASE v3.5 resulted in2059matching to the pharmacophore features. Rigid receptor docking (RRD) was performed to 2059 ligands with GSK-3β. Interactions of top ten leads obtained from ten different clusters through RRD were further studied with QPLD, IFD, and MM-GBSA. GSK-3β-lead1 docked complex was subjected to 10ns MD simulations run.

Results: Among the 69 leads and 20 co-crystal ligands, lead1 had lowest docking score, lower free energy and better binding orientation towards GSK-3β. The 10 ns MD simulations run confirmed the stable nature of GSK-3β-lead1.

Conclusions: Results from RRD, QPLD, IFD and MD simulations confirmed that lead1 might be used as potent antagonist for GSK-3β for the treatment of AD.

Pradeep N, Sandeep S, Hema K, Umamaheswari A. E-Pharmacophore based virtual screening to identify lead molecules for GSK-3β induced Alzheimer's disease. J Clin Sci Res 2014;3(Suppl 1):S33.

Delta C_T, norm finder, genorm and best keeper programming for the validation of reference genes for the quantitative gene expression studies by in the ovarian follicles of sheep

A.V.N.Sivakumar,[1] V. Praveen Chakravarthi,[2] M. Bhaskar,[2] V.H. Rao[1]

[1] Embryo Biotechnology Laboratory, Department of Physiology, College of Veterinary Science, Sri Venkateswara Veterinary University, Tirupati and [2]Department of Zoology, Sri Venkateswara University, Tirupati

Studies on expression pattern of different developmentally important genes in various stages of in vivo and cultured ovarian follicles provides comprehension of the signalling mechanisms and the pathways for follicular development. While relative quantification of expression of genes employing reference genes is a widely used method, it was repeatedly emphasized that the reference genes need be validated for different tissues and experimental conditions. Stability of expression of various commonly used reference genes was never tested in the mammalian ovarian follicles grown in vivo or in vitro. Therefore in the present study six of the commonly used reference genes viz., YZW, TUB, CYP, SDHA, B2M, RPL13 were validated in different development stages of *in vivo* and *in vitro* grown ovarian follicles. Data was analysed by RefFinder that returns a comprehensive ranking based on the results obtained by applying four different methods of data analysis viz. Delta Ct, Norm finder, Genorm and Best Keeper. The results of stability of expression of the reference genes obtained in the present study are as follows (i) granulosa cells from *in vivo* grown follicles YZW, CYP, TUB (ii) oocytes from *in vivo* grown follicles B2M, YZW, TUBB (iii) granulosa cells from *in vitro* grown follicles, CYP, YZW, TUBB (iv) oocytes from *in vitro* grown follicles B2M, CYP, TUB, and (v) ovarian follicles as a whole whether *in vivo* or *in vitro* grown YZW, CYP, TUB may be used as reference genes. From this study that YZW was most suitable gene among these 6 genes in all in vitro or invivo oocytes and granuosa cells.

Sivakumar AVN, Praveen Chakravarthi V, Bhaskar M, Rao VH. Delta C_T, norm finder, genorm and best keeper programming for the validation of reference genes for the quantitative gene expression studies by in the ovarian follicles of sheep. J Clin Sci Res 2014;3(Suppl 1):S34.

2D-QSAR, pharmacophore modelling and molecular docking studies of C-phycocyanin with human Rad9 protein

Rajasekhar Avula[1], Mallikarjuna Thippana[2], Dakshayani Lomada[3], Madhava C Reddy[1]
[1]Department of Biotechnology and Bioinformatics, Yogi Vemana University, Kadapa and
[2]Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherryand
[3]Department of Genetics and Genomics, Yogi Vemana University, Kadapa

