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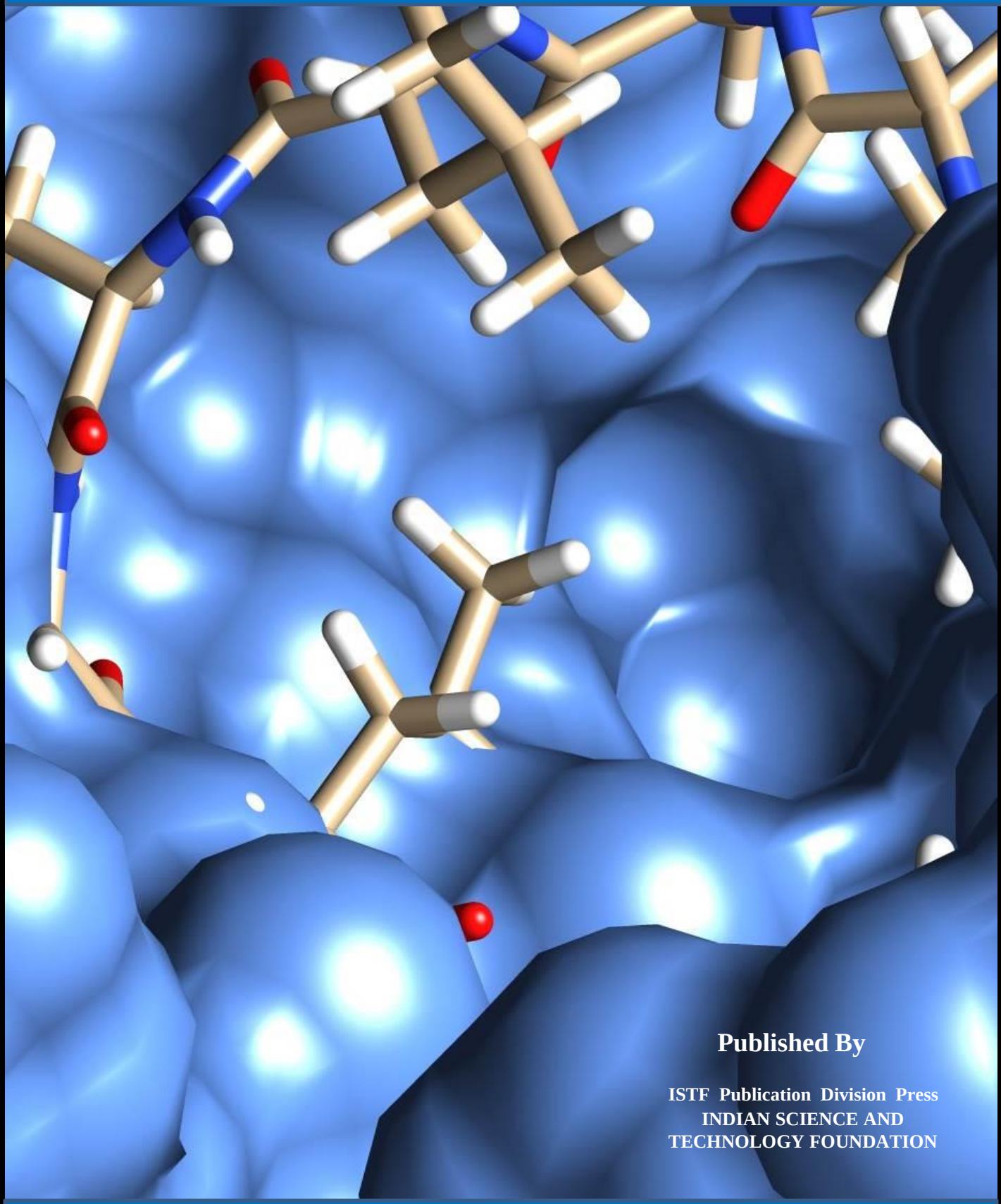

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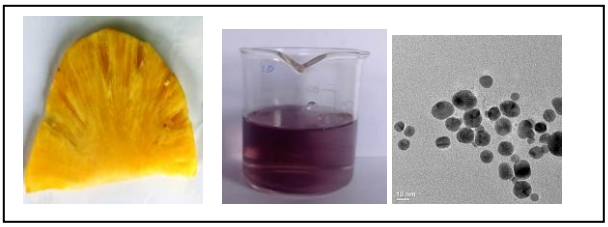
JOS

Microwave Synthesis of Gold Nanoparticles Using Pineapple Extract

Shyamal Mandal[1], Juwesh Binong[2]
[1]Department of Biomedical Engineering, [2]Department of Electronics and Communication Engineering,
North Eastern Hill University, Shillong, Meghalaya, India – 732202. shyamal.mandal.iit@gmail.com,

