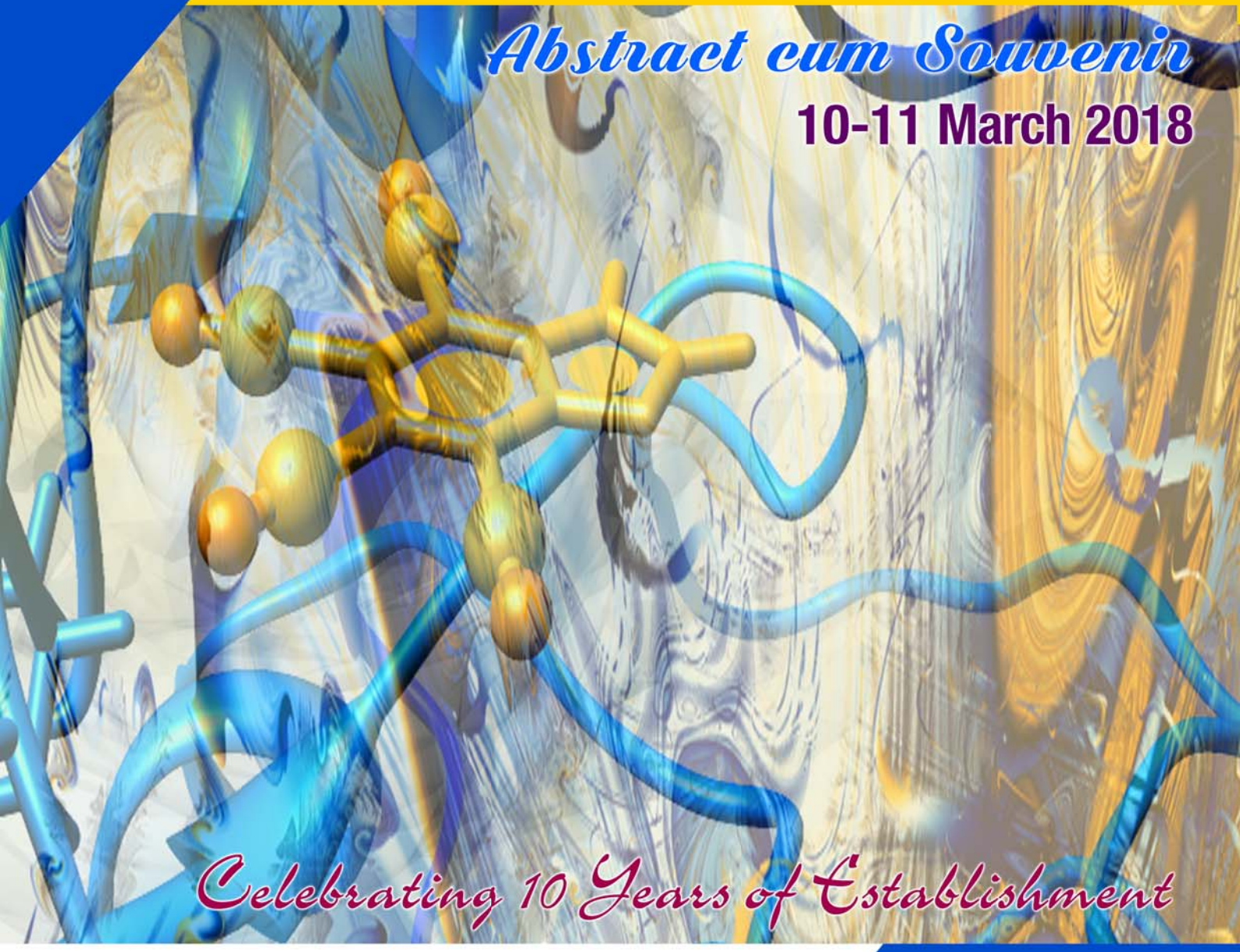
National Conference on
Contemporary Researches in Computer Aided Drug Designing



Abstract cum Souvenir

10-11 March 2018

Celebrating 10 Years of Establishment

Organised by

Bioinformatics Centre (DBT-BIF)
Assam University, Silchar

NORTH EASTERN COUNCIL
Ministry of DoNER

SERB INDIA

National Conference on Contemporary Researches in Computer Aided Drug Designing (CRCADD - 2018)

March 10-11, 2018

ABSTRACT CUM SOUVENIR

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Message

I am delighted to know that Bioinformatics Centre (DBT-BIF), Assam University Silchar is organizing a National Conference on **Contemporary Researches in Computer Aided Drug Designing (CRCADD - 2018)** from 10th to 11th March, 2018.

This conference will be of immensely beneficial for the researchers and scientists working on Bioinformatics, Drug Discovery & Design. I hope this Conference will be a platform to share knowledge, expertise to scholars due to interaction with the resource persons on various aspects of the Researches in Bioinformatics and Computer Aided Drug Design & Discovery. This indeed will help to raise awareness in the field of Biological and Bioinformatics researches.

I have come to know that since establishment, Bioinformatics Centre of Assam University is doing well in teaching and research also conducting Post Graduate Diploma Course in Bioinformatics of two semester duration.

I find myself privileged to welcome all the delegates and speakers to Assam University, Silchar. I convey my best wishes to the organizers for all success of the event.

Dated: 7th March, 2018

Vice Chancellor 7/3/18

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Welcome Address

By
Prof. Manabendra Dutta Choudhury
Chairman
CRCADD, 2018

Honourable Chief Guest of this Inaugural Ceremony; Chief Patron of this Conferfence, Prof. Dilip Chandra Nath, Vice Chancellor, Assam University, Silchar, our guest of honours Prof. G.D. Sharma, Vice Chancellor, Bilaspur University, Chattisgarh; Prof. A. Anand form VIT University, Vellore; Prof. Supriyo Chakraborty, Dean School of Life Sciences, Assam University; all the distinguished delegates; representatives of teaching and nonteaching fraternity of different departments of Assam University, my dear research scholars, participants, students, ladies and gentleman A very good morning and welcome to you all. This is the National Conference on Contemporary Researches in Computer Aided Drug Designing being organised by Assam University Bioinformatics Centre while celebrating the 10 years of establishment of the centre and also when Assam University is celebrating the 25th year of establishment. As you know Bioinformatics Centre is a Department of Biotechnology, Govt. of India funded centre established in Assam University under the School of Life Sciences as project mode. The centre was established in 2008 and we have just completed 10 years of establishment. This was the initiative of DBT, Govt. of India at this moment we have 156 centres like this centre throughout the country and we have a beautiful academic network through all those centres. Our initial mandate was to popularize Bioinformastics by organizing workshops, discussions and invited lectures, we did it for first and second year and thgen we got the mandate of doing in depth rtesearch in Bioinformartics and we have been doing this and you will be happy to know till date the centre has published 67 research papers from the centre only all with high impact factor and in addition we have initriated one academic course under the School of Life Sciences viz Post Graduate Diploma in Bioinformatics (PGDBI) of one year duration and till now we have more than 100 alumni of the centre. You will be happy to know that our present Dean Prof. Supriyo Chakraborty and present DSW Prof. P.B. Mazumder are the alumni of this centre. The centre has been providing the e - journal access facility to the whole university, DBT has given us the DeLCON service with more than 1100 journals and centre has extended the service to whole university. All the journals are now available throughout the university. We are providing studentship and traineeship to the student also. Under the initiative of this centre alongwith another DBT funded centre Biotech Hub in 2016 we organized one International Conference in the name of “ICCAR 2016” and there we resolved to frame a multi

institutional society in the name of Society for Antimicrobial Research. The society was formed and it was resolved in 2016 seminar that in every 2 years there will be a seminar under the society and accordingly it was decided that 2018 seminar will be organized by IIT Kharagpur and IIT Kharagpur has taken all the initiative, this december there will be ICCAR 2018 in IIT Kharagpur. Prof. Anand from VIT University is here, he agreed to organised ICCAR-2020 and we are expecting that it will be organized in VIT University in 2020 and 2022 ICCAR will be organized by BHU. Dr. Tuhina Banerjee from BHU attended the seminar and agreed to organized the same in 2022 and again if everything goes well in 2024 we will be organize ICCAR 2024 here in the Assam University under the joint initiative of Bioinformatics Centre and Assam University Biotech Hub.

