

Day 1, 23rd May 2019

Conference on “**Recent Advances in Bioinformatics**” was organized by Advanced Computation and Data Sciences Division (ACDSD) & Bioinformatics Centre-Biological Sciences and Technological Division (BSTD), CSIR-North East Institute of Science & Technology Jorhat, Assam during 23-26th May 2019. The primary focus of the conference was on state-of-the-art of Artificial Intelligence, Machine Learning, Text mining in Genomic, Proteomics sector, recent Bioinformatics tools, software and Hands-on session on CADD and QSAR.

About Us: ACDSD is a new division of CSIR-NEIST which was inaugurated by **Dr. Shekhar C Mande**, Director General, CSIR & Secretary, DSIR, Govt. of India on 17th March 2019. Under the leadership of **Dr. G. Narahari Sastry**, Director, CSIR-NEIST, this division aims to strengthen the advanced computational and data analytics of the different R&D sectors in CSIR-NEIST, Jorhat by adopting contemporary scientific and technological advances. This helps to explore into different social problems with the proper data driven solution by adopting machine learning (ML) algorithms and artificial intelligence (AI). Also it will undertake the path of documentation, digitization and deposition of data and subject this data for ML and AI.

Inaugural ceremony of the Conference



The program begun with inauguration of “**Passion and Excellence sections of Kids’ World of Science**” by our honourable chief guest **Prof. T.P Singh**, AIIMS, New Delhi and the conference started with the NEIST Song followed by lighting of the lamp by honourable Chief Guest **Prof. T.P Singh**, distinguished Professor, AIIMS, New Delhi, INSA senior fellow, **Dr. G. Narahari Sastry**, Director, CSIR-NEIST along with other visiting faculty. The convenor of the conference, **Dr. Y. Silla Devi** welcomed the dignitaries, invited guests, participants scientist, staffs and students and highlighted the objective of the conference. **Dr. G. Narahari Sastry** delivered the presidential address focusing on the importance of Bioinformatics in the present day scenario. A short note was delivered by **Mr. S.C Kalita**, Chief Scientist which was followed by a brief description of Bioinformatics Infrastructure Facility Centre by **Dr. H.P. Deka Boruah**. The key note lecture was delivered by the chief guest **Prof. T.P Singh**, AIIMS, New Delhi on “Structure and Function relationship of innate immune proteins and their application as protein antibiotics.. In his talk he summarised about the pre, current and post-antibiotic era focussing on dual therapeutic strategy that is antimicrobial protein therapeutics and ligands against bacterial protein targets. The program ends with vote of thanks delivered by **Mr. Debabrata Das**.

Lecture session-I: Theme-Big Data in Biological Space; Chaired by Dr. HP Deka B. BSTD, CSIR-NEIST



The first speaker **Dr. G. Madhavi Sastry** of Schrodinger, LLC delivered a talk on “Boosting Virtual screening enrichment using a new data fusion approach: Coalescing 2D fingerprints. She also demonstrated on CADD using the software developed by her team



The second talk was on “Data driven models for computational biology” by **Dr. Shandar Ahmad, Professor JNU**, New Delhi. His talk focussed on the importance of machine learning and clustering models in biological problems on a large scale of data.



The third scientific talk was delivered by **Dr. Vinod Scaria, Senior Scientist** of CSIR-IGIB, New Delhi. He mentioned about the comprehensive resource of human genetic variation, rare genetic diseases, integrating whole-genome and whole-exon data sets from MENA region.



The last talk was delivered by **Dr. Sucheta Tripathy**, Principal Scientist, CSIR-IICB, Kolkata. Her talk was on Taming the genomics big data by horn-A new perspective. She mentioned about the De-novo genome sequencing of bacterial and fungal species software development.

Lecture Session-II: Theme- Molecular dynamics and CADD



The first speaker of the Day 2 was **Dr. Anupam Nath Jha**, Tezpur University, Assam. He talked on the topic “Nanoparticle-Protein interaction” highlighting how nanoparticles induces protein stability and effective in target based drug delivery.



The second speaker was **Dr. S. Nagamani**, CSIR-NEIST. He explained about the theme of Molecular Property Diagnostic Suite software (MPDS). He explained MPDS software to perform different drug discovery calculations such as descriptor calculations, molecular docking and QSAR.