Nanotechnology emerged as an admirable technology in most of the engineering applications. In other word they are ruling the world for the past few decades and expected to play a dominant hold in future. They have broad class of applications in most fields some predominant includes biotechnology, pharmacology, optics, electronics, energy and environment. The extremely small size of material (1-100nm) creates a large surface area in relation to their volume, which makes them highly reactive, compared to bulk form of the same materials. In recent times nanomaterials are used in various applications such as therapeutics, antimicrobial agents, transfection vectors, and fluorescent labels. Gold nanoparticle synthesis by the green route has become the latest development. Another advantage of synthesize gold nanoparticles with fruit juice as a capping agent less chemical residue. The gold solvent can preserved for long time. Gold nanoparticle (AuNPs) thus synthesised were characterised by transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) to confirm their size, shape and composition. These gold nanoparticles have versatile applications as biomarker and cancer therapy.

Pineapple AuNPs solution AuNPs



Key Word: Microeave, Gold nanoparticles, Pineaaple Juice.

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pH-induced conformational changes in SP6 RNA polymerase: an *in silico* study

Satya Ranjan Singh, Ayaluru Murali*
Department of Bioinformatics, Pondicherry University, Puducherry-605014
*murali@bicpu.edu.in (Corresponding Author)

SP6 RNA polymerase (SP6RNAP) is an essential enzyme for the transcription process in SP6 bacteriophage. SP6RNAP plays a vital role in mRNA vaccine designing technology and other translational biotechnology research due to the high specificity of its promoter. The self-replicating performance also put this polymerase to study extensively. Despite the reports emphasizing the function of this enzyme, a detailed structural and functional understanding of RNA polymerase is not reported so far. Here, we report the first-ever information about SP6RNAP structure and its effect on promoter binding at different pH environments using molecular docking and molecular dynamics simulation (MDS) study. We also report the changes in polymerase conformations in different pH conditions using the *in-silico* approach. The docking study was also performed for SP6RNAP with SP6-promoter at different pH environments using the *in-silico* docking tools. The structural aspects confirmed that the pH 7.9 state favors the polymerase functional activity in the transcription process which was in the range reported using the transcription assay. This polymerase's unique features may play its emerging role as an efficient transcription factor in translative biological research.

Key-words: SP6 RNA polymerase, SP6 promoter, transcription factor, mRNA-vaccine technology, Molecular dynamics simulation

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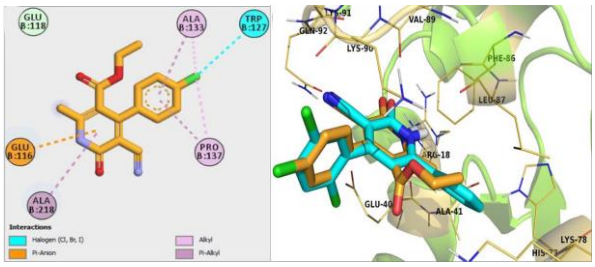
Pyridone based analog synthesis, study and molecular docking studies

Laldingluaia Khiangte[a,b]*, Ved Prakash Singh[a,b]

[a]Department of Chemistry, School of Physical Science, Mizoram University, Aizawl, Mizoram- 796004
[b]Department of Industrial Chemistry, School of Physical Science, Mizoram University, Aizawl, Mizoram- 796004
Email: dinga012@gmail.com

Multicomponent condensation reactions (MCRs) principles are used to synthesis the dihydropyridone, followed by oxidation to synthesis the pyridone. The crystals of both the compounds were determined by using the single-crystal X-ray diffraction method. Dihydropyridone are found as racemic mixture and crystalized as co-crystal. Hirshfeld surface analysis is done in all the structure for analysis of various intermolecular interactions. The synthesised compounds were docked with Kinesin Eg5 protein and Survivin protein to analyse their binding affinities. The binding interactions of all the compounds are found in the cavity of Eg5 with the ester group protrudes outside the cavity. The chlorobenzene ring of compounds **4 & 5** is directed towards the hydrophobic region, but compound **5** favours the hydrophilic region of the active sites of Eg5 protein. The compound **5** interacts with the survivin protein in the allosteric cavity near the dimerization interface and resemble the pose of the reference compound. The results of this studies shows that the crystal compounds **3, 4 & 5** might induce apoptosis through inhibition of survivin and Eg5 proteins, and thus, it could be a promising anticancer agent.