Recalling the initiative we took 10 years back, there was a time in Assam University when we were in temporary accomodation no internat connectivity even proper electricity was not there. At that point of time it was very difficult to think to start the Bioinformatics Centre. I remember one of my Ph.D. Scholar Dr. Pankaj Chetia who is now working as Assistant Professor in Dibrugarh University, at that time he was in Guwahati, he phoned me saying that DBT has floated advertisement for Bioinformnatics Infrastructure Facility and he told "Sir I think Assam University should go for this because we have internet connectivity now". As you all know that the internat connectivity and high end computer are the primary requirement for Bioinformatics work. NKN was not there at that time, only lease line connectivity was available, I downloaded the application form and everything and I remember Prof. G.D. Sharma Sir was Pro Vice Chancellor at that time, I rushed to his room at 7.00 pm and took his signature in the application form. After three months we got the sanction letter and that is the beginning of this centre and since then we have been trying to achieve excellence. With all your support and blessings, hope we will be able to convert the centre to a National Centre of Excellence in near future. You will be happy to know that during these 10 years period of time the centre has organized six conferences and for the three consecutive years the centre got national award for publications. Our centre ranked fifth (5th) in publications in the field of Bioinformatics among all the Bioinformatics Infrastructure Facilities in different Universities in India in 2015. Based on 2014 publication the centre got 1st Rank. Based on 2013 publication the centre got 4^{th} Rank.

Now of course, DBT has changed the strategy and not considering the impact factor but till 2016 it was there and we got national award for 3 years. All the Bioinformatics centres were established by DBT Govt. of India as project mode initially so the Govt. of India recently has decided that the centres will continue till march 2020 and beyond that those centres will be given extension who can absorbe man power.We have 2 regular staff in bioinformatics centre – 1 RA and 1 lab attendant cum cleaner. If the AUS can absorb these 2 positions, then DBT will

consider for continuation of this bioinformatics centre in future. We are thank full to our guest faculties. As we do not have permanent faculty in the centre, we request the faculties of other departments to take classes for our PGDBI student.

With these few words I welcome honourable VC sir Prof. Dilip Ch. Nath, welcome prof. G.D. Sharma, VC of Bilashpur University, Prof. Anand, he has travelled such a long distance from VIT University. We have collaboration with VIT University, whenever we invite him he tries to come, also our welcome to our Dean Prof. Supriyo Chakraborty,Welcome to Dr. Sudha Ramaiah, from VIT, Dr. Garima Khare from Delhi University, all the teaching and non-teaching members presents here. Welcome to AUTA president. We invited president of non-teaching association also, president of student union is present here- we welcome him too. All our departmental. faculty members, faculty members of School of Life sciences and all other Schools, our participants, all our research scholars. With these few words I once again extend hearty welcome to all present over here.

Thank you.

CONTENT

Programme Schedule

10th March, 2018 (Saturday)	
EVENTS	**TIMINGS**
Registration	**9.00 am to 10.00 am**
Inaugural Session	**10.00 am to 11.00 am**
Refreshment	**11.00 am to 11.30 am**
Technical session-I	**11.30 am to 1.00 pm** **Chairman:** Prof. Supriyo Chakraborty **Rapporteur:** Dr. Arun Jyoti Nath **Invited talk by** - Prof. Anand A, VIT University, Vellore Dr. Yashmin Choudhury, Assam University, Silchar
Lunch break	**1.00 pm to 2.00 pm**
Technical session-II	**2.00 pm to 3.30 pm** **Chairman:** Prof. Anand A **Rapporteur:** Dr. Yashmin Choudhury **Invited talk by** - Dr. Garima Khare, University of Delhi South Campus Dr. N. Sanjay Singh, G.P. Women's College, Imphal
Tea	**3.30pm to 3.45pm**
Technical session-III	**3.45 pm to 5.15 pm** **Chairman:** Prof. P.B. Mazumder **Rapporteur:** Dr. Prodipto Das **Invited talk by** – Prof. Sudha Ramaiah, VIT University, Vellore Dr. Pankaj Chetia, Dibrugarh University, Dibrugarh
Evening Tea	**5.15 pm to 5.30 pm**
Cultural programme	**5.30 pm to 7.00 pm**
Dinner	**7.00 pm onwards**
11th March, 2018 (Sunday)	
Breakfast	**9.00 am -10.00 am**
Technical session-IV	**10.00 am to 1.30 pm** **Chairman:** Prof. Piyush Pandey **Rapporteur:** Dr. Pankaj Chetia **Talk by** – Prof. M. Dutta Choudhury, Assam University, Silchar Dr. Anupam Nath Jha, Tezpur University, Tezpur Prof. Supriyo Chakraborty, Assam University, Silchar Dr. Sudip Choudhury, Assam University, Silchar
Lunch break	**1.30 pm to 2.30 pm**
Technical session-V	**2.30 pm to 3.30 pm** **Chairman:** Dr. Anupam Nath Jha **Rapporteur:** Dr. Pinak Pani Nath Choudhury **Invited talk by** - Prof. Paritosh Mandal, Assam University, Silchar Dr. Jagajjit Sahu, Assam Agricultural University, Jorhat
Tea	**3.30 pm to 3.45 pm**
Technical session-VI	**3.45 pm to 5.00 pm** **Oral presentations** **Chairman:** Prof. M. Dutta Choudhury **Rapporteur:** Dr. Sudip Choudhury **Poster Session** **Judges:** Prof. Paritosh Mandol Dr. Pankaj Chetia Dr. Anupam Das Talukdar
Valedictory Session	**5.00 pm to 5.30 pm**

INVITED TALKS (IT)

IT 1

In silico approaches for understanding the molecular basis of antibiotic resistance in pathogenic bacteria and to exploit vital bacterial mechanisms for new drug discovery

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Abstract

Computational analysis of bio-molecular interaction networks is now gaining a lot of importance to understand the functions of novel genes/proteins. Gene interaction (GI) network analysis and protein-protein interaction (PPI) network analysis play a major role in predicting the functionality of interacting genes or proteins and gives an insight into the functional relationships and evolutionary conservation of interactions among the genes. An interaction network is a graphical representation of gene/protein interactome, where each gene/protein is a node, and interaction between gene/protein is an edge. We employed popular open source databases that serve as data repositories to search and collect protein/gene interaction data, and also tools available for the generation of interaction network, visualisation and network analysis. Also, various network analysis approaches like topological approach and clustering approach to study the network properties and functional enrichment server which illustrates the functions and pathway of the genes and proteins have been used. The results presented provide an overview on the antibiotic resistance mechanisms and the gene and protein-protein interaction (PPI) networks involved in resisting antibiotics among pathogenic bacteria. The methodology used in the present study can be used to extract useful and meaningful information from the gene and protein interaction networks.

IT 2

In silico approaches to locate potential anti-malarial compounds: A study on quinolinyl chalcone derivatives and heterocyclic substituted chalcone derivatives

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Abstract

The malarial infection causes consistent loss of million people every year, imposing sincere responsibility to research scientists and healthcare professionals to safeguard the life by eliminating the infection at the earliest. This responsibility shall be fulfilled only by the design and development of novel, potent and safe anti-malarial compounds especially against *P. falciparum*, the causative agent of severe malaria, which has gained resistance to most of the anti-malarial compounds, including artemisinin derivatives. Considering these facts, molecular modeling studies are carried out. In this present study, the molecular docking and 3D-QSAR CoMFA analyses have been successfully carried out with novel quinolinyl chalcone derivatives and heterocyclic substituted chalcone derivatives. These studies are executed to examine the critical structural requirements for the design and development of more active inhibitors against P*f* lactate dehydrogenase and *Pf* cysteine proteases. The binding mode of the novel inhibitors is assessed by Surflex-docking program. The output of the docking study recommends that the hydrogen bond interactions are the major interaction which could be considered as critical in the alteration of inhibitory activities of novel quinolinyl chalcone derivatives and heterocyclic substituted chalcone derivatives. Based on the finest docked poses, best predictive CoMFA models are developed. The model provides statistically significant results in terms of cross-validated coefficient q^2 of 0.850, conventional coefficient r^2 of 0.912, $r^2_{(pred)}$ of 0.855, correlation graph and small *SEE* of 0.280 for novel quinolinyl chalcone derivatives. Cross-validated coefficient q^2 of 0.912, conventional coefficient r^2 of 0.901, $r^2_{(pred)}$ of 0.924, correlation graph and small *SEE* of 0.210 for novel heterocyclic substituted chalcone derivatives indicating the presence of better statistical relationship between the descriptors and inhibitory activity. The results from the current study could be utilized for design and development of lead and potent *P. falciparum* lactate dehydrogenase and cysteine protease inhibitors to combat malaria.

IT 3

Virtual screening with soft docking: an integrative approach against adenosine 2A receptor

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Abstract

Integration of computational strategies and biological knowledge has paved the way for screening out therapeutics against various diseases. Here we have applied different computational techniques to virtually screen out molecules against the agonist conformation of the Adenosine A2A receptor involved in the modulation of inflammation and insulin resistance. A dataset of 143 phytochemicals has been created belonging to different categories like Flavonoids, Alkaloids, Terpenes, Sulfonylurea.

