Department of Chemical Engineering

Three Days Online Workshop on

In Silico Drug design and Development

REPORT

Dec 8-10, 2021

Inauguration of the Workshop

The three days Online Workshop on Drug design and development was organized in the Microsoft teams Meetings. Dr. B. Vivekanandan, Associate Professor and HOD, Department of Chemical Engineering inaugurated the workshop and welcomed the gathering.

Day 1

The first session was conducted by **Dr. G. Dicky John Davis** on the topic "Computational Methods for Protein Structure Prediction". He first outlined general idea on why and how protein structure prediction has to be done. He also explained the different techniques of protein structure prediction by wet lab as well as by computational methods. He then demonstrated a homology modelling software for tertiary structure prediction of protein.

In the second session **Dr. Bijo Mathew** (Associate Professor, Department of Pharmaceutical Chemistry, Amrita School of Pharmacy, Amrita Vishwa Vidyapeetham, Kochi, India) shared his views on the topic of 'Overview of drug receptor interaction'. He emphasized on the different bonds involved in drug receptor interactions. He also highlighted the lipinskys rule of 5 which helps in figuring out the best fit of the drug.

The third session was delivered by **Dr. P. Yogeeshwari** (Professor, Department of Pharmacy, Birla Institute of Technology & Science, Pilani, Hyderabad campus) on the topic of 'Insights on drug design methods and outcomes in cancer therapeutics'. She explained how computer-aided drug discovery (CADD) has emerged as a powerful, and promising technology for faster, cheaper, and more effective drug design. She also discussed the

different subareas of the computer-aided drug discovery process with a focus on anticancer drugs with emphasis on structure-based drug discovery and ligand-based drug discovery.

The fourth session was held by **Dr. Anshuman Dixit** (Senior Scientist, Institute of Life Science, (An Autonomous Institute of DBT, Govt. of India), Bhubaneswar. on "Deciphering the regulatory roles of non-coding RNA in cancers". He discussed the regulatory role exerted by ncRNAs on metabolic enzymes and pathways involved in glucose, lipid, and amino acid metabolism. He also explained the therapeutic potential of metabolism-related ncRNAs in cancer.

Day 2

The second day of the workshop started with the session conducted by **Dr. Lipi Thukral** (Senior Scientist and Assistant Professor, CSIR-Institute of Genomics and Integrative Biology (IGIB), New Delhi) on "How molecular dynamics simulation work?". She gave a very interesting, animated tutorial on different molecular dynamics simulations on how protein motion can be studied by following their conformational changes through time. She also mentioned certain simulation software's and choices that has to be made prior to running the simulation and which molecules to be included and the force field used to describe their behavior.

In the second session, **Dr. Xavier Suresh** (Associate Professor, School of Advanced Sciences and languages, VIT Bhopal University) delivered a tutorial and hands on workshop on the software "Autodock". The participants were instructed to download the free software "Autodock vina" and "MGL tools" before the workshop started. He also gave a short introduction on docking and the various types of docking prior to the tutorial.

The third session was handled by **Dr. Ganesh Bagler** (Associate Professor, Computational Biology, Indraprastha Institute of Information Technology Delhi, New Delhi) on the topic "Network Pharmacology: A systems approach for drug discovery". He explained the combination of two fields Network biology and pharmacology as a method for data