Key-words: Crystal, pyridone, docking, Hirshfeld surface analysis, non-covalent interactions



(a) (b)

Figure:(a) 2D representation of compound **5** interaction with Eg5 protein, (b) Overlay of compounds **5** (orange) and **2** (reference compound; blue).

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Fungal Xylanase produced using *Amorphophallus paeoniifolius* peels as substrate which aided in the making of bread dough fluffy

Richa Nenava[1], Sadhana Nighojkar[2], Anil Kumar[1] and Anand Nighojkar[3*]

[1] School of Biotechnology, Devi Ahilya University, Takshshila Campus, Khandwa Indore 45200, India.
[2] Mata Gujri College of Professional Studies, A.B. Road, Indore 452001, India.
[3*]Maharaja Ranjit Singh College of Professional Sciences, Hemkunt Campus, Khandwa Road, Indore 452001, India.

The present research investigation on fungal xylanase isolated from elephant dung holds great potential for hemicellulose bioconversions. Xylanase works on the arabinoxylans present in cereals, which binds the water in the dough and thus provides better crumb structure and reduces stickiness of the dough [1]. The isolated fungus was utilized for the production of endo1,4 β-xylanase enzyme using *Amorphophallus* peels (elephant foot yam) in Solid State Fermentation. The produced enzyme was optimized using OFAT approach (One Factor at a Time) and RSM (Response Surface Methodology) based on Box Behnken Design exhibiting optimized values of 121 ± 2.5 U/ml and 12 ± 1.2 U/ml respectively [2]. The optimum xylanase activity was obtained at 60°C, pH 8.0 in 96 h culture with inoculum size of 1x 10^6 spores/ml, 90% moisture and 2 mm particle size in SSF. The enzyme was then partially purified using ammonium sulphate fractionation and DEAE-cellulose and then used for its application in making the dough fluffy [3]. 0.5 ml of xylanase was added to the 10 gm of wheat flour and the dough is kneaded and observed after 4 h, 8 h and 12 h of incubation. The dough rising was observed in the test sample after 4 and 8 hours of incubation at 35±1.5°C of 10 mm and 21 mm respectively. The xylanase is attributed to improve the texture, softness and increased bread dough volume while maintaining proper moistness and fluffiness by means of formation of air pores [4,5,6]. This must be considered for further analysis and primary usage in the bakery industry as a substitute of chemical agents implied to bread manufacturing units.

Key-words: *Amorphophallus paeoniifolius* peels, *Aspergillus terreus* Thom, Baking, Dough mixing, Xylanase.

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Targeting moaA1 gene is a potential target for multi-drug resistance in *Mycobacterium tuberculosis*.

Rohini Kumari, Pramod katara

Computational Omics Lab, Center of Bioinformatics, IIDS, University of Allahabad, India. E-mail addresses: Rohini Kumari (rohini009kumari@gmail.com), Pramod Katara (pmkatara@gmail.com)

The conventional drug treatments of *Mycobacterium tuberculosis* result in more drug resistance. Identification of the new target molecules can drive novel therapeutic agents to overcome multi-drug resistance. Computational analysis can accelerate the major research for the identification of potential therapeutic targets and drugs. Therefore, we performed the gene expression analysis and single nucleotide polymorphism (SNP) of potential genes from multiple drug-treated patients such as capreomycin (CAP), isoniazid (INH) and rifampicin (RIF) (GEO-GSE53843). The DEGs data revealed that about 11 genes are commonly dysregulated by above conventional drug treatments. While 37 genes are INH-specific treatment dysregulated. Pathway analysis revealed that these dysregulated genes have an essential role in the drug metabolic process and influx mechanism. Further, overall genomics analysis suggested that the moaA1 gene could serve as a potential target inhibitor of *M.tuberculosis*. The moaA1 gene is over expressed in multiple drug resistance patients. It is known as a catalyzes the cyclization of GTP to (8s)-3'-8-cyclo-7,8-dihydroguanosine 5'-triphosphate which play important role in the molybdopterin biosynthesis.