Initially 118 molecules showing druglike properties have been screened. 2D QSAR study involving a Multiple Linear Regression analysis was performed to estimate the correlation between the physicochemical properties and the experimental values of LD_{50}. Less toxic molecules predicted through QSAR have been selected. Six bioactive compounds satisfying ADMET properties were considered for further analysis.

A multi-template homology modeling has been applied to model the missing residues of the target protein. Minimized conformation of both the modelled receptor and the ligands has been considered to identify the bound conformations of the ligand to the receptor. The binding affinity has been estimated through different docking approaches: i) rigid docking ii) with an explicit hydration to ligands iii) flexibility at active site. Through water mediated docking simulations, we have analysed the binding behavior in presence of water molecules. The possible conformational space of the active site has been explored by keeping the binding site residues as flexible. The stability of these docked complex structures has been evaluated through quantifying the non-covalent interactions. It has been observed that the reported active site residues are involved in the intermolecular interactions.

This integrative approach has revealed that four selected compounds might be efficient inhibitors for adenosine A2A receptor. The molecules screened through the above method are undergoing *in-vitro* experiments.

IT 4

Identification and evaluation of inhibitors against important drug targets of *Mycobacterium tuberculosis* by employing structure based virtual screening

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Abstract

Mycobacterium tuberculosis (*M. tb*), the causative agent of tuberculosis, killed ~1.7 million people in the year 2016 worldwide with an additional 0.4 million people that were co infected with HIV. These massive numbers highlight the high rate of morbidity and mortality caused by tuberculosis worldwide. Despite the availability of an effective frontline chemotherapeutic regimen comprising of four frontline drugs namely isoniazid, pyrazinamide, rifampicin and ethambutol, the morbidity and mortality rates associated with TB patients remain very high. Moreover, the lengthy treatment of 6–9 months leads to non-compliance by the patients leading to an inexorable increase in the multi drug resistant and extremely drug resistant strains of *Mycobacterium tuberculosis*. Thus, the need to fill the drug pipeline with as many new scaffolds with distinct mechanisms of action cannot be overemphasized in order to curtail this deadly disease. Structure based virtual screening has been a very powerful tool for the identification of inhibitors agains important targets with known structures. All pathogens require a tight regulation of the intracellular levels of iron, which in *M. tuberculosis*is performed by the transcription factor IdeR that regulates the synthesis of mycobactins (siderophores) as well as bacterioferritins (iron storage proteins) to maintain iron homeostasis. IdeR has been shown to be importance for the growth and survival of *M. tuberculosis*making it an attractive drug target. Another important target in mycobacteria is an enzyme PptT (4’ Phosphopantetheinyltransferase) involved in 4′ phosphopantetheinylation, which is a post translation modification that immensely contributes to the survival and virulence of the pathogen. Studies with a conditional mutant of PptT in *M. tb* demonstrated that PptT is required for the growth and persistence of *M. tb* in the mice model of tuberculosis infection emphasizing its crucial role of PptT as a drug target.We employed a structure based inhibitor identification approach against IdeR and PptT, which included virtual screening followed by inhibition assays to evaluate the inhibitory potential of various shortlisted molecules against the activity ofIdeR and PptT, separately. Subsequently, the leads obtained from this approach were further utilized for structure based similarity search approach that resulted in molecules with potent *in vitro* inhibition. Further, the molecules were evaluated

against the growth of *M. tuberculosis* in broth culture and inside macrophages followed by cytotoxicity studies and a few promising hits have been identified that can be employed as starting points for further optimization to identify novel and potent anti-tubercular molecules.

IT 5

King chilli (*Capsicum chinense* Jacq.) as a source of therapeutic agents to fight MDR *Shigella* strains: a computational study

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Abstract

The emergence and propagation of multidrug resistant bacteria is a major problem worldwide. One of the mechanisms of resistance in bacteria is the over-expression of efflux pump proteins. The major efflux system responsible for resistance in *Shigella* spp. is the RND efflux pump AcrAB-TolC. In this study, we tried to assess the efflux pump inhibitory activity of one traditionally important medicinal plant, i.e. *Capsicum chinense* Jacq., which is popularly known as King Chilli.

King chilli is prescribed by herbal practitioners (against *Helicobacter pylori* infection) in peptic ulcer. But we were more interested to find suitable natural products to combat multidrug resistant *Shigella* spp. To assess the Efflux Pump Inhibitory (EPI) activity of King chilli, a preliminary test was performed *in vitro* using crude extracts of *C. chinense* Jacq. For this study, MDR *Shigella* spp. was obtained from AMCH and antibiotic susceptibility test was done by Kirby Bauer disk diffusion method. Activity of crude extract was tested by well diffusion method after serial dilution of the extract. As the crude extracts showed EPI activity, *in silico* studies were carried out to understand probable mode of action of compounds present in king chilli as Efflux Pump Inhibitors. From Dr. Duke's Phytochemical and Ethnobotanical Database, 10 compounds already isolated from King chilli were collected and their structures were obtained from ChEMBL and PubChem Compound databases. These compounds were docked against the most crucial efflux pump protein AcrB present in *Shigella* spp. using AutoDock 4.2. The docking scores were compared to that of known inhibitor of AcrB, i.e. Carbonyl cyanide m-chlorophenyl hydrazone (CCCP). It was found that dihydrocapsaicin is the most potent compound as EPI inhibitor extracted from *C. Chinense* Jacq. Molecular

Dynamics simulation studies were also carried out using GROMACS 5.1 for better understanding of the binding efficacy.

Keywords: *Shigella* spp., Efflux Pump, Molecular Docking, MD Simulation

IT 6
Computer aided peptide vaccine designing using reverse vaccinology

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Abstract

Availability of complete genome sequences of disease causing organisms has made it possible to design peptide vaccines. Reverse vaccinology involves the designing of peptide vaccines from genomic sequences. The complete proteome of a pathogen can be determined by *in silico* transcription and translation. Usually the cell surface proteins or porins are good candidates for peptide vaccine research and design. Several algorithms are now available to identify the potential T cell and B cell epitopes on target pathogenic proteins. These epitopes may vary in length from 6 to 24 amino acids. The peptide epitopes can be synthesized and formulated as multiple-epitope-based-vaccines at low cost. The epitopes should possess high antigenicity and immunogenicity scores despite having high hydrophilicity, high stability and high proportion of aliphatic amino acids. The peptide epitopes must not be toxic to human and amyloid in nature. Peptide vaccines do not need low temperature storage condition and can be transported easily. Synthetic peptide vaccines have great potential in combating the pathogen induced diseases against which no vaccine or drug is yet available in the market.

IT 7

Artificial Neural Network in predicting Bioactivity of new compound

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Abstract

A revolutionary change in conventional methods of testing bioactivity of plant materials has taken place with the intervention of computing. The computer-aided tools have significantly reduced the time necessary for bioactivity assessments. Quick and cost-effective prediction of biological activity of plant materials is now possible based on physicochemical properties. Although Computer-Aided Drug Discovery (CADD) has emerged as a broad subject in the field of medicinal plants research, computational molecular docking and computational target fishing are the specific techniques applied in this field. Above all, Artificial Neural Networks (ANNs) have become one of the latest techniques for direct prediction of a specific property of specific bio-molecules. This chapter, utilizing a specific example, describes how ANNs could be used to predict possible biological activity of a few drug molecules using computational tools. Results obtained from ANNs have been cross-validated using molecular docking technique. Six gossypol derivatives, whose biological activities have not been studied before, were taken for the study. Their physicochemical properties were considered as input and biological activities as output. Chemical descriptors and their respective biological activities of a number of compounds were recorded from NCBI PubChem compound database. The data were divided into 70% and 30% as training set and test set, respectively. On successful validation of the training by adjusting different layers and nodes of ANNs and after setting out final networks, descriptors of six unknown gossypol derivatives were used as experimental set for prediction of their bioactivity. Based on ANNs prediction, out of the six, three derivatives, whose predicted biological activities were the same, were taken for finding their activity using BiosolveIT FlexX 1.3.0 software to cross validate the prediction of ANNs. It was observed that ANN prediction for contraceptive activity of gossylic lactone, gossypol tetra acetic acid, and gossypol-6,6'-dimethyl ether matched with cross validation result obtained from BiosolveIT FlexX 1.3.0. The cross validation study also suggested that by inhibiting acrosin and hyaluronidase enzymes, these three derivatives might exert contraceptive activity.

