

**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

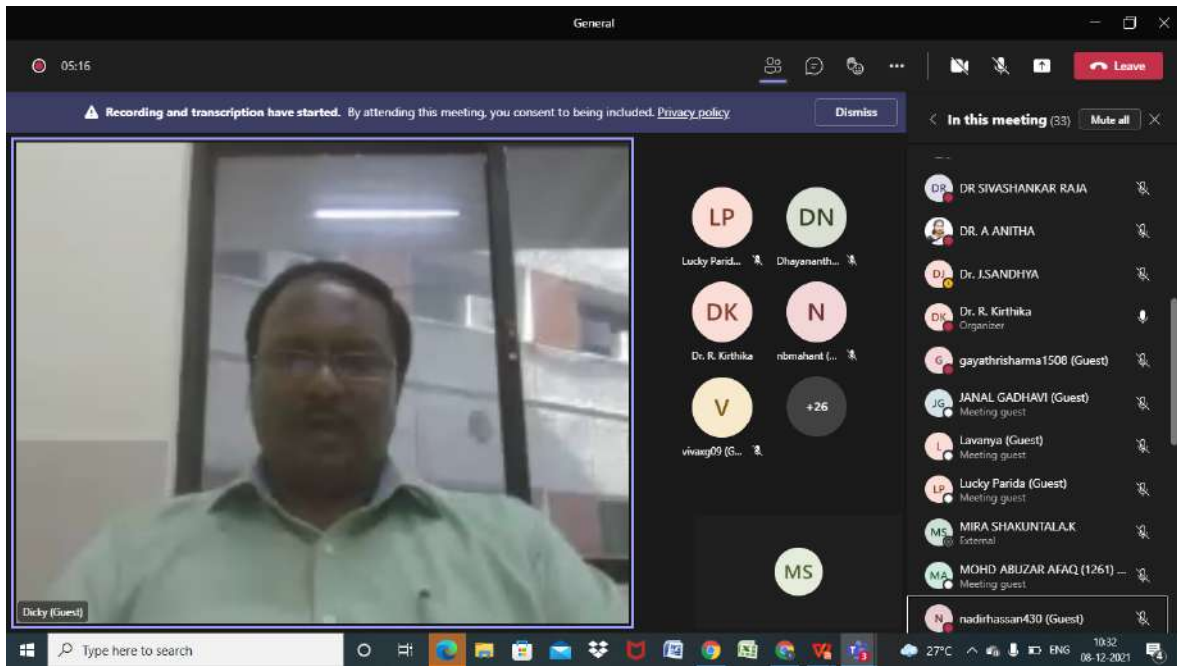
integration and multitarget drug development. He also emphasized on this particular field for the promise of expanding the current opportunity space for druggable targets

### **Day 3**

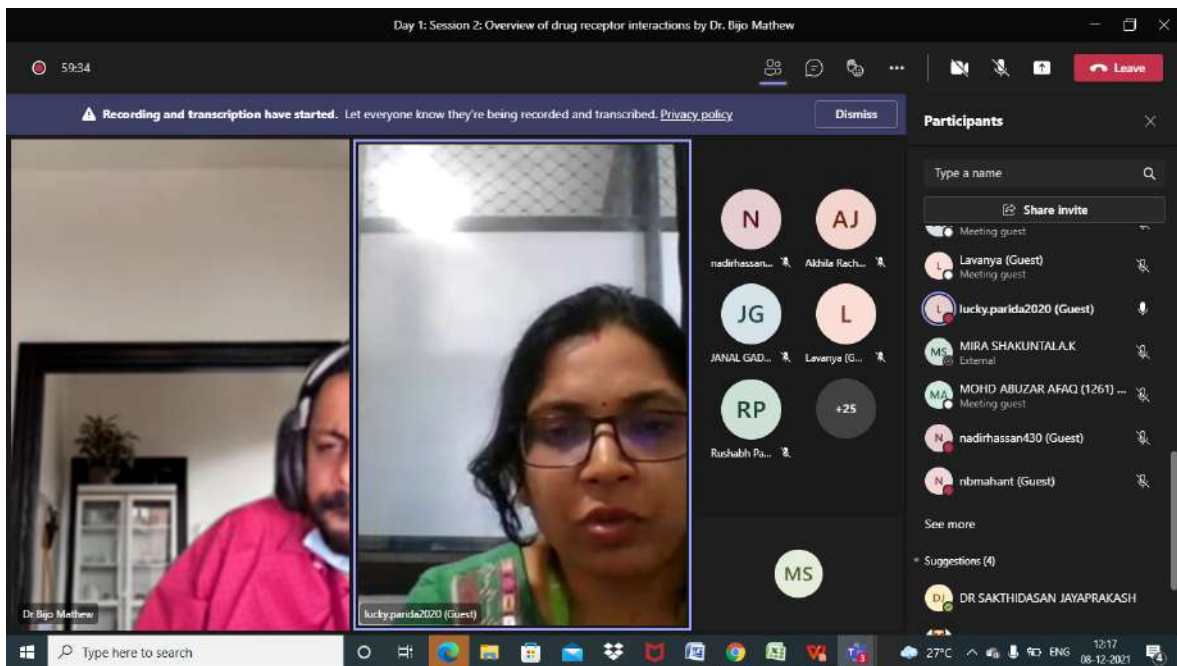
In the final day of the workshop, **Dr. Mukesh Doble** (Professor, Biotechnology, IIT, Chennai) delivered three hours of hands-on workshop on “Quantitative Structure Activity Relation”. He described how QSAR can be used to identify chemical structures that could have good inhibitory effect on specific 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

