



**HSNC UNIVERSITY**  
**KISHINCHAND CHELLARAM COLLEGE**

**DEPARTMENT OF STATISTICS, LIFE SCIENCES,  
CHEMISTRY AND MATHEMATICS**  
**UNDER THE AEGIS OF DBT STAR STATUS AND STAR SCHEME ORGANIZED**  
**A TWO-DAY STATE LEVEL ONLINE WORKSHOP**

ON

**MATHEMATICAL & COMPUTATIONAL APPLICATIONS IN  
BIOLOGICAL, CHEMICAL AND RELATED SCIENCES**

---

An Interdepartmental Workshop on 'Mathematical & Computational Applications in Biological, Chemical and Related Sciences' was organized under the aegis of DBT Star Status and Star Scheme by the association of the Departments of Statistics, Life Sciences, Chemistry and Mathematics, K. C. College, HSNC University on 8<sup>th</sup> and 9<sup>th</sup> of July 2021. 200 curious minds from all over the state of Maharashtra actively participated in this workshop. Dr. Virupaksha A. Bastikar, Associate Professor, Amity Institute of Biotechnology and Dr. Pramod Kumar P. Gupta, Assistant Professor, D. Y. Patil deemed to be University were invited as the resource persons for the sessions. The workshop was organized with an aim to help students, researchers and people from all spheres working in the field of science learn the aspects crucial in the functioning and building of science in the future.

Mrs. Usha Gollakota, Head, Department of Mathematics gave the welcome address and expressed her best wishes to the participants of the workshop. Dr. Shalini R. Sinha, Coordinator, DBT-Star-Scheme and Vice-Principal, K. C. College gave the insights on DBT-Star Scheme grant earned by the organizing departments for their undying effort. The workshop was graced through the address by Dr. Hemlata K. Bagla, Principal, K. C. College and Sr. Dean, Faculty of Sciences, HSNC University. The astounding expertise of the resource persons were introduced to the participants by student volunteers of the workshop. Vote of thanks for the Inaugural session was given by Dr. (Ms.) Aashu Vajpai to express gratitude the eminent dignitaries for their valuable time.

Dr. Virupaksha A. Bastikar commenced the first session with an introduction to data science and its evolving nature. With this, he moved on to explaining Bioinformatics as a type of data science where the domain knowledge is biology. Dr. Bastikar exposed the participants to the aspect of integration of different field of science. He further explained that knowledge about nature of data is mandatory for the application of mathematics which is used for its modelling and computation is needed for handling the data and necessary designing. He briefed about the biological databases. Application based approach was given to the workshop with apt examples of

the databases – NCBI, PDB and UniProtKB. The session ended with a question-and-answer session where Dr. Bastikar patiently cleared the doubts of the participants.

Dr. Pramod Kumar P. Gupta began the second session by connecting the importance of understanding and implementation of databases. He explained that database search provides a vast number of results, it is very important to know how to convert this data into knowledge. The resource person shed light on the fact that a computational, mathematical and statistical approach to interpret biological data has reduced time and effort. The importance of computational analysis was learnt in understanding various characteristics of the gene or protein such as biological function, structure and evolution. Dr. Gupta explained the process of reading GenBank Pages using glycoproteins in coronavirus as an example. Further, demonstration of BLAST as a tool used for Pairwise sequence analysis was done. He explained the various parameters that need to be set before running blast and provided a elucidate explanation of the results obtained after running BLAST, covering the description, graphical summary, alignments and taxonomy. All questions of participants were answered very patiently, simplified and detailed explanations were provided for every query. The sessions of the first day were a novel experience for everyone and the participants were eager for another day of skillful learning.