Keywords: Artificial Neural Networks (ANNs), Biological activity, Gossypol derivatives, Computer-Aided Drug Discovery (CADD)

IT 8

Mode of action of Ruthenium metal based anticancer drugs at molecular level

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Abstract

Cancer is a class of diseases characterized by the uncontrolled division of abnormal cells to form lumps or masses of tissue called tumor in a multicellular organism. Roughly, one person in eight of world dies of cancer. Hence, treatment of cancer is very challenging. Therefore, understanding the mode of action of chemotherapeutics with biomolecules such as DNA and proteins are very important in the drug designing research. Interaction of anticancer ruthenium complexes such as, [trans-RuCl3(H2O)(3H-imidazole)(dmso-S)] I, [trans-RuCl2(H2O)2(3H-imidazole)(dmso-S)]+1 II, [trans-RuCl3(H2O)(4-amino-1,2,4-triazole)(dmso-S)] III and [trans-RuCl2(H2O)2(4-amino-1,2,4-triazole)(dmso-S)]+1 IV, which are generated after intracellular aquation of their respective complexes, with human serum albumin (HSA) by using Docking and QM/MM methods. It is observed that the binding energies of monoaqua adduct I-HSA and III-HAS are -4.52 kcalmol-1 and -4.58 kcalmol-1, whereas that of diaqua adduct II-HSA and IV-HAS are found to be -4.74 kcalmol-1 and -4.91 kcalmol-1, respectively. Again, quantum chemical investigation on the hydrolysis of NAMI-A in NAMI-A-HSA and nitrosylation of hydrolyzed NAMIA-HSA adduct show that the free energy of activation (ΔG) and rate constant (k) for the hydrolysis process in aqueous medium are 24.85 kcal mol−1 and 3.81×10-6 s−1, respectively. Nitrosylation of hydrolyzed NAMI-A-HSA adduct with nitric oxide is found to be thermodynamically more favorable with the incorporation of solvent effect and suggests the antimetastatic activity of the NAMI-A drug. It is also seen that nitric oxide coordinates linearly to NAMI-A-HAS leading to the reduction of Ru(III) to more active Ru(II), with the reduction potential of −2.32 V. On the other hand, interaction of I and III with the normal (GC and AT) and mismatch base pairs (GG, AA, TT, CC) shows that normal and mismatch base pairs lose their planarity upon interaction with ruthenium complexes and both the complexes interact strongly with the mismatch base pair GG than the normal base pairs.

While, Interaction of Ru(II) complexes of the type [Ru(tmp)2(dpq)]2+, [Ru(tmp)2(dppz)]2+ and [Ru(tmp)2(11,12-dmdppz)]2+ with two B-DNA hexamers of alternative AT and GC sequences, namely d(ATATAT)2 and d(GCGCGC)2 respectively, reveals that the Ru(II) complexes show intercalative minor groove binding mode with DNA base pairs as well as their preferential binding to d(ATATAT)2 over d(GCGCGC)2. Further, DFT investigation reveals that the [Ru(tmp)2(11,12-dmdppz)]2+ shows greater affinity towards DNA sequences. This result indicates that the methyl substituent of the ligands increase the binding affinity towards the DNA duplex.

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IT 9
Recent trends in cancer therapeutics

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Abstract

For decades, intravenous cytotoxic drugs have been the mainstay of cancer treatment. These drugs work by eliminating rapidly profilerating cells, including cancer cells and some normal tissues. Hence, they are responsible for the classic toxicities of alopecia, gastrointestinal symptoms and myelosuppression in several patients. In addition, their success rate in the treatment of several cancers is questionable, with a high rate of distant metastases and loco-regional recurrences reported in cancers such as those of the head and neck region after non-surgical treatment with radiotherapy and/ or chemotherapy. The treatment of cancer has therefore undergone a paradigm shift in the past decade with greater emphasis on drug discovery in the realm of therapies tailored to exploit inherent differences between cancer cells and normal cells, and based on an understanding of the underlying regulatory networks of a cancer cell. The altered metabolism and adaptations of cancer cells create a phenotype required

to promote tumor cell growth and survival by exaggerated anabolic metabolism. Several new chemotherapeutic approaches target the aberrant metabolism of cancers, either by indirectly targeting the signalling pathways that are preferentially activated or repressed in cancer, or by directly targeting the metabolic enzymes involved. Furthermore, targeted cancer therapies use pharmacological agents that interfere with specific proteins involved in tumorigenesis, and are hence safer and more effective. Computational approaches have had a major impact on the design of anticancer drugs and identification of drug candidates over the years and have provided fruitful insights into cancer in general. The ramifications of these recent approaches in cancer therapy will be discussed.

IT 10

Garnering Drug Discovery Research Outputs from India: A Scientometrics Assessment

Jagajjit Sahu

Abstract

Drug discovery is the fastest developing research field as it is one of the vital chapters in the healthcare sector. With the advancement of new technologies, huge piles of data have been gathered on public domains needed to be structured. The difficulty to handle the complexity of these kind of data is most often known as the issue of “Big Data”. Prioritizing these issues, researchers have been using data mining techniques such as artificial intelligence (AI) to fetch meaningful information out of these data. Scientometrics is an efficient approach to deal with large amount of literature data to perform meta-analysis to evaluate the research outputs. The context of the talk will be basic introduction to the data driven science and scientometrics approach including a case study on the drug discovery researches from India. In an attempt to evaluate the research outputs, PubMed reports till 28th February 2018 were collected and screened based upon their availability in Web of Science (WoS). The selected reports were then analyzed using Bioconductor packages such as “pubmed.mineR”, “RISmed” and“bibliometrix” in R to infer into several statistical parameters. The findings of this study will reveal information about the annual growth in publications, collaboration with other countries and various important aspects to provide an insight into the research outputs in the field of drug discovery.

IT 11

Structure based design strategy in development of Bioactive molecules

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Abstract

The amalgamation of *in silico* and experimental strategies has beenof great value in the design and development of novel promising candidate compounds. This approach of Structure based design strategy critically evaluatesthe key phenomena involved in theintermolecular recognition process involved in ligand-receptor interactions.Thus,an appropriate integration of computationaland experimental methods are being capable to providean elaborate understanding of the convolutedaspects of intermolecular recognition [1]. Molecular docking, structure-based virtual screening and molecular dynamics(MD) are among the ajor components in structure based molecular design strategies due to their wide range of applications inthe analysis of drug-target binding energetics, molecular interactions andinduced conformational changes [2,3]. Essentially, is a cyclic process consisting of stepwise knowledge acquisition and feedback - starting from aknown target structure, to identification of potential ligands by conducting*in silico*studies - followed by the synthesis of the most promising candidate structures [4,5].

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IT 12

Feature Selection for QSAR studies using R software

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Abstract

The Quantitative Structure-Activity Relationship (QSAR) has become important tools for drug designing and natural product research in the last few decades. Out of the various models developed, Multiple Linear Regression is a popular choice for many researchers. However, there are many issues that are frequently overlooked in this study. With the advancement of bioinformatics and chemiinformatics tools, hundreds of descriptors have been generated. Searching the potential independent variables that can describe and relate to the dependent response variable, is another challenging task. There are various descriptor selection procedures, out of which, Boruta, approach, all subset regression, anova approach, AIC method, Stepwise Regression and Genetic Algorithm have been used in described in the present study. The approaches highlighted in the present paper could provide an easy, extendable and customizable approach in the MLR analysis for the QSAR study using open source software tools.

Keywords: QSAR, Feature Selection, R software, MLR, Drug Designing

ORAL PRESENTATIONS (OP)

OP 1

In silico screening of some dietary phytoestrogens for estrogenicity and prediction of their potential as lead molecules for human estrogen receptors

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Abstract

Phytoestrogens are plant-derived non-steroidal compounds found in many fruits, beans and vegetables having affinity for binding to the estrogen receptors and thus mediate estrogenic activity. Although many *in vivo* and *in vitro* studies have shown comparable estrogenic activity of some of these compounds with respect to endogenous estrogens, reports are rare with regard to their *in-silico* estrogenicity. In the present study, estrogenic potential of 27 phytoestrogens and their metabolites have been studied keeping 17β-estradiol (E_2), estrone (E_1) and estriol (E_3) as reference endogenous estrogens. Binding affinity to the hERα and hERβ has been studied using Molecular Docking using BioSolveIT/LeadIT (FlexX). Quantitative Structure activity Relationship (QSAR) approach (Easy QSAR 1.0) and ADME-Tox screening (Mobyle@RPBS) have been used to prepare activity-IC_{50} and toxicity profile respectively of the selected compounds. In addition, the drug likeness scores of the compounds were recorded using Molsoft. All the compounds passed the ADME-Tox screening. A total of 10 (ten) out of 27 (twenty seven) compounds exhibited higher binding affinity than E_2 for both hERα and hERβ, but only 7 (seven) of them shared the same binding cavity with most potent estrogen E_2 for binding to the receptors. Interestingly, QSAR analysis revealed that almost all the compounds exhibited relatively higher activity with hERβ than hERα. However, they exhibited differential activity and drug-likeness scores. Finally, 3 (three) isoflavones viz., genistein, daidzein and formononetin have been sorted on the basis of their higher binding affinities than E_2, similarity in binding with E_2 and positive drug-likeness scores. The results clearly indicate that dietarily derived phytoestrogens exhibit differential estrogenicity with respect to both potency and activity. Therefore, estrogenic activity together with the toxicity and drug likeness profiles of phytoestrogens may provide important clues as a first step towards exploring their

potential as lead molecules with a goal of designing single or combinatorial drugs in preventing estrogen-dependent cancers or as natural alternative to hormone replacement therapy (HRT) in alleviating post-menopausal syndromes in women.