Keywords: Tuberculosis, drug resistance, expression profiling and virulence genes,

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EspB is a membrane binding effector of the Mycobacterial Type VII secretion system

Nayanika Sengupta and Somnath Dutta
Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560012 email ID: nayanikas@iisc.ac.in

EspB, denoted by Rv3881c, is a PE/PPE family secreted substrate of the ESX-1 apparatus of the T7SS. Full length EspB is a 48 kDa polypeptide (460 amino acids) chain which is cleaved at its C-terminal domain by MycP protease in the periplasm of Mycobacterial cells. In 2013, Chen et al. showed that recombinantly purified mature form of EspB selectively bound phosphatidic acid (PA) and phosphatidylserine (PS) in contrast with the full length EspB. However, till date further knowledge representing the mode of interaction between processed EspB and PA or PS remains unaddressed. This poses an important structural question – does mature EspB have a specific binding pocket for PA and PS or is the binding mediated between EspB and biological membranes composed of PA and PS? Based on the long withstanding debate on the functional role of EspB, we designed a cryo-EM based study to elucidate EspB-lipid affinity. Recombinant mature EspB was purified by two-step affinity and SEC purification. The peak fractions were analysed by NS-TEM and the fraction corresponding to discrete heptameric particles was vitrified to perform cryo-EM structural analysis. Cryo-EM data were collected in the presence of 0.03% fluorinated octyl maltoside to address the challenge of strong preferred orientation in vitreous ice. Through single particle reconstruction, we were able to resolve heptameric EspB at 5.9 Å. We deployed several biophysical tools to screen different target lipids. Microscale thermophoresis (MST) and NS-TEM illustrated strongest binding with PA. Intriguingly, cryo-EM micrographs revealed PA vesicles decorated with side views of EspB. Our current cryo-EM 3D reconstruction of EspB with PA shows the presence of extra densities near the otherwise unstructured C-terminal disordered region (CTD). We hypothesise that lipid binding may induce order in the intrinsically disordered CTD and thus EspB may elicit pathophysiological response by PA and PS mediated host membrane binding.

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Allele frequencies data and statistic parameters for 15 STR loci in a southern Moroccan population

Noura Dahbi[1*], Khadija Cheffi[1], Abderrazak El khair[1], Lamiaa Habbibeddine[2], Jalal Talbi[2], Abderraouf Hilali[1], Hicham El ossmani[1, 3]

[1]Hassan First University of Settat, Higher Institute of Health Sciences, Laboratory of Health Sciences and Technologies, 26000, Settat, Morocco.
[2]Mohammed V Agdal University, Faculty of Sciences, Rabat, Morocco.
[3]Royal Gendarmerie Criminalistics Institute, Rabat, Morocco.

Short tandem repeats (STRs) are particularly informative markers with a high level of variability. They are widely used in anthropological studies to quantitatively characterize the relationships between individuals in the same or distinct populations. In this study, 15 autosomal STR markers (D5S818, FGA, D8S1179, D21S11, D7S820, CSF1PO, D3S1358, TH01, D13S317, D16S539, D2S1338, D19S433, VWA, TPOX, and D18S51) were PCR amplified using AmpFlSTR® Identifiler™ Kit (Applied Biosystems, Foster City, CA, USA) [1] in order to study the genetic diversity of a population in the south of Morocco. A sample of over 100 healthy unrelated individuals was studied. Allele frequencies, Hardy-Weinberg equilibrium and forensic parameters were calculated using Arlequin v3.5.2.2 [2] and STRAF (1.0.5: STR Analysis for Forensics) [3]. The findings show a significant deviation from equilibrium for three markers even after Bonferroni correction: TH01, VWA, and D18S51. All loci are highly polymorphic, with D18S51 showing the highest polymorphism. The combined power of discrimination and exclusion was significantly high, suggesting that this panel is relevant for forensic casework.

Key-words: Morocco; Short Tandem Repeat; allele frequencies; forensic, population data.

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Paludisphaera soli sp. nov., a new member of the family Isosphaeraceae isolated from high altitude soil in the Western Himalaya; a possible bio-control against exotic invasive *Prosopis juliflora*

Meesha Sharma[1, 2], Rishabh Kaushik[1, 2], Ch. Sasikala[3], Ch. V. Ramana[4] and Maharaj K. Pandit[1, 2]

1. Department of Environmental Studies, University of Delhi, Delhi, 110007, India.
2. Centre for Interdisciplinary Studies of Mountain & Hill Environment, University of Delhi, Delhi, 110007, India.
3. Bacterial Discovery Laboratory, Centre for Environment, Institute of Science and Technology, J. N. T. University Hyderabad, Kukatpally, Hyderabad 500085, India
4. Department of Plant Sciences, School of Life Sciences, University of Hyderabad, P.O. Central University, Hyderabad 500046, India