After lunch break, **Dr. Vinod Scaria**, CSIR-IGIB demonstrated on IndiGen programme launched by CSIR-IGIB which focused on “Genomics for Public Health in India”. This session was followed by blood sample collection under IndiGen programme from volunteers, and also collected blood samples.

Dr. Vinod Scaria collected blood sample for IndiGen programme, which aim is to perform whole genome sequencing of thousands of individuals representing diverse ethnic groups from India.



The last and special lecture of the session was followed by **Dr. V. Subramanian**, CSIR – CLRI, Chennai. He delivered a talk on the origin of the stability of Asp in X_{AA} and Y_{AA} positions on collagen-like peptide using the molecular dynamics method. He also mentioned about the structural basis for the stability of collage-like peptide, hydrogen bonding and mechanism of action of the collagenase enzyme for degradation of collagen.



Session-III: Hands on: Molecular Docking & CADD



The first speaker of Day 3 was **Dr. Amit Kumar Yadav**, THISTI, Faridabad. He delivered a lecture on functionality of genetic code is expanded by various post-translational modifications (PTMs) and study the “PTM code” which provides an additional layer of encoding to the heredity information.



After the tea break, hands on session was carried out by **Mr. Nandan Kumar** and **Mr. Y. Bhargav Kumar** on CADD related software, i.e. AutoDock, MPDS modules. They demonstrated the AutoDock and MPDS tools, meanwhile they also gave a short overview on the docking methodologies, file preparation & handling, visualization, protein data bank and their file format, line notation, i.e. SMILE notation, InChI key, fingerprints and compound library.



After session was **Dr. Prajwal Nandekar**, Schrodinger Inc Bangalore, gave a brief description on the topic “Transforming Drug Discovery with Advanced Computational Modeling” followed by hands on session on 3D QSAR using Schrodinger software. He described about the basics of QSAR like the chemical fingerprints and molecular descriptors. He gave a brief introduction about the different types of molecular descriptors starting from the 0 dimensional descriptors like molecular weight, melting/boiling point etc. to higher dimensional descriptors like bond lengths, bond angles, torsion angles etc. Then he talked about the common yet extremely important terms in computer aided drug design like ‘Hit’, ‘Lead’, ‘Lead Optimization’, ‘Virtual Screening’ and ‘QSAR’ etc. Then he proceeded to the demonstration and a hands-on session on 3D QSAR using Schrodinger software.



In the last session, we had interactive discussion with Dr. G.N.Sastry, Director, CSIR-NEIST and other invited delegates along with participants.

Day 4, 26th May 2019

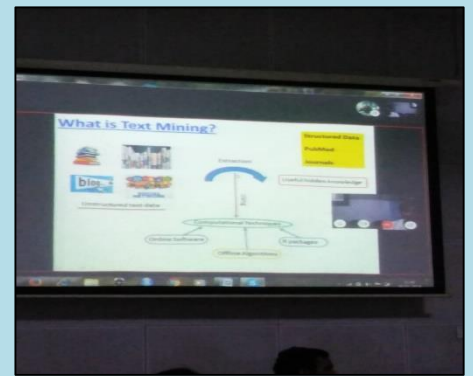
Lecture Session-IV: Theme- Applications of Text mining and Molecular mechanics in Biological field.



First speaker of the Day 4 was **Dr. R. Parthasarathi**, CSIR-IITR, Lucknow. He delivered lecture on the role of quantum mechanics and classical mechanics in different fields such as metabolic pathways in plants, nanomaterials and biofuels. He also explained the toxicity prediction and available different platform in IITR.



Second lecture was delivered by **Dr. S. Ramachandran** (CSIR-IGIB, New Delhi) on Text mining in R via video conference. Especially he explained the pubmed mine R package. He also showed different scripts in R which helpful to analyse the pubmed abstracts. He explained the disease co-occurrence, word frequency analysis using R code.



The lectures were followed by closing ceremony which includes taking feedbacks from the participants and distributing certificate of participation. After this, lunch was served for all the participants.



Group photo of the participants, Organising committee members, ACDS scholars with **Dr. G. Narahari Sastry**, Director, CSIR NEIST and invited delegates.