Key Words: Phytoestrogens, 17β-estradiol, Docking, QSAR, ADME-Tox, Drug-likeness.

OP 2

HRAS-GTPase inhibition mediated anti-carcinogenic potential of quercetin, luteolin and their derivatives: A Computational appraisal

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Abstract

The ras-signaling pathway has gathered considerable attraction as a target for anticancer therapy because of its important role in carcinogenesis. Oncogenic mutations in GTP-bound mutant form of H-Ras (Harvey Ras) proteins are found in 30% of human tumors. Point mutation in the codons 12, 13, 59 and/or 61 of H-Ras gene converts it into active oncogenes. The highest incidences of H-Ras gene mutations are found in adrenocarcinomas (90%), the colon (50%), and the lung (30%) cancers, in thyroid tumors (50%) and in myeloid leukemia (30%). Keeping such an alarming situation under consideration, we have attempted to design suitable anti carcinogenic drug by using computation tool. Though there are different lead molecules available that can inhibit the function of *H-Ras* P^{21} protein and in turn arrest the process of cell growth and proliferation of the cancer cell, there is always a need to find better alternatve. Moreover the plant extract of *Sonchus brachyotus* DC has been acclaimed as potential anti carcinogenic agent in many traditional medicines. The plant is reported to have quarcetin and leuteolin as its important constituents. In this present study an attempt has been taken to elucidate the anti-carcinogenic potential of quarcetin, leuteolin and their derivatives using computational tool.

Key words: *In silico*, H-Ras, anticarcinogenic drug, Quarcetin, Luteolin, *Sonchus brachyotus* DC.

OP 3

Exploring the role of mutations in fabG1 of *M. Tuberculosis* using Molecular Dynamic Simulations

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Abstract

Tuberculosis (TB) still remains as the most deadly infectious disease in the world. In 2015, the WHO estimated that over 1.4 million deaths are caused world-wide due to *M. tuberculosis* infection. Therefore, there is an urgent need for developing new drugs to combat *M. tuberculosis*. The β-ketoacyl-ACP reductase (fabG1) is one of the complex enzymes that is responsible for the production of long chain fatty acid derivatives (key precursors to mycolic acid,) which are the main constituents of *M. tuberculosis* cell wall. The structural features of fabG1, especially its affinity for long-chain substrates, pave the way towards the development of fabG1-specific substrate analogues, which can lead to the design of novel anti-tuberculosis drugs. According to some of the recent reports, it was proposed that the mutant fabG1 structure should be considered for the *in silico* drug development instead of wild-type one. Hence, to understand the structural and dynamic behaviour of the mutant(s) and wild-type fabG1, long-range molecular dynamics simulation were performed. The finding of this study indicates that the $fabG1^{WT}$ was found to be more stable in comparison to the mutant ones. Overall, this study will help in understanding the effect of the mutation(s) in fabG1 and will also help in designing novel analogues to combat the *M. tuberculosis*.

Keywords: Tuberculosis; fabG1; molecular dynamics simulation; mutant; WHO

OP 4

Finding the most prominent targets of Benzo(a)pyrene interaction: an immunological perspective of cancer promotion

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Abstract

Benzo(a)pyrene [B(a)P] belongs to the class of polycyclic aromatic hydrocarbon is one of the main components of tobacco smoke that plays lung along with head and neck carcinogenesis. B(a)P is metabolized by cytochrome P4501A1 (CYP1A1) that activates it into epoxide which can form DNA adduct and produce reactive species which results in the production of pro-inflammatory cytokines and chemokines. Cancer-related inflammation is an essential component of tumorigenesis, with common and defined players at different stages of initiation and progression. Thus, cancer and inflammation are very much related by epidemiology, histopathology, inflammatory profiles, and thus efficacy of immunomodulatory drugs are prophylaxis. So, identification of key inflammatory pathways associated with carcinogenesis of benzo(a)pyrene will try to define any possible interaction of B(a)P and inflammatory mediators using the *in silico* technique. The study provide evidence that ADAM 17, a membrane-anchored metalloproteinase alternatively also called as tumor necrosis factor-α converting enzyme (TACE) is a possible target of B(a)P mediated inflammation.Understanding the modes of interaction will provide a better strategy for targeting ADAM 17 for anticancer therapy.

Keywords: Benzo(a)pyrene, ADAM 17, *in silico,* Cancer, inflammation

OP 5

Identifying potential drug targets against carbapenem resistance through *in silico* gene network analysis

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Abstract

With the increasing incidences of resistance towards 1st, 2nd, 3rd line of antibiotics, the health care settings had to shift to the last line of resort- carbapenems. However, the ever evolving nature of bacteria has led to the emergence of New Delhi-metallo-beta-lactamases (NDM-1) which can hydrolyze carbapenem. These NDM genes interact with each other or their gene products i.e. proteins by either inducing or repressing each other though a chain of proteins and metabolites which provides protection to the bacteria against the antibiotics. Thus, screening of the interacting proteins can give an idea about the genes which are actively participating in imparting carbapenem resistance. In this study an attempt was made to design a holistic model which could show the genes which are most influential in creating carbapenem resistance. Total 420 NDM genes of *E. coli* were obtained from the NCBI database of which only 59 had shown interaction in STRING. These 59 genes had 1679 functional partners of which 1165, 319 and 195 had medium, high and highest confidence scores respectively The 59 genes were then subjected to clustering analysis which gave 71 clusters having 804 functional partners while, the rest remained unclustered. Furthermore, *in silico* analysis of the topological properties like Betweeness Centrality and Average Shortest Path Length of all the functional partners and functional enrichment analysis for gene ontological (GO) analysis showed only 21 functional partners (umuC, umuD, ssb, groS, arcB, insG, lon, nth, insD, traI, folA, ccdB, finO, espP, rspA, folP, repA2, repFIB, tus, sugE, ampC). These 21 genes can be thought to have an important role in imparting carbapenem resistance and thus can be regarded as potential antibiotic targets for future.

Keywords: NDM, Carbapenem, antibiotic resistance, gene network analysis

POSTER PRESENTATIONS (PP)

PP 1

A quantum chemical study of structure and reactivity on ruthenium (III) based anticancer complexes

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Abstract

Density functional theory (DFT) study is performed to investigate the structure and reactivity of ruthenium (III) complexes. To understand the reactivity of ruthenium (III) complexes, global reactivity descriptors such as global hardness, electrophilicity and chemical potential are evaluated. DFT based reactivity descriptors reveal that Indazolium[*trans*-$RuCl_4$(1H-indazole)(dmso-*S*)] shows the highest reactivity in gas phase as well as in solvent phase. The geometrical parameters obtained from DFT calculation are also correlated well with available experimental results. By using the multiple linear regression technique a quantitative structure-activity relationship (QSAR) model have been built up with the help of DFT based descriptors, such as electrophilicity (ω), energy of the lowest unoccupied molecular orbital (E_L) and molecular mechanics descriptor namely surface area (SA) etc against HT-29 colon carcinoma cell line. The derived QSAR model reveal that these DFT based descriptors are highly correlated with experimental cytotoxicity, having r = 0.959 and 0.999 in gas and solvent phases, respectively. Docking study suggests that the mode of action of the complex is changed when reduction of ruthenium (III) complexes occur. The study also suggest that complex-enzyme adduct is proceeded by formation of aqua derivatives irrespective of the oxidation state of the metal ion

Keywords Anticancer, DFT, QSAR, Ruthenium complexes, docking.