Human Rad9 (hRad9) plays a crucial role in maintaining genetic stability by regulating cell cycle phase checkpoints, DNA repair mechanisms, telomere stability and apoptosis. hRad9 over expression has been linked to breast, lung, prostate, thyroid, and skin tumorigenesis. Up-regulated hRad9 interacts with the antiapoptotic Bcl2 proteins (Bcl2 and Bcl-xL), that interaction block the binding sites of Bcl2 family proteins with chemotherapeutic drugs these leads to drug resistance. The present study aims to identify novel small molecules that bind Rad9 and makes Bcl2 more susceptible to drugs. Due to its well-known antioxidant, anti-arthritic, anti-inflammatory and anti-cancer properties of C-Phycocyanin (CPC) was selected as a candidate drug molecule in this study. Different molecules containing CPC backbone were created by 2D QSAR from Discovery studio, ligand training and pharmacophore modeling were done using Ligand scout. Finally docking studies were carried out by Autodock Vina. Our study shows that CPC analogs (4-chloro-1-oxophenazine-5-carbonitrile) can effectively bind hRad9. It is for further investigations to confirm these results *in vitro* and *in vivo*.

Rajasekhar Avula, Thippana M, Lomada D, Reddy MC. 2D-QSAR, pharmacophore modelling and molecular docking studies of C-phycocyanin with human Rad9 protein. J Clin Sci Res 2014;3(Suppl 1):S35.

Identification of potent inhibitors for RuvA through different docking strategies

Manne Munikumar, Vani Priyadarshini, Dibyabhaba Pradhan and Amineni Umamaheswari*
Bioinformatics Centre, Department of Bioinformatics,
Sri Venkateswara Institute of Medical Sciences University, Tirupati

Background: Bacterial meningitis is an inflammation of the membranes (meninges) surrounding the brain and spinal cord which is a major cause of death and disability worldwide. *Streptococcus pneumonia*, *Neisseria meningitidis*, *Haemophilus influenzae* type b and *Staphylococcus aureus* are the predominant pathogens of bacterial meningitis. Holliday junction DNA helicase (RuvA), involved in homologous recombination was identified as a common drug target in pathogens of bacterial meningitis. Homologous recombination is crucial for genetic diversity and repairing in damaged chromosome.

Methods: Three dimensional (3D) structure of RuvA was generated based on the crystal structure of 1C7Y using Modeller 9v12. PHASEv3.5 was used to set up an in-house 3D ligand database comprising of more than one million small molecules from nine small molecule meta database. Two existing inhibitors of RuvA were searched in the 3D ligand database through shape screening and obtained nine hundred ligands were streamlined through three different docking strategies of RRD, QPLD and IFD. Free energies of ligand binding (“G) for compounds obtained through extra precision docking were computed using Prime v3.2. Molecular dynamics simulations for RuvA-lead1 complex was carried out for 10ns.

Results: Top ten lead molecules, which have better binding affinity (the lowest XP Gscore), orientations compared to existing RuvA inhibitors and with good pharmacological properties were identified. MD simulations of RuvA-lead1 complex revealed that the complex was stable in all 2084 trajectories.

Conclusions: Results of RRD, QPLD, IFD, Prime MM/GBSA and MD simulations affirmed that lead1 as potent inhibitor against RuvA pathogens of bacterial meningitis.

Munikumar M, Priyadarshini V, Pradhan D, Umamaheswari A. Identification of potent inhibitors for RuvA through different docking strategies. J Clin Sci Res 2014;3(Suppl 1):S36.

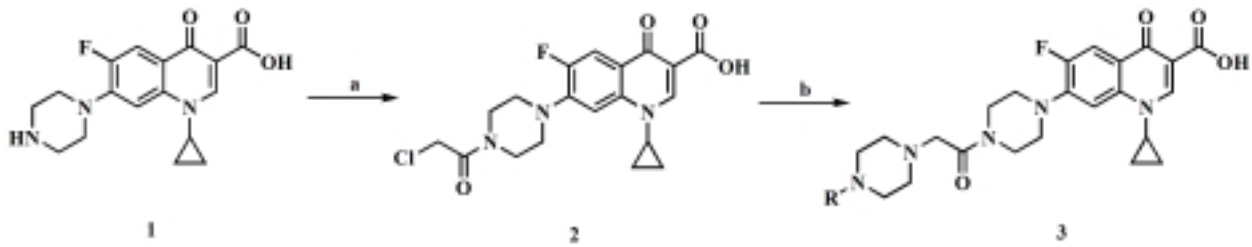
Design, synthesis and *in vitro* antifungal evaluation of novel ciprofloxacin derivatives