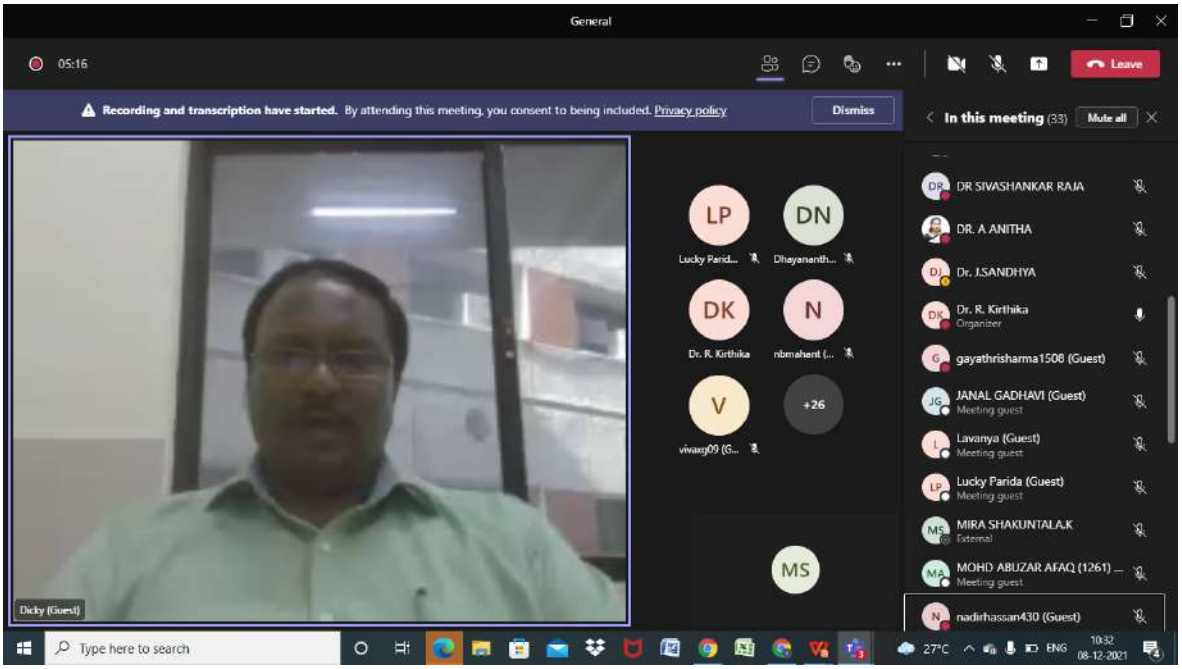
integration and multitarget drug development. He also emphasized on this particular field for the promise of expanding the current opportunity space for druggable targets

Day 3

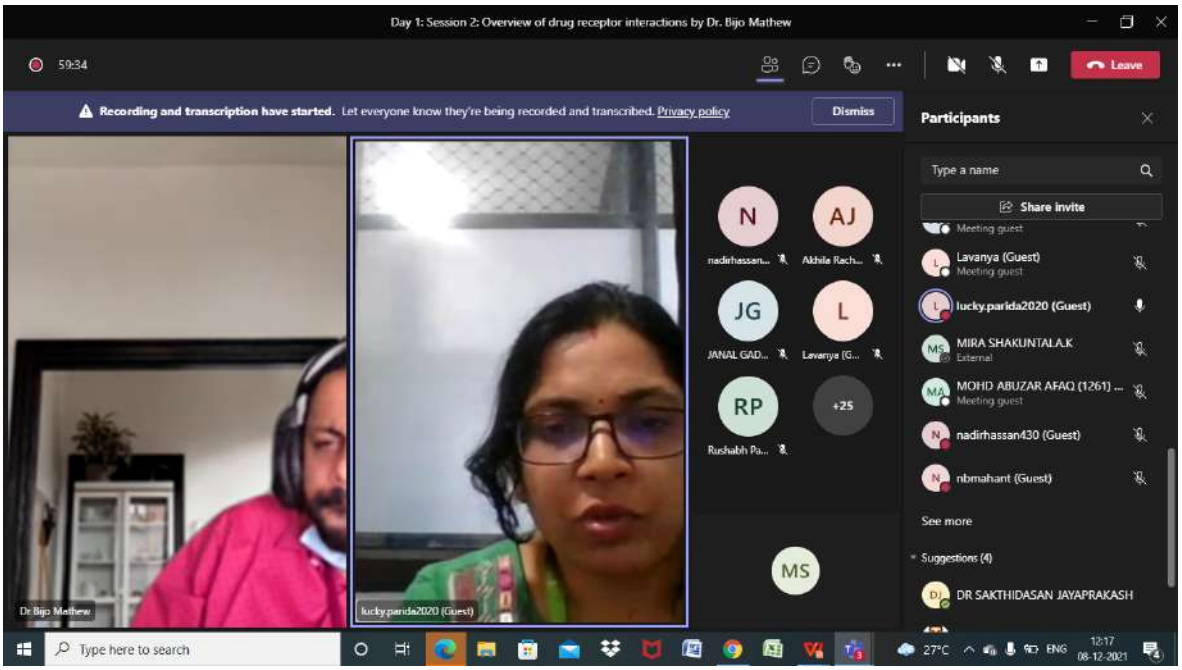
In the final day of the workshop, **Dr. Mukesh Doble** (Professor, Biotechnology, IIT, Chennai) delivered three hours of hands-on workshop on "Quantitative Structure Activity Relation". He described how QSAR can be used to identify chemical structures that could have good inhibitory effect on specific targets and have low toxicity. He also gave a detailed description on QSAR based virtual screening to filter out large libraries of small molecules for best hits with desired properties that can be tested experimentally.

