A brief report of the Lecture Workshop on

Applications of Bioinformatics in Drug Designing

Two day lecture workshop was organized on 22nd and 23rd Jan, 2015 in School of Biotechnology and Bioinformatics, D.Y.Patil University.

22nd Jan, 2015-Day 1

10.30 am-11.30 am

The session started with Prof. KVR Chary (TIFR) talk on Bioinformatics and NMR spectroscopy.

- This talk mainly discuss about the current growth of genebank sequences and crystal structures were detailed.
- The methods used behind the data generation like X-ray and NMR was discussed. Further the role of NMR was discussed in detail.
- In addition to this, the problems of NMR, sensitivity, resolution, water resonance. A tracked approach for automated NMR assignments in proteins (TATAPRO). Many motifs were discussed which includes crystallines and greekey.

11.30 am-12.30pm

Lecture delivered by Dr. Smitha Mahe (NIRRH) on Structural, Molecular and Cellular Aspects of Ligand-Receptor Interaction: Step Towards Drug Designing.

- The talk mainly discusses about the steps towards drug designing in in-silico database.
- it was also about computer aided drug discovery, drug target identification and validation, gene expression and molecular pathway.
- Identifying binding sites, lead identification, ADME studies, toxicity, QSAR and designing antagonist for histamine receptor. Finally fragment screening.

( Dr. Deepti Deobbkar could not take the lecture due to health issues)

1.30pm -2.30 pm

Lecture given by Selvaa kumar C. The title of the talk was Identification of leads from marine seaweeds using Bioinformatics softwares.

- This talk was mainly on the identification of leads from marine seaweeds using Bioinformatics softwares which includes homology modelling of human beta tubulin and virtual screening of seaweed secondary metabolites
- Conformers were generated and docked against human beta tubulin.
• ADME properties were calculated for these selected compounds
• Further Compounds from higher and lower plants with cytotoxic properties were docked against human beta tubulin so as to identify their binding affinity.

2.30pm-3.30pm

Next talk was by Selvaa Kumar C. This was a demo session which deals with the homology modelling of the human tubulin, their structural validation. All the participants were provided with the work flow of the demo session (work flow attached).

23rd Jan, 2015-Day 2

10.30am -12.00pm

This lecture was given by Dr. M.V Hosur (ACTREC) titled X-ray crystallography of Biological Molecules HIV-1 protease
• He gave a brief summary of advances in structure determination by crystallography which includes crystallization, X-ray sources, detection and phasing.
• There was also emphasis on structural Biology of HIV-protease and structural mapping of proteins and unfolding.

12.00 pm - 1.00pm

This lecture was given by Mr. Naveen padmas gave a talk on “Identification of potential Drug Targets”
Very often, the route to new therapeutics ends in costly failure. It is very important to identify drug targets with true potential to see success. Many different approaches have been established for identification of potential drug targets and validation. The drug target fails mainly for two reasons, they either don't work or they prove to be unsafe. Both the reasons are directly related to sloppy drug target identification. We have tried a novel approach, by starting our screening at the Genomic level. Human Gene Mutation database was considered for identifying the mutations reported in colorectal cancer. The CDS regions were identified from the Genbank and was searched in PDB for reported structures. A model was generated and validated using swiss-model. The drug binding potential pockets were identified using CASTP server and cross checked with Drug bank. A live demonstration of the same was provided to the audience.
2.00 pm-3.00pm

This lecture was delivered by Mr. Shine Devraj. The title of the talk was “Molecular modeling studies on Aβ(42) protein in Alzheimer’s disease”

- This talk was about the study of beta amyloid protein (Aβ42) in Alzheimer’s disease by using molecular dynamics simulation to explore the mechanism behind Aβ42 with GM1 ganglioside in lipid membrane and to construct a molecular model called ‘GAβ42’ complex in membrane environment.
- Moreover, the presentation was also emphasized on the role of Aβ42 in apoptosis pathway in Alzheimer’s disease. Thus, the talk concluded that the preset computational studies enhance the structural biologists to resolve such type of complex biological models.

3.00 pm-4.00pm

This lecture was delivered by Prasanna Venkatraman (ACTREC) on “Converting non-Druggable genes/proteins to Druggable targets-role of hot spot sites”

- Main emphasis was on trapping kinase targets in an inactive conformation-design of allosteric inhibitors
- Global conformation flexibility versus local accessibility of phosphosite and conformation trapping by inhibitors.
Lecture Cum Workshop on
Application of Bioinformatics in Drug designing
22\textsuperscript{nd} - 23\textsuperscript{rd} Jan, 2015

Participants Details

Total Participants: 59
Students: 38
Teachers: 21

Colleges:

1. School of Biotechnology and Bioinformatics, D.Y.Patil University
2. Bharati Vidyapeeth, Navi Mumbai
3. Mahama Gandhi Medical College, Kamothe, Navi Mumbai
4. Medical College, D.Y.Patil University, Nerul, Navi Mumbai
5. Khalsa College, Matunga, Mumbai