K. Mahalakshmi Naidu, A.Suresh, N.Suresh, H.N. Nagesh, K.V.G. Chandra Sekhar*

Department of Chemistry, Birla Institute of Technology & Science-Pilani, Hyderabad

A series of novel 1-cyclopropyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid derivatives were synthesized, characterized (^{1}H NMR, ^{13}C NMR, IR and ESI MS) and evaluated for their activities against four fungal strains by agar well diffusion method and zone of inhibition (mm) are recorded after 48h of incubation. The compounds 3a-v showed moderate to good activity against *C. albicans* and *S. cerevisiae*. The compounds 3t and 2 displayed good activity against *C. albicans* (23 and 26mm respectively) at 150µg concentration in comparison with standard ciprofloxacin. The compounds 3d, 3f, 3i, 3j, 3k, 3l, 3m, 3n, and 3o showed moderate activity against both *C. albicans* and *S. cerevisiae.*

Scheme 1 Synthetic route to achieve title compounds **(3a-v)**



Reagents and conditions: (a) Et_3N, $ClCH_2COCl$, CH_2Cl_2, 0°C-RT; (b) Et_3N, KI, substituted piperazines, 125 °C.

Mahalakshmi Naidu K, Suresh A, Suresh N, Nagesh HN, Chandra Sekhar KVG. Design, synthesis and *in vitro* antifungal evaluation of novel ciprofloxacin derivatives. J Clin Sci Res 2014;3(Suppl 1):S37.

Homology modelling, molecular dynamics and drug docking studies of ATP-sensitive K+ channel (KATP)

Peddanna Kotha, Chippada Appa Rao

Department of Biochemistry, Sri Venkateshwara University, Tirupati

The pancreatic â-cell ATP-sensitive K+ channel (KATP) plays a critical role in glucose homeostasis and Insulin secretion. Mutations in these genes can result in permanent neonatal diabetes mellitus (PNDM). Expression of genes of KATP channels in vector system is difficult. KATP channel protein cannot be isolate and purify in amounts for X-ray crystallography and nuclear magnetic resonance (NMR) studies, and so a few ion channel structures are deposited in the PDB database. The scarcity of atomic resolution 3D structures of channels is a problem for understanding their molecular mechanisms of action and for designing new compounds. Here we generated the 3 dimensional structure (3D), molecular dynamic simulation and drug docking studies for KATP channels. The protein sequence of KATP channel from homosapiens was retrieved from uniprot protein database. The selected protein was searched for related protein to be used as template by basic local alghinment tool (BLAST) against protein data bank (PDB). Sequence analysis has shown that maximum identity with high score and low e-value which was aligned and used as reference structure. The 3D model of KATP channel was generated based on the crystal structure of template protein by using Modeller 9v8. With the aid of the molecular mechanics and molecular dynamic methods, the final refined model was obtained and further assessed by protein structure validation suite (PSVS), which showed that the refined model was reliable. With this model flexible docking studies were performed with the glibenclamide and natural products using GOLD software, important residues were determined.

Kotha P, Appa Rao C. Homology modelling, molecular dynamics and drug docking studies of ATP-sensitive K+ channel (KATP). J Clin Sci Res 2014;3(Suppl 1):S38.

Structured based drug designing approach on *Berberis aristata*

Valentina P, Sushrut Sharma
Department of Pharmaceutical Chemistry, SRM College of Pharmacy, SRM University, Kattankulathur, Tamil Nadu

Objective: *Berberis Aristata* is a notable plant for antidiabetic activity. An approach of structure based drug design was carried out for its *Amylase* and *Glucosidase* inhibitory activity.

Method: Berberine, berbamine, oxyberberine, oxycanthine and aromoline are the alkaloids reported in *Berberis aristata*. These alkaloids are the ligand for our study and was drawn in Chemsketch and saved as mole file. The enzyme alpha amylase and apha glucosidase were downloaded from PDB (1HVX and 4B9Y). Molecular docking was performed in Argus lab12 version and hydrogen bonds were measured in Pymol.