The second session was "Simulating the kinetic process of drug target binding in Real Time" by **Dr. Jagannath Mondal** (Associate Professor, Tata Institute of Fundamental Research, Hyderabad). He introduced the potential benefits of drug-target kinetics, such as the ability to delineate both thermodynamic and kinetic selectivity. He also described factors, such as target vulnerability, that impact the utility of kinetic selectivity.

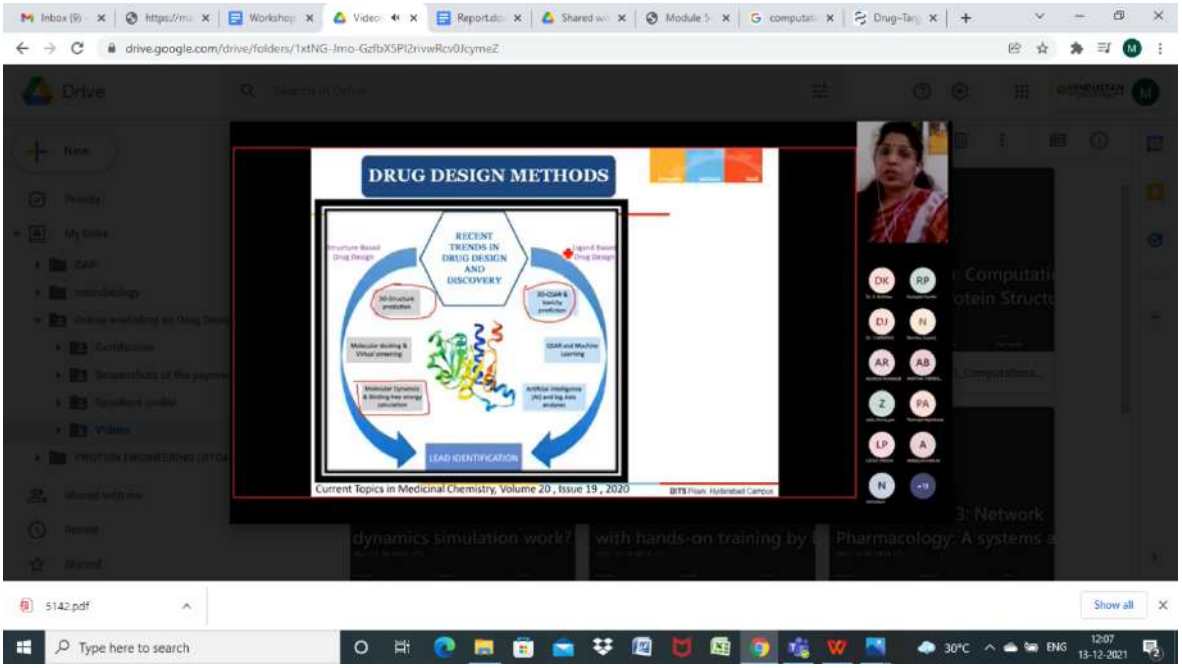
At the end of the workshop, Dr. R. Krithika (Assistant Professor S.G., Department of Chemical Engineering, HITS) gave the vote of thanks.