PP 2

Unequal usage of synonymous codons in mitochondrial protein coding genes of *Andrias davidianus*

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Abstract

Codon usage bias is the phenomenon of unequal usage of synonymous codons encoding an amino acid in which some codons are more preferred to others.Analysis of codon usage bias (CUB) is useful as it helps in better understanding of the molecular biology, new gene discovery, design of primers and gene evolution. To understand the patterns of codon usage in mitochondrial protein coding genes in *Andrias davidianus***,**we used *in-silico* approaches to analyze the protein coding sequences.*Andrias davidianus*is commonly known as Chinese giant salamander, is the world's largest amphibian. It is currently listed as Critically Endangered by the IUCN. From nucleotide composition analysisof mitochondrial protein coding genes of *Andrias davidianus*, we report that mitochondrial protein coding genes are AT rich, and A/T-ended codons are more preferred to G/C -ended codons. RSCU values for the 60 sense codons in mitochondrial genes indicated that nucleobases A and Toccurred most frequently than C and G at the third codon position. CUB was not significant as reflected by high value of effective number of codons (46.62).Correspondence analysis showed that besides mutationother factors such as natural selection might also affect the codon usage pattern. This study would help in understanding nucleotide composition dynamics and molecular evolution of mitochondrial protein coding genes of *Andrias davidianus*

Key words: Codon usage bias, *Andrias davidianus*, molecular evolution, mutation pressure and natural selection.

PP 3

Codon usage trend of mitochondrial protein coding genes of *Pseudanoplocephala crawfordi*

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Abstract

The unequal usage of synonymous codons that encode the same amino acid during translation of a gene is known as codon usage bias (CUB). The present study was undertaken to perform nucleotide composition and CUB in different mitochondrial protein coding genes of *Pseudanoplocephala crawfordi*, an important zoonotic cestode, as no work was reported yet. The mean synonymous codon usage order (SCUO) value was found to be < 0.5 (*i.e*. 0.42), which reflects existence of lower codon bias in the species. The overall AT was higher than overall GC content in mitochondrial genes of the species. Highly significant correlation was found between A% and A3%, and negative correlation between A% and T3%and G% and A3% which suggests that both natural selection and mutation pressure might affect the CUB on *P. crawfordi*. Parity rule (PR2) analysis suggests the more usage of G and C at the four-fold degenerate codon family. Relative synonymous codon usage (RSCU) analysis revealed15 over-represented codons. Neutrality analysis suggests the dominating role of natural selection over mutation pressure in the codon usage variation. Positive mean value of mutational responsive index (MRI) and translational selection (P2) value less than 0.5 which suggest both mutation and selection for translational efficiency moderately affected the codon usage bias in *P. crawfordi*.

Key words: Codon usage bias, mutation pressure, natural selection and synonymous codon usage order

PP 4

GSK3β Inhibitory Potential of Some Phytoconstituents Relevance to Neuro-degenerative Diseases: An *In Silico* Approach

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Abstract

Alzheimer disease (AD) is the most common form of age-related dementia. The etiology of AD is considered to be multifactorial as only a negligible percentage of cases have a familial or genetic origin. Glycogen synthase kinase-3 (GSK-3) is regarded as a critical molecular link between the two histopathological hallmarks of the disease, namely senile plaques and neurofibrillary tangles. Glucose Synthase Kinase 3 beta plays an important role in the phosphorylation process of Tau protein which is very vital for the integrity of the neurons. Our present study emphasises on the blocking of the target GSK3β, so that phosphorylation of Tau protein will not take place and normal neural structure will be maintained that in turn helps in preventing neuro-degenerative diseases including Alzheimer's disease.

Keywords: GSK-3β, Alzheimer disease, kinase, neurodegeneration, tau proteins.

PP 5

Enhancement of Taxol production by endophytic fungi

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Abstract

Taxol, an important drug for cancer chemotherapy, was originally found in the bark of *Taxusbrevifolia,* a threatened species of gymnosperm. Following the first discovery of the compound in 1970s, it has been reported from other species of *Taxus* too. A major breakthrough has emerged with discovery of taxol from endophytic fungi *Taxomycesandreanae*in 1993. Further, not only *Taxus*spp, fungi associated with many other plant species namely *Aeglemarmelos*, *Tectonagrandis*, *Salaciaoblonga* , *Corchorusolitorius*,

produce taxol. While the mechanism of taxol production by endophytic fungi is still not clear, it is now almost universally agreed that endophytic fungi can produce taxol independently.

On the 25th year of this great discovery of fungal taxol, it may be worthwhile to assess the present status of the compound, computational approaches for the enhanced production of taxol with an overview of genomic databases, prediction software and computational tools. At present many genomes of endophytic fungi are available for analysis. In the database, genome data through bioinformatic tools help in prediction of new molecules and enzymes. Development of genomic database would help in contextual genomics and co-expression analysis. The genomic database research in study of fungal metabolism is becoming more and more feasible. In case of fungal taxol the availability of completed genome is rapidly increasing and providing opportunity to study fungal enzymes, pathways and metabolic networks. Further, the development of algorithms for mining meta genomic data isfound to be useful for large scale genome mining.Further, potential methods for identification of taxol biosynthetic gene cluster in genome sequences of endophytic fungi and technique for prediction of taxadiene from genomic data are also discussed.

PP 6
Computational analysis of LDLR for exploring its disease networks

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Abstract

CerebroVascular Diseases (CVD), the disorder of heart and blood vessels, is the leading cause of mortality worldwide. It causes 17.7 million deaths, which accounts for 31% of all diseases globally. The major manifestation of CVD is atherosclerosis. A good number of scientific publications have correlated consumption of areca nut with CVD like stroke. It is documented in many papers that the impairment of LDLR may cause atherosclerosis. Since biological processes are controlled by genes and those genes in turn are influenced by each other therefore, alteration in the expression of LDLR gene may have effect on other related genes and in turn different physiological pathways. Thus, in the present study computational gene

networks were created to analyze LDLR gene along with its functional partners in order to get an idea about the effect of LDLR gene on other associated diseases. For this purpose, protein-protein interaction data obtained using STRING (v10.5) revealed 10 functional partners at medium confidence score. Clustering analysis using MCODE app of the Cytoscape software (v 3.5.1) showed single cluster with 8 nodes (genes). Parameters like average shortest path length and betweenness centrality were calculated using Network Analyzer plug-in. Gene Ontology (GO) analysis and disease network was done using DAVID 6.7 and KEGG DISEASE database. From all these analyses genes apoB and apoE were found to be most influential. As LDLR gene is found to be closely interacting with ApoB and ApoE which in turn are associated with Hypercholesterolemia, Familial hypobetalipoproteinemia (FHBL), Alzheimer's disease, Lipoprotein glomerulopathy, Sea-blue histiocyte disease, Macular degeneration, thus patients with these disease may be prone to atherosclerosis and CVD.

Keywords: CerebroVascular Diseases, atherosclerosis, LDLR, Gene network analysis.

PP 7

Docking Study of Important Phytoconstituents from *Flacourtia Indica* Plant Against the Treatment of Tuberculosis

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Abstract

Tuberculosis, an ancient disease of mankind remains a major cause of morbidity and mortality worldwide. Though many drugs are available, yet the complete avoidance of this disease has not been achieved. *Flacourtia indica*, an indigenous shrub have been reported to have anti-bacterial activity. Therefore the current aim of this work was to perform an *in silico* analysis of six isolated phyto-compounds from *Flacourtia indica* for their anti-tubercular activity.Enoyl acyl carrier protein reductase (InhA), involved in bacterial fatty acid synthesis has been considered as the desired drug target and Isoniazid is taken as the known inhibitor. The drug targets and ligands were chosen from Protein Data Bank and PubChem respectively. Molecular

docking was performed using FlexX. Molsoft online software was used for calculating the drug-likeness score. Thestudyrevealed thatCatechin-[5,6-e]-4b-(3,4dihydroxyphenyl)dihydro-2(3H)-pyranone (P1), a phytocompound from this plant showed better results with a docking score of -29.7110Kcal/mol when compared to the control (Isoniazid) which showed -18.8969Kcal/mol. Therefore, P1 may be considered to have a better binding affinity with the target and thus a potential drug lead for future tuberculosis treatment after validated with *in vitro* and *in vivo* experimentation.

Keywords: Tuberculosis, *Flacourtia indica*, InhA, Isoniazid, Molecular docking, Catechin-[5,6-e]-4b-(3,4dihydroxyphenyl)dihydro-2(3H)-pyranone.