Result: The docking score for Berberine , Berbamine,Oxyberberine , Oxycanthine and Aaromoline were -9.42623 , -9.0379 , -8.46393, -11.0619, -9.70657 for Alpha Amylase inhibitory activity and -9.34786, -9.70657, -8.3348, -11.4367 -8.90261 for Alpha Glucosidase inhibitory activity respectively.

Conclusion: From the above result, it is concluded that Berberine, Berbamine and Aromoline are potent Alpha Amylase and Alpha Glucosidase inhibitor and can be promising moiety for controlling the digestion of starch and post parandial glycemia.

Valentina P, Sushrut Sharma. Structured based drug designing approach on *Berberis aristata*. J Clin Sci Res 2014;3(Suppl 1):S39.

Molecular dynamics study of the TSH receptor with small molecule antagonists

Lavanya S, Kavya Kannan, Shalini Dasgupta

Department of Bioinformatics, SRM University

The Thyroid Stimulating Hormone Receptor (TSHR) is a member of rhodopsin/adrenergic receptor family in the GPCR superfamily. The TSH Receptor is critical in the development, growth, and function of the thyroid. Numerous mutations in the TSHR gene have been identiûed and associated with speciûc thyroid diseases, such as hypothyroidism (Atrophic Thyroiditis), Autoimmune Hyperthyroidism (Graves' disease), thyroid cancer etc. Our work aims to study the interactions of small molecule antagonists with the TSH receptor. The low molecular weight (LMW) ligands were obtained through literature survey and various other chemical databases. Virtual screening was performed to these compounds by docking them against the target receptor in LigandFit and Molegro Virtual Docker, followed by ADMET property calculation. Molecular dynamics simulation was then performed in Desmond to study the interactions of the most potent ligand with the target receptor in a dynamic solvent based system.

Lavanya S, Kannan K, Shalini Dasgupta. Molecular dynamics study of the TSH receptor with small molecule antagonists. J Clin Sci Res 2014;3(Suppl 1):S40.

Docking studies to explore novel inhibitors against human beta-site APP cleaving enzyme (BACE-1) involved in Alzheimer's disease

[1]S. Anjum Mobeen, [2]Manne Munikumar, [2]Amineni Umamaheswari*
[1]Department. of Biotechnology & Bioinformatics, Yogi Vemana University, Kadapa and
[2]Department of Bioinformatics, Bioinformatics Centre, SVIMS, Tirupati

Alzheimer's disease (AD) is one of the most prominent neurodegenerative disorder, particularly in elder persons over 65 age. It is characterized by progressive cognitive deterioration together with declining activities. Amyloid precursor protein (APP) cleaves at A-beta (Aβ) peptide by rate limiting factor of Beta-site APP cleaving enzyme (BACE-1) in amyloidogenic pathway. Elevated level of BACE-1 leads to the accumulation of insoluble form of Aβ peptides (Senile Plaques) an important hallmark in the pathogenesis of Alzheimer disease. Five published inhibitors of BACE-1such as thiazolidinediones, rosiglitazone, pioglitazone, Sc7 and tartaric acid are available with poor pharmacological properties and intolerable side effects. Therefore, a computational approach was undertaken to design novel inhibitors against human BACE-1. The crystal structure of human BACE-1 was retrieved from the protein data bank and optimized by applying OPLS force field in Maestro v9.2. An ASINEX database (115,000 ligands) was downloaded and compounds were prepared using LigPrep. The optimized ligand dataset was docked into the BACE-1 through sequential application of Glide HTVS, SP and XP methods that penalizes more stringently for minor steric classes subsequently. Finally, seven leads were reported and ranked based on XPGscore with better binding affinity and good pharmacological properties compared with existing inhibitors and six leads were proposed for human BACE-1. Among the six leads, lead 1 with XPGscore -8.051 kcal/mol, would be intriguing for rational drug design against Alzheimer's disease and would be highly encouraging for future Alzheimer's therapy if tested in animal models.

Mobeen SA, Muni Kumar M, Umamaheswari A. Docking studies to explore novel inhibitors against human beta-site APP cleaving enzyme (BACE-1) involved in Alzheimer's disease. J Clin Sci Res 2014;3(Suppl 1):S41.