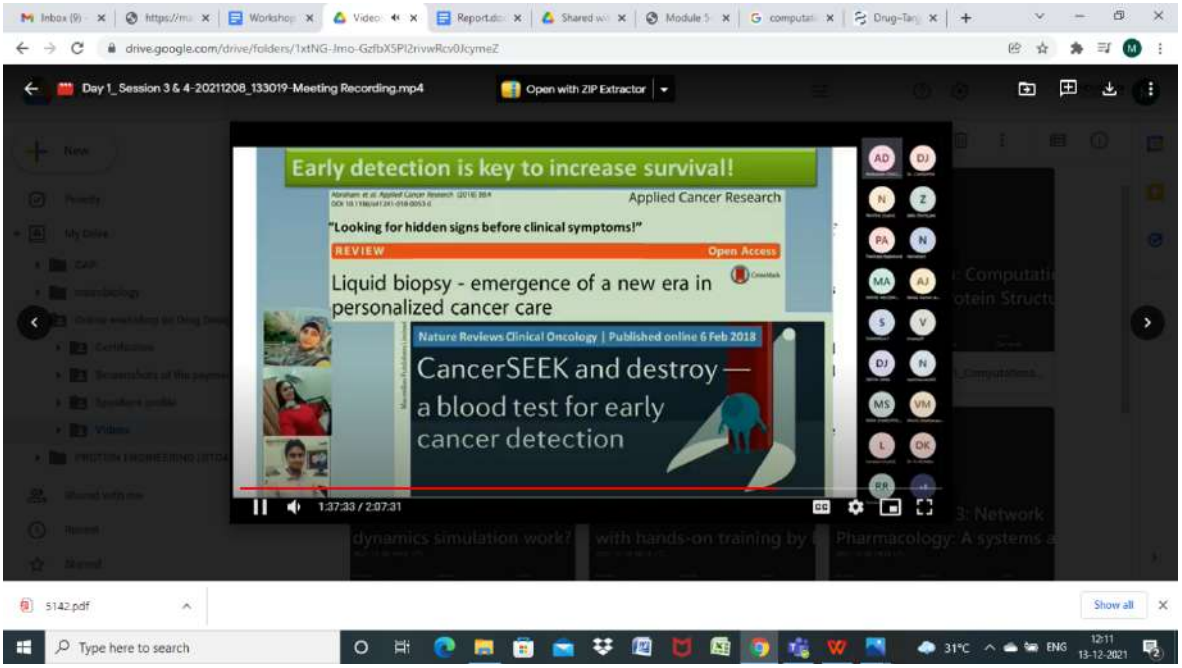
Dr. G.Dicky Davis explaining the different computer prediction methods



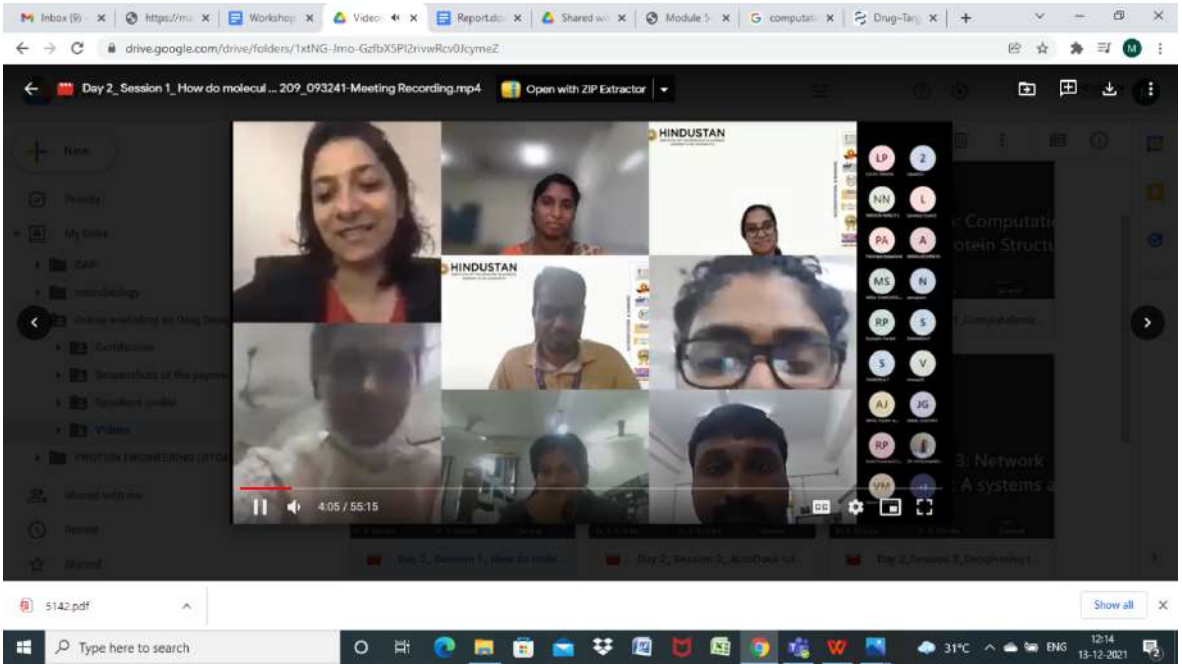
Dr. Bijo Mathew answering a query raised by a participant