PP 8

Screening of certain phytochemicals for anti-amoebic potential: An *in silico* approach

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Abstract

Protozoal infections such as that caused by *Entamoeba histolytica* has worldwide occurrence. Amoebic dysentery, associated with amoebic liver abscess is one of the leading cause of mortality worldwide and it is also a great concern for India and its neighboring countries. *Cysteine proteinase 5* or *EhCP5* is responsible for intestinal mucin degradation and hence tissue invasion in infected individuals and is one of the main virulence factor of *E. histolytica*. In the present study, EhCP5 was considered as the target protein whose tentative structure was predicted and generated by *Easy Modeller* using *Trypanosoma* Cathepsin protein (PDB ID-3MOR) as the template peptide chain. About 70 anti protozoal compounds were listed out based on reports. 20 inhibitors which were supposed to act as control were adopted from Binding data base. The *ADMETox* screening of the compounds were done using *Mobyle RBPS.* Molecular docking of the compounds and target was performed using *FlexX* software. The generated protein model of EhCP5 was found to comprise of two chains. From ADMETox screening it was found that most of the compounds obeyed Lipinski's rule. Drug likeliness analysis was done using Molsoft LLC server. Molecular docking revealed the greater scores of the phytochemicals i.e. greater binding affinity of the phytochemicals with the target protein as

compared to the inhibitors. Epoxygaertneroside and Ellagic acid displayed strongest binding with the target protein having docking score -28.1192 kcal/mol and -27.75 kcal/mol whereas the docking score of the strongest inhibitor was -26.555 kcal/mol. The drug likeliness score of epoxigaertneroside and ellagic acid was found to be 0.62 and -0.98 respectively. Epoxygaertneroside has been reported in plats such as *Morinda sp.*, *Pentas lanceolata* whereas ellagic acid is found in strawberries, raspberries, cranberries, pomegranate, walnuts etc. Thus, these plant products may prove alternate remedies against amoebic infections or dysentery and lower the incidences of drug resistance of *E. histolytica* and side effects posed by marketed drugs.

Keywords: *Entamoeba histolytica*, molecular docking, Epoxygaertneroside, Ellagic acid.

PP 9
In Silico Designing of Suitable Domperidone Derivative

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Abstract

Gastrointestinal problems are major complications that a human being suffers in theglobal scenario. The problem includes ailment in gastrointestinal tract and associated different accessory organ of digestion. As remedy, diverse types of prokinetic or gastro kinetic medication have been developed through years but most of them are no longer in the market uses because of their reported toxicity.

Domperidone is one such promising gastro kinetic medicine that acts antagonists of dopaminergic receptor D2. But due to wider use of this medication, presently it has been found to have Potassium Channel Binding (hERG) toxicity that may lead to Ventricular Arrhythmia, even including Sudden Cardiac Death (SCD). For all these reasons, the compound was already banned by Food and Drug Administration Authority (FDA) in United States and is under continuous periodic monitoring in some other nations. So, the necessity has arisen to develop an alternative to this compound (Domperidone) at earliest.

The present work takes a challenge of designing novel Domperidone derivative molecules by CADD (computer-aided drug design) which can minimize the hERG toxicity. The most fundamental aim in CADD is to analyze the ability of compounds to hit biological target and to measure the extent of binding. It can even measure the conformational changes in the small molecules after binding to target. The results showed that the designed compound D28 was very much active against Dopamine-D2 receptor but less towards hERG. The present work is a proposal to take newly designed Domperidone derivative in the pipeline after further post-design treatments.

Keywords: Domperidone, hERG, Dopamine-D2, CADD, Arrhythmia

PP 10
In silico screening of some Enamines and their derivatives in Combating persistent Tuberculosis

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Abstract

Tuberculosis (TB) is a communicable disease which is one of the leading causes of deaths all over the world. The causative agent of TB is *Mycobacterium tuberculosis* (Mtb). In most of the cases inhaled bacilli are destroyed by body's defence mechanism whereas some cause active TB that are able to evade the cell-mediated immune response. In such a condition drugs are prescribed which destroy the active disease causing Mtb. But some mycobacterium may also enter into another phase known as non-replicating phase or latent stage. Reactivation of latent infection occurs more frequently which is about 5-15% per year and approximately 50% over a lifetime in human immunodeficiency virus (HIV) co-infected individuals (Pawlowski*et al*, 2012). According to World Health Organisation, Global tuberculosis report (2012), the reactivation of latent infection is largely responsible for active TB in many countries and nearly 8.7 million new and relapse cases of active TB occurred in 2011. In the latent phase, the Mtb remains persistent inside the phagosome of macrophage. The phagosomes are glucose-deficient and Mtb requires β-oxidation of fatty acids, glyoxylate shunt and gluconeogenesis for its survival. Glyoxylate shunt is essential for gluconeogenesis. Glyoxylate shunt requires two

enzymes namely isocitratelyase (ICL) and malate synthase (MS). Both the enzymes arerequired for survival of Mtb. MS catalyses the formation of Malate which is finally converted to glucose by gluconeogenesis and it is also absent in the vertebrates. Therefore, MS is an attractive target and its inhibition can prevent persistence. In the present study, computational techniques were used to analyse the inhibitory activity of some enamines and their derivatives on Malate Synthase (MS). The study reveals that one of the enamines (Ethyl(2Z)-2-(4-chlorophenyl)-3-[(4-hydroxyphenyl)amino]prop-2-enoate) and its derivatives have high MS inhibiting potential and may be able to deal with the problem of persistence and reactivation of TB in patients better than the commonly prescribed drugs namely Rifampicin, Isoniazid and Pyrazinamide.

Keywords: Persistent tuberculosis, Malate synthase, Enamines, CADD

PP 11

Screening of some phytochemicals for their anti-Leishmaniasis activity targeting Trypanothione Reductase: An *In silico* approach

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Abstract

Background: Leishmaniasis is a major public health problem and about 20-30 thousand peoples are dying annually worldwide. Certain types of sand flies are responsible for spreading the disease-causing protozoa, i.e. ***Leishmania sp***. There are mainly 3 forms of infections, viz. visceral (kala-azar, the most serious form of the disease), cutaneous (the most common), and mucocutaneous. Till date, there is no such effective vaccines are available. Chemotherapy is relying solely on the infected people as a control strategy. **Trypanothione Reductase (TR)** is a key molecule against oxidative stress and maintaining the redox potential of the cell for the survival of *Leishmania* & *Trypanosome* protozoans. By obstructing the **TR** enzyme in Trypanothione pathway of the pathogen may possible to prevent the survival of the parasite.

Method: To screen the phytochemicals against Leishmaniasis, bioinformatical tools were used. **35** known inhibitors of leishmanias were taken from the '**Binding DB'** databse. Toxicity of **100** selected phytochemicals was screened using **mobyl@rpbs** server. The protein structure

of **TR** enzyme was downloaded from **'Protein Data Bank (PDB)** server. Activity profiling (**IC50**) of phytochemicals was done by QSAR using **easyQSAR** software. Molecular docking was performed by **'Flex X'** within phytochemicals and known inhibitor with **TR** protein separately.

Result: Out of **100** Phytochemicals, **Quarcetin** showing the good binding affinity with target protein chain A with a docking score of-**36.6761** and it is also showing good binding affinity with target protein chain B with a docking score of **-30.7994**. Predicted IC50 values of the phytochemical is almost similar to the known inhibitor.

Conclusion: By analysing docking score and IC50 value of Quarcetin showing the better results than knowing inhibitors, and it may be a good drug against Leishmaniasis.

Keywords: Leishmaniasis, Trypanothione reductase, Phytochemicals, Quarcetin, Molecular Docking, IC50, QSAR.

Vote of Thanks

By
Dr Anupam Das Talukdar
Organizing Secretary, CRCADD

Honourable Chief Guest, Vice Chancellor of Assam University, Silchar, Prof. Dilip Chandra Nath; our Guest of Honour, Vice Chancellor of Bilaspur University, Chhattisgarh, Prof G. D. Sharma; Honourable Dean, School of Life Sciences, Assam University, Silchar, Prof. Supriyo Chakraborty; our most valued invited guests, distinguished delegates, my dear research scholar participants from various Northeastern Institutes, students, ladies and gentleman; its my immense pleasure on being asked to deliver the vote of thanks on this occasion.

I extend my sincere thanks to Prof. Dilip Chandra Nath, Hon'ble Vice Chancellor of Assam University, Silchar, for his gracious presence in this inaugural ceremony and his valuable words. His vision and guidance helped us to organize this event.

On behalf of the Organizing Committee of the Conference, I convey my deep regards and gratitude to Prof. G. D. Sharma, Hon'ble Vice Chancellor of Bilaspur University, Chhattisgarh, who happens to be the Ex Pro-Vice Chancellor of Assam University, Silchar as well as the founder Coordinator of our Bioinformatics Centre, for gracing the inaugural ceremony of the conference as our Guest of Honour and sharing his visions.