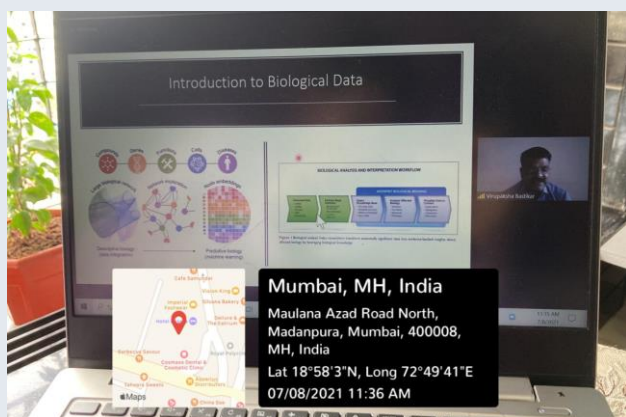
The second day commenced with enthusiasm with the curiosity birthed after day one wherein Dr. Virupaksha A. Bastikar taught how to visualise different chains in the molecule, ligands, receptor-ligand interactions as well as 2-D interactions of the receptor. He walked the participants through the entire process of docking, step by step, in all details. He prepared the molecule and cleaned the receptor for docking. He also illustrated the computer-based drug design pipeline along with ligand fitting and fragment-based drug design. The session end with the illustration of molecular modelling techniques. After the question-and-answer session, the last session was commenced by Dr. Pramod Kumar P. Gupta. He explained procedure to perform amino acid and protein MD simulation in presence of water molecules and interpreting output using Discovery studio visualizer, VMD, DCD, RMSD and NAMD. Further, he explained how to remove water molecules and save the protein structure in different conformations. This went along with understanding the evaluation needed to interpret the optimum conformation of a protein molecule. Relevance was brought in concept with analyzing contribution of simulation in COVID-19 research. The sessions were concluded where the curiosity in minds of the participants was satisfied with simplified answers given through the expertise of the resource persons in the question and answer session.

As the workshop came to an end, an overview of workshop was given by Dr. Satish Kolte, Associate Professor, Department of Chemistry, K. C. College & Director- NSS and DSD, HSNC University. Participants were invited to give their feedback. The participants appreciated the expertise of the speaker in explaining vast concepts through simple explanation and also thanked the organizing committee for arranging the workshop. At the end of the webinar Dr. Tejashree Shanbhag, Vice Principal, K.C. College, HSNC University expressed her thoughts and congratulated all the participants of the workshop.

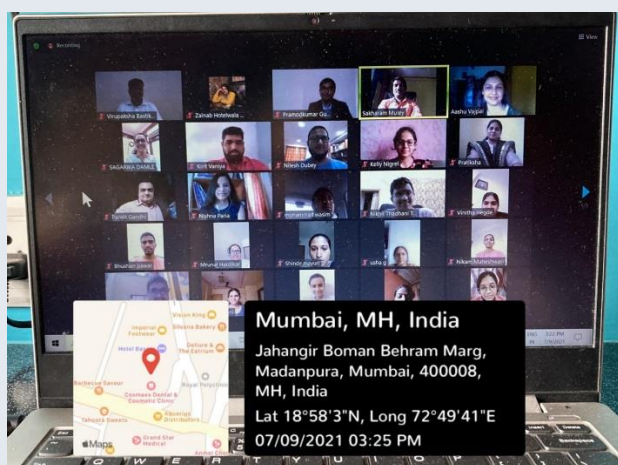
Expressing gratitude and appreciation is almost as important as the event. The workshop was closed by proposing a vote of thanks, given by Dr. Sakharam Muley who thanked everyone involved in the successful execution of the workshop. A group photo was taken to remember this momentous and novel experience. The workshop was informative and advantageous for the participants wherein they received application-based knowledge. The purpose of this workshop was served as it enlightened the curious minds of the participants into interdisciplinary learning.

The success of this workshop is the outcome of the collaborative efforts taken in the organization and execution by the organizing teams of the four departments. The departments aspire to continue this approach to learning in future and look forward to working collaboratively for passing on the gift of knowledge to people of all spheres.

- Department of Statistics, Life Sciences, Chemistry and Mathematics  
Kishinchand Chellaram College,  
HSNC University



Dr. Virupaksha Bastikar explaining the Importance of Biological Data



A group photo with all the participants and Resource persons at the end of Workshop

---