Planctomycetes represent a unique phylum of the domain bacteria, which have intrigued the scientific community with their unusual properties like internal compartmentalisation and the absence of peptidoglycan in their cell wall due to which they were mis-classified as 'floating fungus' in the last century (1). Here, we describe a novel strain of Planctomycetes designated as JC670^T, which was isolated from a high altitude soil sample (~2900m m a.s.l) in the Western Himalayas and represents the first report of a Planctomycetes from this region (2). Colonies of the strain were observed to be light pink coloured with spherical to oval shaped cells that exhibit budding and have crateriform structures all over the cell surface (2, 3). Cells were found to grow well at pH 7.0 and pH 8.0 and could tolerate up to 2% NaCl (w/v). MK6 was the only respiratory quinone identified and the major fatty acids identified were $C_{18:1\omega9c}$, $C_{18:0}$ and $C_{16:0}$, and phosphatidylcholine, two unidentified phospholipids and six unidentified lipids were identified as the polar lipids. Polyamines like putrescine and *sym*-homospermidine were also detected. The draft genome of this strain is 7.97 Mb, with GC content of 70.4 mol%. Based on phylogenetic analyses with the sequences of ninety-two core genes, low *d*DDH value (20.6%), low gANI (76.8%) and low AAI (69.1%) (Auch et al. 2010) results along with differential chemotaxonomic and physiological properties, strain JC670^T (= KCTC 72850^T = NBRC 114339^T) was recognised as the type strain of a new species of the genus *Paludisphaera*, for which the name *Paludisphaera soli* sp. nov. was proposed and accepted. Moreover, based on microcosm experiments (unpublished data), we suggest that this isolate can act as a putative biocontrol agent as exhibited by its negative impact on the seedlings of a global invasive plant *Prosopis juliflora*.

Key-words: Soil bacteria, Planctomycetes, Paludisphaera, Invasive, *Prosopis juliflora*

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Current Cell and Tissues Based In vitro Models and Applications

Dr Dhrubojyoti Sen [1], Shouvik Sarkar [2]

[1]Department of Pharmaceutical Chemistry, School of Pharmacy, Techno India University, Salt Lake Sector, EM–4/1, Sector–V, Kolkata–700091, West Bengal, India.
[2] Department of Pharmaceutical Chemistry, School of Pharmacy, Techno India University, Salt Lake Sector, EM–4/1, Sector–V, Kolkata–700091, West Bengal, India.

The purpose of in vitro models is to address paradigm shifts in research related to the following: i) a trend toward saying goodbye to flat biology, i.e. developing tools that mimic human tissues/organs and diseases, and ii) reducing/eliminating the need for animal experiments in research. Models can be developed at different scales (macro, meso, micro, and nano) depending on whether they explain behavior at the whole system level, behavior at the level of molecular clusters, or behavior at the molecular level. The ultimate objective is to reduce the cost and time of experimental measurements and get satisfactory results. Drugs and therapeutics are pharmacokinetically influenced by the anatomy of the vascular system, which contributes to the functioning of all essential organs, including ADME. In this way, experimental models of blood vessels can significantly contribute to developing drug formulations that are tailored to the individual. It has also been used in food testing and developing neutraceuticals. The growing availability of human-induced pluripotent stem cells (hiPSCs) from healthy individuals and patients has driven advances in the development of experimental in vitro models of vascular structures: endothelial cells, pericytes, and vascular smooth muscle cells can now be generated from hiPSCs and used in ‘microfluidic chips’ (also known as ‘organ-on-chip’ technology) as a basis for in vitro blood vessel models. The use of natural, synthetic, and hybrid material-based hydrogels in 3D culture provides 'close-to-in-vivo' structures because of the high water content and flexibility they provide, which mimic natural tissues and can be used for various organs. The in vitro simulation models have also been upgraded to study the metabolism of phytochemical absorption using various working models. In vitro models have thereby proven essential to improving the quality of life for patients with a wide range of comorbidities.

Keywords: 3D culture, hiPSC, pharmacokinetics, organ-on-chip, phytochemicals

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Understanding properties of endocrine disruption chemicals using molecular docking approach

Abira Dey [1, 3], Ruoya Li [2], Nathalie Larzat [2], Jean Bernard Idoipe [2], Ashwani Sharma [1, 2,3 *]

[1]Indian Science and Technology Foundation, New Delhi, India
[2]Insight Biosolutions (IBS), Biopole Rennes, 35000, Rennes, France
[3]Moldoc Biotech Pvt. Ltd., Yamuna Vihar, Delhi-110053, India
[*] Corresponding Author: director@isto-india.org

The endocrine system is a message carrier complex composed of feedback loops of hormones that are distributed by different internal glands of a living organism right into the circulatory system. It is responsible for the production, storage, and secretion of hormones inside the body.[1] Endocrine disruption chemicals are a category of unnatural chemical compounds which obstruct the normal functioning of the hormones inside the body. The effects of chemicals in the body include metabolic issues, infertility, obesity, early puberty, insufficient growth, heart disease, less immunity, learning disorder, and so on.[2] These chemicals get inside the body through the contamination of the food chain, inhalation of the contaminated house dust, pesticides and herbicides that are spread on the crops, industrial solvents and their by-products, plastic containers, pharmaceuticals, dietary components, personal care products, and even through clothing.[3]