Prediction and analysis of endocrine disruptors interacting with human gonadotropin-releasing hormone (GnRH)

Kranthi Kumar K, Kumaraswamy Naidu C, Suneetha Y

Department of Zoology, Sri Venkateswara University, Tirupati

Manmade chemicals or pollutants that disrupt the human reproduction by mimicking the hormones and activating the cell signaling pathways are called endocrine-disrupting compounds (EDCs). These EDCs are able to interact with hormonal receptors and hormone transport proteins leading to disruption in hormone metabolic pathways. Most of these EDCs are involved in GnRH (Gonadotropin-releasing hormone) signaling pathway and cause hypogonadotropic hypogonadism and testicular cancer. The mechanism of these chemical interactions and pathway allotment was little known. In the present study, we aim to identify the hormonal receptor/protein from KEGG disease database and binding affinity of selected EDCs interacting with gonadotropin-releasing hormone receptor (GnRHR) using homology modeling. The present study may be useful for future drug design and identification of novel drugs for hypogonadotropic hypogonadism and testicular cancers.

Kranthi Kumar K , Naidu CK, Suneetha Y. Prediction and analysis of endocrine disruptors interacting with human gonadotropin-releasing hormone (GnRH). J Clin Sci Res 2014;3(Suppl 1):S42.

Virtual screening of selected endocrine disrupting chemicals against StAR protein

D. Trinath, C. Kumara Swamy Naidu, Y. suneetha*

Department of Zoology., Sri Venkateswara University, Tirupati

Endocrine disrupting chemicals (EDCs) are known to interfere with the hormonal action. Some of the EDCs include; pesticides, plastics, industrial chemicals and many other chemicals. These EDCs can mimic hormones participating in the steroidogenic pathway. StAR protein transfers the cholesterol into mitochondria for the synthesis of steroid hormones. In the present study, selected EDCs were docked into the active site of StAR protein using molecular docking approach.

Trinath D, Naidu CK, Suneetha Y. Virtual screening of selected endocrine disrupting chemicals against StAR protein. J Clin Sci Res 2014;3(Suppl 1):S43.

Polycystic ovary syndrome

Devagudi Pujitha, Dubbaka Nidhi, Maanthula Jhansi Reddy
Department of Bioinformatics, Sathayabama University, Chennai

Polycystic ovary syndrome (PCOS) is one of the most common endocrine disorders among females. PCOS produces symptoms in approximately 5% to 10% of women of reproductive age (approximately 12 to 45 years old). It is thought to be one of the leading causes of female subfertility and the most frequent endocrine problem in women of reproductive age.

Polycystic ovary syndrome (PCOS) in women, with early prenatal T excess programming a permanent PCOS-like phenotype characterized by luteinizing hormone (LH) hypersecretion from reduced hypothalamic sensitivity to steroid negative feedback and relative insulin excess from increased abdominal adiposity. These combined reproductive and metabolic abnormalities are associated with ovarian hyperandrogenism and follicular arrest in adulthood, as well as premature follicle differentiation and impaired embryo development during gonadotropin therapy for in vitro fertilization (IVF). Miscarriage rates among women with PCOS are believed to be increased compared with normal fertile women, although supporting evidence is limited. Pregnant women with PCOS experience a higher incidence of perinatal morbidity from gestational diabetes, pregnancy-induced hypertension, and preeclampsia. After puberty, as each menstrual cycle begins, FSH concentrations rise beyond a critical 'threshold' and multiple follicles are recruited to begin pre-ovulatory development. The assembly of the primordial follicles early in ovarian development and the subsequent development and transition of the primordial follicle to the primary follicle are critical processes in ovarian biology. These processes directly affect the number of oocytes available to a female throughout her reproductive life. Elucidation of the molecular and cellular control of primordial follicle assembly and the primordial to primary follicle transition provides therapeutic targets to regulate ovarian function and treat ovarian disease. There is an increasing body of evidence indicating that PCOS may have significant implications for pregnancy outcomes and long-term health of a woman and her offspring. The use of insulin sensitizing drugs to decrease hyperinsulinemic insulin resistance has been proposed during pregnancy to reduce the risk of developing preeclampsia or gestational diabetes. Although metformin appears to be safe, there are too few data from prospective, randomized controlled trials to support treatment during pregnancy.