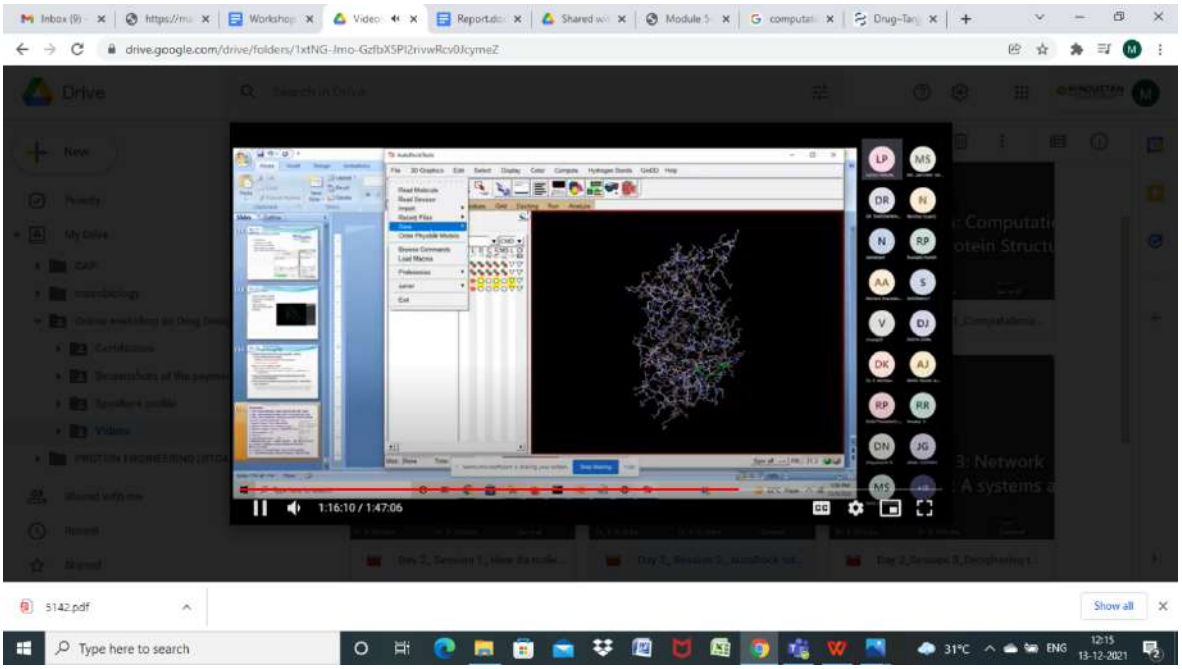
Dr. P. Yogeeshwari explaining the different methods in drug design