In this study, Estrogen alpha and Estrogen Beta receptor proteins were docked against a natural hormone, Estradiol, and three non-natural chemical compounds, Bisphenol A, Bisphenol B, and Hexestrol. Estradiol produced strong binding affinities with docking energy of -7.7 kcal/mol against Estrogen alpha and -8.8 kcal/mol against Estrogen Beta. It was observed that the non – natural chemical compounds had comparable binding affinities with that of the natural hormone. Bisphenol A produced binding affinities with docking energy of -8.1 kcal/mol against Estrogen alpha and -7.9 kcal/mol against Estrogen Beta, Bisphenol B produced binding affinities with docking energy of -8.2 kcal/mol against Estrogen alpha and -8.2 kcal/mol against Estrogen Beta, and Hexestrol produced binding affinities with docking energy of -6.2 kcal/mol against Estrogen alpha and -8.5kcal/mol against Estrogen Beta.

Therefore, our study confers that the non – natural chemical compounds compete with the natural hormone to interact with the Estrogen alpha and Estrogen Beta receptor proteins and interfere with the normal functioning of the hormones. Hence, this study can be valuable in sketching the *in – vitro* assessments for predicting the participation of the non–natural chemical compounds in Endocrine Disruption.

Key-words: Endocrine system, endocrine disruption chemicals, hormonal imbalance, estrogen receptor, molecular docking.

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JOS

Designing of Antimicrobial compounds and finding their mechanism of inhibition on *Pseudomonas aeruginosa* by in-silico approach

[1]Tanmai Agasam@, [1]Anshul Nigam, [2]Ashwani Sharma#

[1]Amity Institute of Biotechnology, Amity University Mumbai, Mumbai - Pune Expressway, Bhatan Post - Somathne, Panvel, Mumbai, Maharashtra 410206, India

[2]Indian Science and Technology Foundation, Delhi, 110053, India

@Presenting author: email: agasamt3@gmail.com, #Corresponding author: email: director@isto-india.org

Pseudomonas aeruginosa is a common opportunistic pathogen known for causing highly problematic, chronic infections in cystic fibrosis (CF) patient's lungs. Patients with chronic obstructive pulmonary disease (COPD). Complications from intractable Pseudomonas aeruginosa infections eventually compromise lung function. Particularly in CF patients, resulting in death on average, 38 years old. *Pseudomonas aeruginosa* has a remarkable ability to resist multiple first line antibiotics, either intrinsically or because of Resistance genes are acquired. When *Pseudomonas aeruginosa* occurs, it is nearly impossible to eradicate the organism. Many antibiotics have been employed to kill bacteria, but the mechanisms of their activities are still unknown. As a result, determining the mechanism of antimicrobial action of those compounds by analysing their interaction with proteins targets in various pathways is critical. This study focuses on the interaction between the antimicrobial compounds with various proteins of *Pseudomonas aeruginosa*. A total of 20 protein [1] targets were selected from different pathways of *Pseudomonas aeruginosa* in this research. Propranolol and N-acetylcysteine were the selected antimicrobial compounds. Propranolol and N-acetylcysteine [2] have multiple target sites with various proteins of Pseudomonas aeruginosa. They have good interaction with the proteins. Homology modelling was performed for some of the proteins to predict the structure of the protein. Binding site residues of all the proteins were found from pdbsum or ProFunc. Docking was performed for all proteins with antimicrobial compounds by use of AUTODOCK VINA. Docking was performed to find out the binding of the compounds with various proteins. Toxicity analysis of the drugs was performed by use of VEGA QSAR. After analysing the results, we found that Propranolol has a stronger binding with proteins of *Pseudomonas aeruginosa*. Propranolol is not a mutagenic substance. Therefore, it is safer to use Propranolol for treating Pseudomonas disease.