Pujitha D, Nidhi D, Reddy MJ. Polycystic ovary syndrome. J Clin Sci Res 2014;3(Suppl 1):S44.

In silico design of novel leads against p55 protein domain of VacA toxin

Pasala Chiranjeevi*, Sandeep Swargam, Dibyabhaba Pradhan and Amineni Umamaheswari**

Department of Bioinformatics, Bioinformatics Centre, SVIMS University, Tirupati

Background: The pre-mature VacA toxin released by the *H. pylori* matures in the acidic or alkaline conditions in the lumen of the human gut. The matured toxin is cleaved into p55 and p33 domains by enterokinase. The p33 domain further reunites with p55 domain, away from 110 amino acids in the N-terminal region to form pathogenic vacuolation on the plasma membrane leading to gastritis and adenocarcinoma. Herein, rational drug design method was implemented to discover lead molecules which would interfere in p33 attachment with p55 domain of VacA.

Methods: X-ray crystal structure of p55 domain (PDB ID: 2QV3) was retrieved from the protein data bank. The structure was prepared and minimized using protein preparation wizard tool present in the Maestro v9.4. A grid was generated on p33 binding site. Virtual screening was performed from the Asinex database using three accuracy mode of docking using Glide v5.9 (high throughput, standard precision and extra precision) implemented in Maestro.

Results: Five lead molecules revealed good binding affinity with p55. The binding affinities were expressed in term of XP Gscore for the best five lead molecules are -5.5 kcal/mol, -5.3 kcal/mol, -4.9 kcal/mol, -4.2 kcal/mol and -4.2 kcal/mol respectively. Analysis of p55-lead1 docking complex showed that the lead molecules were interacting with p33 binding site residues directly through three intermolecular hydrogen bonds (Asp455, Asn515 (2), Arg592).

Conclusions: The five proposed leads interacted with VacA protein at p33 binding site. Therefore, drug molecules, if designed, based on these molecules, would contribute to loss of pathogenicity of *H. pylori*.

Chiranjeevi P, Swargam S, Pradhan D, Umamaheswari A. *In silico* design of novel leads against p55 protein domain of VacA toxin. J Clin Sci Res 2014;3(Suppl 1):S45.

Application of bioinformatics in peanut genomics

Y. Amaravathi, Sai Shruthi, R.P. Vasanthi

Institute of Frontier technologies, RARS, ANGRAU, Tirupati

The discovery of next generation sequencing like 454 pyrosequencing and Illumina SBS, more and more transcriptome sequences are available for peanut. Bioinformatics makes it possible to analyse even large genome size crops like groundnut (2800 Mb) at DNA sequence level. Due to the low genetic diversity, complex genetic behaviours and large tetraploid genome, peanut remains to be one of less-studied crops with limited genomic resources. Transcriptome sequencing results in generation of sequence data to a large number of expressed sequence tags. This sequence information will be largely helpful in analysis of the sequence for microsatellites with the help of computational tools like microsatellite finder and we can convert them in to molecular marker by designing primers to unique flanking sequences. Molecular marker segregation in the population allows estimating chromosome pairing behaviour. Genetic mapping in polyploids like groundnut presents unique problems with respect to large genome size and amphidiploids nature. Therefore, large segregating populations are needed to obtain reliable genetic distance estimates. Comprehensive studies using multidisciplinary approaches like genomics, bioinformatics and statistical tools will push the boundaries of current methodologies to translate the knowledge gained into practical applications like marker assisted selection. One of the ways to look for genes controlling traits of agronomical importance is to pre-select in silico EST sequences with a putative interesting function, and to genetically map the corresponding cDNAs to look for co-localization with QTLs. In this study, we have analyzed about thousand EST sequenced which are available in the public database for the primer binding sites, PCR amplification product size and annealing temperatures. This will help to design our experiment in such a way that we can run PAGE gels for all the primers with same size amplification product (in bp). Surprisingly, some of the ESTs (0.08%) with only one binding site and some EST's (1.08%) don't have the primer binding site at all. In conclusion, we can employ bioinformatic tools for sequence analysis *in silico* which can speed up the genotyping in QTL mapping in segregating population.