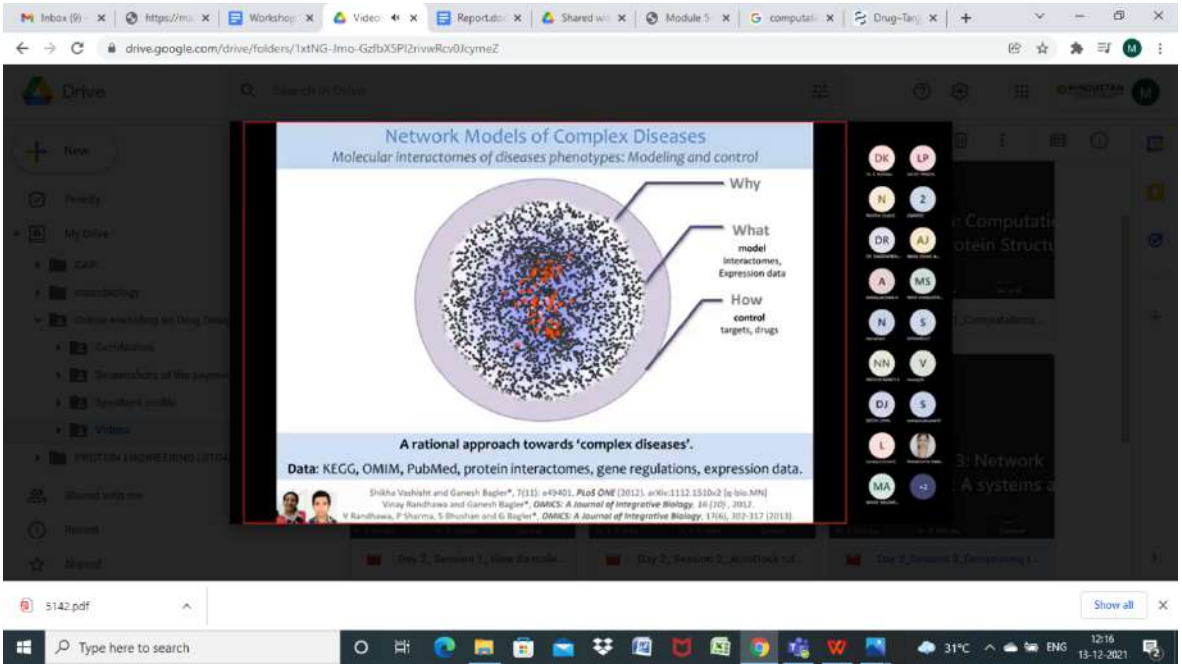
Dr. Anshuman Dixit explaining the different techniques in cancer survival



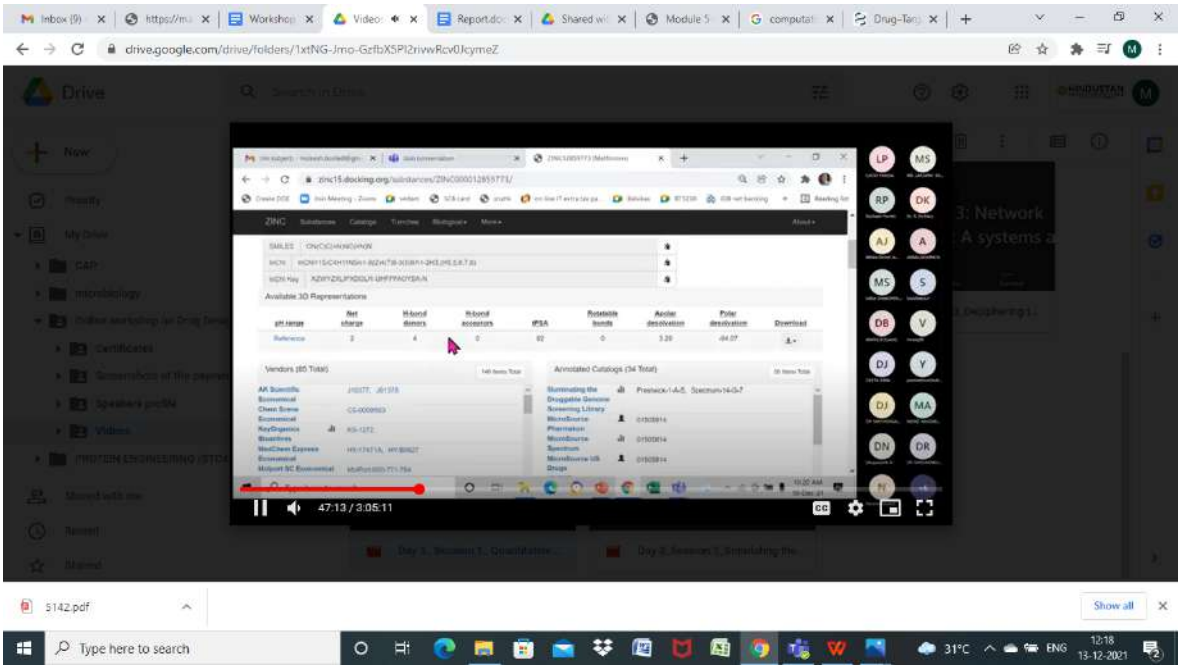
Dr. Lipi Thukral interacting with the participants



Dr. Xavier Suresh demonstrating the Autodock software



Dr. Ganesh Bagler citing references based on network pharmacology



Dr. Mukesh Doble explaining the different drug databases