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Understanding the mechanism of anti-microbial action of non-antibiotic drugs omeprazole and lansoprazole against *H.pylori*

Dibyendu Biswas[1], Dr. Ashwani Sharma[2]
[1]MSc student of JIS Institute of advanced studies and research, JIS university, Kolkata, India
[2] Director, Indian Science and Technology Foundation, India

H. pylori is a Gram-negative bacterium. The outer membrane is the outer barrier of Gram-negative bacteria, which consists of two highly asymmetric layers-the inner monolayer contains only phospholipids and the outer monolayer consists mainly of outer membrane proteins (OMPs) that are resistant to the external environment. The study of *H. pylori* OMPs will contribute to the development of vaccine and drug targets. OMPs in *H. pylori* mainly include lipoproteins, porins, iron-regulated proteins, efflux pump proteins, and adhesins. Many drugs have been used against *H.pylori*, However, no clear mechanism of inhibition has been reported against H. pylori. For our project, we have chosen 2 compounds namely Lansoprazole and Omeprazole to understand their mechanism of inhibition on *H. pylori* by Molecular modeling approach. These are two drugs which are well known for the treatment of infection created by *H. pylori*. We have chosen different pathway proteins from the H. pylori life cycle such as membrane proteins, efflux protein, DNA, RNA and metabolite synthesis proteins, transporter proteins etc. The affinity was predicted by the Molecular docking approach. Our in-silico study concludes that Lansoprazole produced very strong affinities with 16 proteins from different pathways with free energy of binding of -7 to -9 kcal/mol. However, Omeprazole produced affinities with 9 proteins from different pathways with free energy of binding of -7 to -9 kcal/mol. Therefore, our docking study predicted that Lansoprazole effectively inhibits several pathway proteins in the *H. pylori* and is able to kill the *H.Pylori* more efficiently as compared to Omeprazole. Our in-silico study will help the biologist to design very precise experiments to validate our in-silico approach and be able to reduce time and cost to perform many assays.

Key-words: drugs, anti-microbial, in-silico, proteins, affinity

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Molecular Docking And Toxicity Analysis of FDA Approved Drugs And Plant Metabolites Against Potential Biomarkers To Target Human Hepatocellular Carcinoma

Jasbir kaur Simak[1*], Ashwani Sharma[2*], Anshul Nigam[3]

[1*]Amity Institute of Biotechnology, Amity University Mumbai, Mumbai - Pune Expressway, Bhatan Post - Somathne, Panvel, Mumbai, Maharashtra 410206, India
[2*]Indian Science and Technology Foundation, Delhi, 110053, India
2* Insight Biosolutions, Biopole Rennes, 35000, Rennes, France
2* Moldoc Biotech Pvt. Ltd., Yamuna Vihar, 110053, Delji, India
[3]FBE Technologies Pvt Ltd, Kidwai Nagar, Kanpur, Uttar Pradesh, 208011, India

Hepatocellular carcinoma (HCC) also known as malignant hepatoma is a severe illness occurring in patients suffering from chronic hepatitis B and hepatitis C. FDA approved drugs for the treatment of HCC including sorafenib, regorafenib, levatinib, cabozantinib, and ramucirumab come with inevitable side effects ranging from diarrhea, fatigue, hand-foot skin reactions, hypertension, blurred vision, and numbness [1]. Other major challenges that aid in the development of prevalent HCC are resistance to FDA approved drugs and diagnosis of HCC at a later stage. Thus, the development of potential biomarkers and drug alternatives is necessary. In our study, we selected two potential biomarkers namely, Bromodomain and PHD finger containing 1 and Transglutaminase 2, 6 FDA-approved drugs and 157 plant compounds and performed docking with the help of AutoDock VINA to predict their binding affinities to the proteins. The top ranked compounds were then subject to toxicity analysis using VEGA QSAR. After analyzing the results, it was found that plant compounds have stronger affinity towards the proteins in comparison to the FDA approved drugs. Abyssinone and Kaempferol were the plant compounds having stronger affinity to BRPF1 and TGM2, respectively. Also it was found that Cepharanthine, was the only plant compound having good affinity to both of the proteins. Moreover, after the toxicity prediction, it was revealed that the top ranking plant compounds were mostly non-mutagenic and non-carcinogenic and active in *in vitro* micronucleus activity whereas the results varied for each of the FDA approved drug. The purpose of performing molecular docking and toxicity analysis was to understand the affinity of plant compounds and FDA drugs to the two potential biomarkers and analyze their toxicity to find a potential biomarker as well as a potential candidate targeting human hepatocellular carcinoma. This work helped us find potential plant metabolites for treatment of hepatic cancer which are less toxic than FDA drugs.