DRUG DESIGN METHODS

RECENT TRENDS IN DRUG DESIGN AND DISCOVERY

LEAD IDENTIFICATION

Structure Based Drug Design

Ligand Based Drug Design

AI/ML and Machine Learning

Molecular Modeling & Virtual Screening

Current Topics in Medicinal Chemistry, Volume 20, Issue 19, 2020

BITS Pilani, Hyderabad Campus

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

Early detection is key to increase survival!

Applied Cancer Research

"Looking for hidden signs before clinical symptoms!"

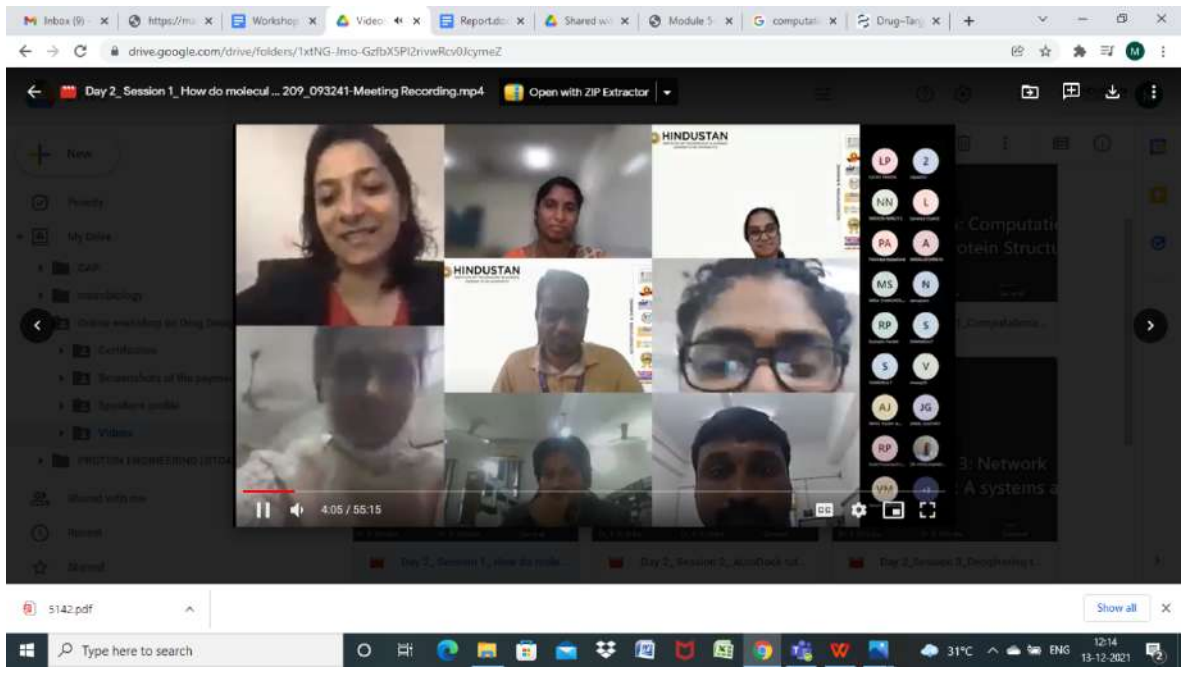
REVIEW Open Access

Liquid biopsy - emergence of a new era in personalized cancer care

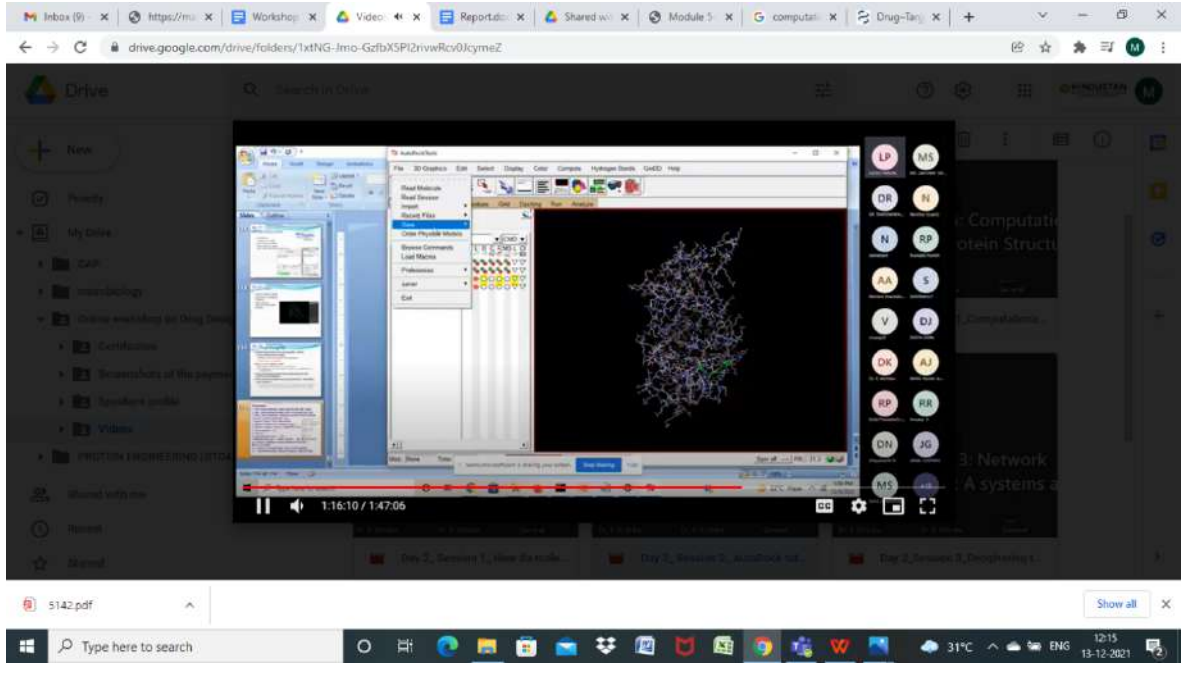
CancerSEEK and destroy - a blood test for early cancer detection

Nature Reviews Clinical Oncology | Published online 6 Feb 2018

Dr. Anshuman Dixit explaining the different techniques in cancer survival



Dr. Lipi Thukral interacting with the participants



Dr. Xavier Suresh demonstrating the Autodock software

The slide is titled "Network Models of Complex Diseases" with the subtitle "Molecular interactomes of diseases phenotypes: Modeling and control". It features a central network diagram with nodes and edges. Three callouts point to the diagram: "Why", "What model Interactomes, Expression data", and "How control targets, drugs". Below the diagram, it states "A rational approach towards 'complex diseases'." and lists "Data: KEGG, OMIM, PubMed, protein interactomes, gene regulations, expression data." At the bottom, it cites two references: "Shikha Vashist and Ganesh Bagler\*, 7(11): e49401, PLoS ONE (2012), doi:10.1371/journal.pone.0161102" and "Vishay Ranaivosoa and Ganesh Bagler\*, OMICS: A Journal of Integrative Biology, 14(10) : 2017." and "S. Bandaru, P. Sharma, S. Bhushan and G. Bagler\*, OMICS: A Journal of Integrative Biology, 11(6), 303-317 (2013)".

Dr. Ganesh Bagler citing references based on network pharmacology

The video player shows a browser window displaying the ZINC database search results for ZINC15. The search criteria include SMILES: C1=CC=C(C=C1)N, MW: 146.15, and other parameters. The results table shows 2 hits. The first hit is ZINC15, with a molecular weight of 146.15 and a molecular formula of C10H9N. The second hit is ZINC16, with a molecular weight of 146.15 and a molecular formula of C10H9N. The video player shows a progress bar at 47:19 / 3:05:11.

Dr. Mukesh Doble explaining the different drug databases