Amaravathi Y, Sai Shruthi, Vasanthi RP. Application of bioinformatics in peanut genomics. J Clin Sci Res 2014;3(Suppl 1):S46.

Manganese induced changes in cholinergic system and energy metabolism in specific regions of rat brain: reversal effect of vitamin E

C. Bhuvaneswari Devi[1], K. Kiran Kumari[2], G. Indravathi[2]

[1]Department of Biotechnology, SVIMS University, Tirupati

[2]S.P.W. Degree & PG College, Tirupati

Manganese (Mn) is an essential nutrient and it is important for optimal cellular function. However, exceedingly high brain manganese concentrations are known to cause neurotoxicity. The present study was aimed at examining the impact of Mn exposure on cholinergic system and energy metabolism. In the present study the male albino rats of 3 months age were exposed to low dose (2.5mg/kg body weight) and high dose (5mg/kg body weight) of Mn through intraperitoneal injection daily for a period of 3 weeks. After the period of dosage, the Mn exposed animals were divided into two groups of which one group of both the doses were given Vit E at a dose for a period of one week. The specific activity of enzyme AChE and ACh content were estimated in synaptosomal fractions of cerebral cortex, hippocampus and cerebellum of control and all Mn exposed rats. The specific activity of enzymes $Mg2^{+}$ATPase and $Na^{+}K^{+}$ATPase were determined in the mitochondrial fractions of cerebral cortex, hippocampus and cerebellum of control and all Mn exposed rats. It was observed that AChE, Mg^{2+}ATPase and $Na^{+}K^{+}$ATPase activities were decreased and ACh content was increased in cerebral cortex, hippocampus and cerebellum of Mn-exposed (both low and high dose) rats when compared to control rats. The effect of Mn exposure was highly pronounced in high dose Mn exposed animals compared to the low dose exposed rats. However, AChE, Mg^{2+}ATPase and $Na^{+}K^{+}$ATPase activities were increased and ACh content was decreased in the rats supplemented with Vitamin E along with low and high dose Mn-exposure. Among the different brain regions cerebral cortex was found to be more susceptible region towards manganese induced toxicity compared to the other two brain regions. This study demonstrates exposure to manganese provoked neuronal injury by inducing alteration in enzymes of cholinergic system and energy metabolism in dose dependent manner, where high dose exposure showed significant alteration compared to the low dose exposure. However, vitamin E treatment have partial ameliorative effects on these disturbance caused by Mn toxicity.

Bhuvaneswari Devi C, Kiran Kumari K, Indravathi G. Manganese induced changes in cholinergic system and energy metabolism in specific regions of rat brain: reversal effect of Vitamin E. J Clin Sci Res 2014;3(Suppl 1):S47.

Biological synthesis of silicon nanoparticles from leaf extracts of *Cynodon dactylon* and *Cymbopogon coloratus*

R. Hari Babu, N. Savithramma

Department of Botany, S.V. University, Tirupati

The recent technological advancement in nanotechnology has opened new avenues for research and development in the field of herbal and medicinal plants biology. Development of reliable and eco-friendly processes for synthesis of nanoparticles is an important step for introduction of nanotechnology in to herbal research. In the past decade, there has been much concern about the methodological advancement of technology for synthesis and characterization of herbal and medicinal plants mediated nanoparticles. Mesoporous silica nanoparticles (MSNs) are a highly promising platform for intracellular controlled release of drugs and bio molecules. Despite that the application of MSNs in the field of intracellular drug delivery is still at its infancy very exciting breakthroughs have been achieved in the last years. Recently, the development of new delivery vehicles based on inorganic nanomaterials has brought new possibilities to this area of research. In the case of mesoporous silica nanoparticles recent breakthroughs have demonstrated its high potential in this field. *Cynodon dactylon* and *Cymbopogon coloratus* are belongs to poaceae family. The nanoparticles are subjected to SEM and EDAX, UV, XRD, AFM and TEM for identification size and shape of nanoparticles.

Hari babu R, Savithramma N. Biological synthesis of silicon nanoparticles from leaf extracts of *Cynodon dactylon* and *Cymbopogon coloratus*. J Clin Sci Res 2014;3(Suppl 1):S48.