Key-words: Hepatocellular Carcinoma, Bromodomain and PHD finger containing 1, Transglutaminase 2, Cepharanthine, Docking, QSAR

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In Silico Analysis of Candidate Drugs Against BSEP and MRP2 for their Roles in the Development of DILI

Suparna Dey[1] and Ashwani Sharma[2,*] (✉)
[1] Department of Biotechnology, St. Xavier's College (Autonomous), Kolkata, West Bengal, India
[2] Indian Science and Technology Foundation (ISTF) and Moldoc Biotech Pvt. Ltd., New Delhi-110053, India
2 Insight Biosolutions, Biopole Rennes, 35000, Rennes, France
*(✉)Corresponding author: email: Director@isto-india.org

Hepatocytes are polarized cells with specialized transport systems in the canalicular and sinusoidal membrane to maintain hepatic bile acid homeostasis and detoxify endogenous and xenobiotic toxins. The bile salt export pump (BSEP) and Multidrug resistance-associated protein 2 (MRP2) are the two proteins that mediate an ATP-dependent export of conjugated xenobiotic drugs and bilirubin across the canalicular membrane into bile. Functional impairment of BSEP and MRP2 has been hypothesized to play a role in the development of liver injury as a side effect of drug therapy due to their central role in the hepatic excretion of bile acids and toxins. While several experimental studies have confirmed potential BSEP drug inhibitors, the lack of an experimentally validated structure of MRP2 in the Protein Data Bank restricts the scope of extensive ligand binding studies with the protein. Consequently, in silico approaches combined with homology modelling revealed the identity of potential drug inhibitors for the two transporters. Interestingly, studies have supported the hypothesis that the risk of Drug-induced Liver Injury (DILI) may be increased if a compound inhibits not one but both the transporters BSEP and MRP2. In our work, we have attempted to find a correlation between the experimentally determined IC50 values of candidate inhibitors of the two transporters, and their respective in silico binding affinities. Our molecular docking studies revealed that Cyclosporine A, a known inhibitor of the BSEP as well as MRP2 has binding energies of -7.8 kcal/mol and -7.1 kcal/mol respectively for the two proteins. Also, Zafirlukast, another inhibitor of the same transporters has binding energies of -9.2 kcal/mol and -10.3 kcal/mol for BSEP and MRP2 respectively. Both Cyclosporine A and Zafirlukast were predicted to possess developmental toxicity and hepatoxicity. As binding energies are related to magnitude of inhibition, in vitro mutational studies are required to validate the in-silico findings.

Key-words: BSEP, MRP2, drug inhibitors, homology modelling, hepatotoxicity.

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In silico Prediction of Binding Affinity Between Test Substances and Enzyme ß-secretase for the Treatment of Alzheimer's Disease

Aniket Gandotra[1], Ashwani Sharma[2,3,4] and Jean Bernard Idoipe[3]*

[1] Sher-e-Kashmir University of Agricultural Sciences and Technology of Jammu, India
[2] Indian Science and Technology Foundation (ISTF), New Delhi, 110053, India.
[3*]Insight BioSolutions, Biopole Rennes, 35000, France
[4]Moldoc Biotech pvt. Ltd., New Delhi 110053, India

Alzheimer's disease (AD) is the progressive neurodegenerative disease of ageing that causes severe suffering for patients, including progressive memory loss with difficulty in performing daily activities.[1] FDA-approved drugs for the treatment of Alzheimer's including tacrine (approved in 1993), donepezil (approved in 1996), rivastigmine (1998), and galantamine (approved in 2001) come with inevitable side effects ranging from diarrhea, vomiting, cough, skin reactions, nausea, pruritis (itching) etc.[2] Thus, the development of potential drug alternatives is necessary. Plant compounds offer numerous alternatives to diminish the advanced and side effects of numerous sorts of diseases, counting Alzheimer's. Simultaneously, plant compound structures, including flavonoids, tannins, polyphenols, triterpenes, sterols, and alkaloids, have anti-inflammatory, antioxidant, anti-amyloidogenic, and anticholinesterase activities.[3] In this study, we selected ß-secretase, 20 FDA-approved drugs and 22 plant compounds and performed docking with the help of Auto Dock VINA to predict their binding affinities to the proteins. The top-ranked compounds were then subject to toxicity analysis using VEGA QSAR. After analyzing the results, it was found that plant compounds have stronger affinity towards the protein in comparison to the FDA-approved drugs. Hesperidin was the plant compound having a stronger affinity to ß-secretase. Also, it was found that Hesperidin, was the only plant compound having a good affinity for the protein. Moreover, after the toxicity prediction, it was found that the top-ranking plant compound was mostly non-mutagenic and non-carcinogenic and active in in-vitro micronucleus activity whereas the results varied for each of the FDA-approved drugs. The purpose of performing molecular docking and toxicity analysis was to understand the affinity of plant compounds and FDA drugs to the potential protein and analyze their toxicity to find a potential candidate targeting Alzheimer's disease.

Key-words: Hesperidin, FDA-approved drugs, Alzheimer's, ß-secretase, Plant compounds.

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