I am grateful to Honourable Dean, School of Life Sciences, Prof. Supriyo Chakraborty for his kind presence in this august gathering and saying valuable words. He is also going to act as one of the invited speakers in the technical session.

Heartiest thanks are due to all the invited speakers who are going to share with us their knowledge, philosophy and experiences on different aspects and allied areas of the conference theme. Thanks are also due to all the Chairpersons and Rapporteurs who are going to conduct the technical sessions of the conference. We understand that you have taken time out of your very important schedules to contribute to this meet and some of you have even travelled a very long distance to come over here. Thank you for your invaluable contribution.

I am thankful to all the invited guests in the audience, my colleagues, teaching and non teaching staffs of the University for gracing this occasion and inspiring us to move forward.

My sincere thanks to all the research scholar participants from different institutes who are the main reason for existence of this event. This is a unique opportunity to share scientific thoughts and experiences with each other and learn a lot from the invited speakers. My

special thanks are due to all those who are going to present their papers in the technical session of this conference.

Organizing this conference wouldn't have been possible without the financial assistance from North Eastern Council (NEC), SERB and DBT, Govt. of India. I wish to thank all those funding agencies and sources in order to facilitate smooth running of this national conference.

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Once again I offer my heartiest thanks to all the guests, delegates, participants and paper presenters on behalf of the organizing committee. Its really a great pleasure to have all of you in this National Conference.

Thanks a lot.

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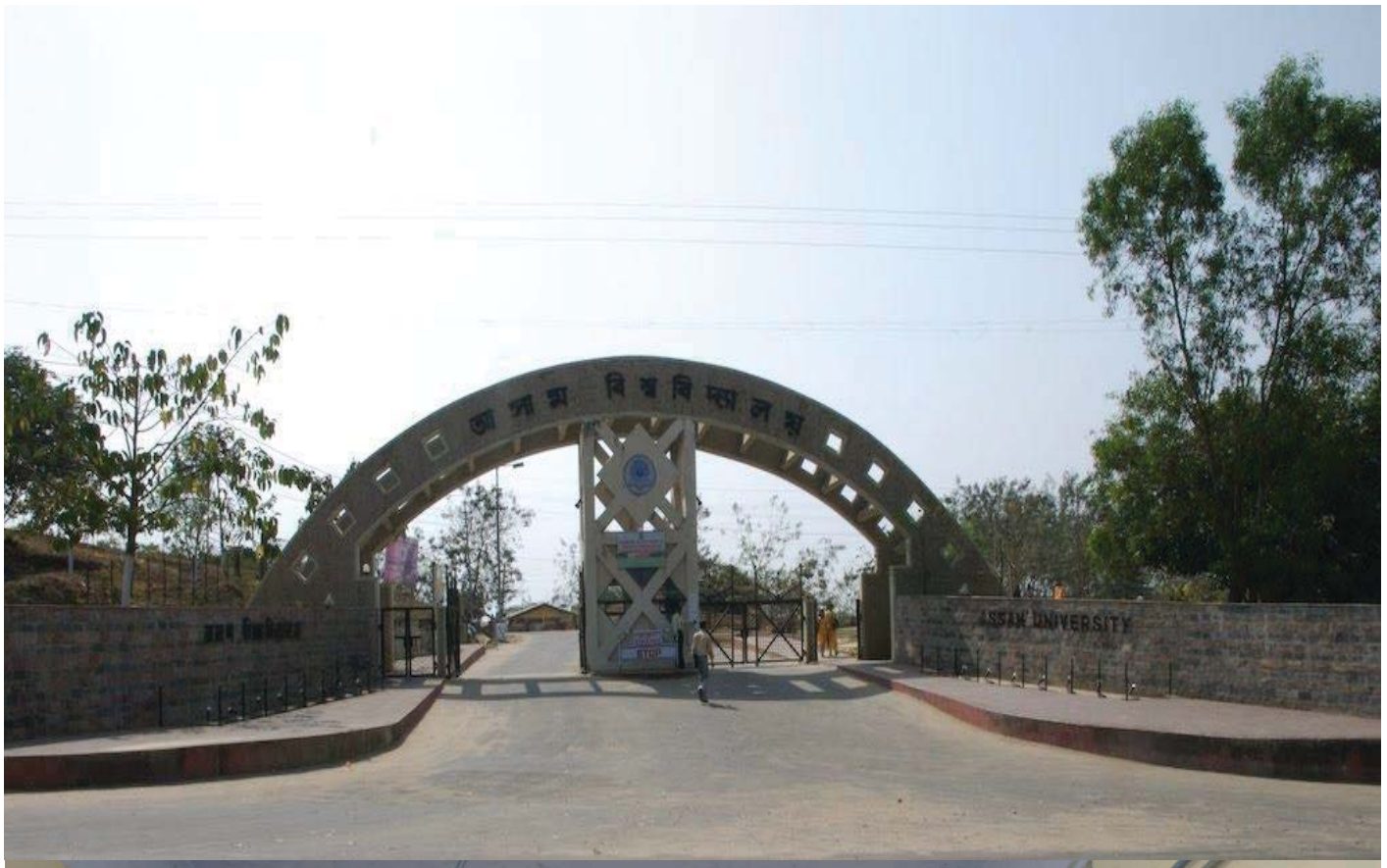

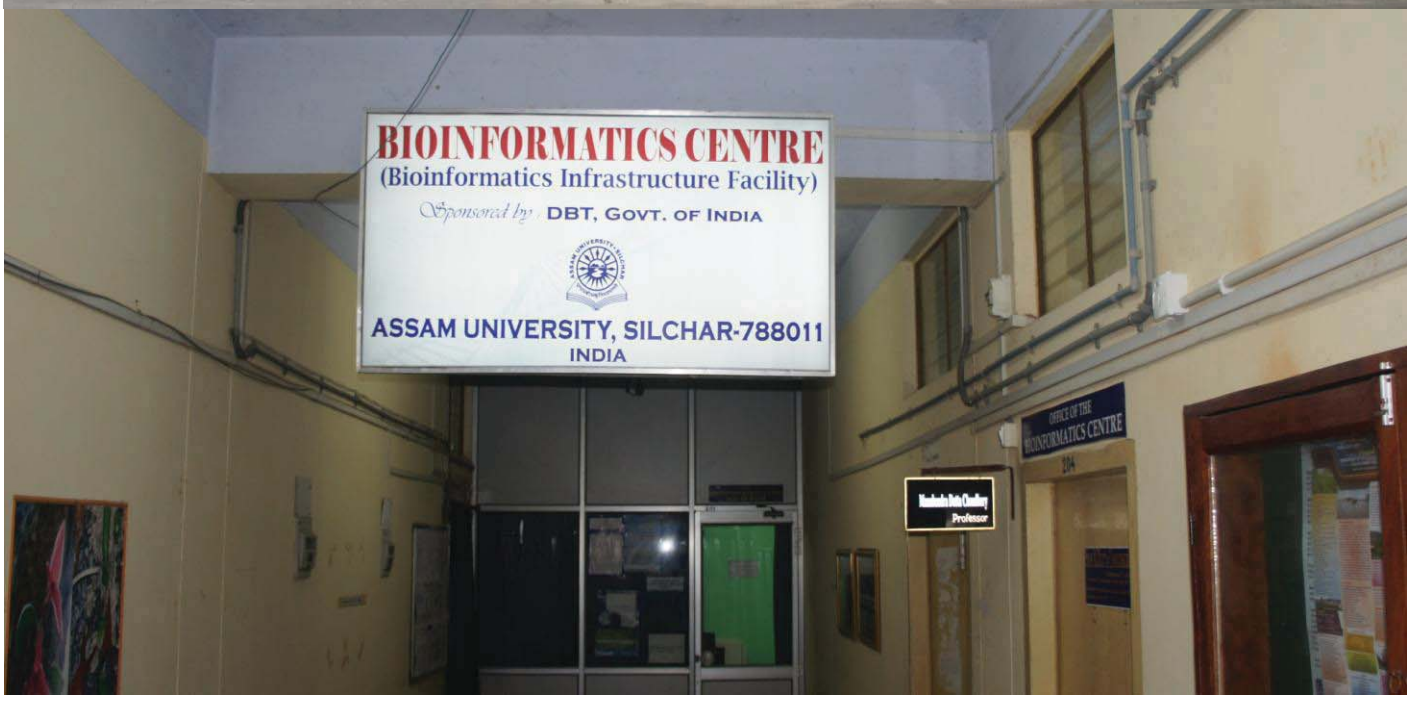

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