

Skill Development Workshop on Computational Drug Discovery and Development



Welcome of the resource person by Principal, Dr. H. N. More
(From left Dr. H. N. More, Mr. Amit Bedi, Dr. Mohsin Khan Pathan, Dr. M. S. Bhatia,
Anchoring by co-ordinator of the workshop Dr. Mrs. S. A. Arvindekar)



Welcome of guest Mr. Amit Bedi by Vice-Principal (Academics) Dr. M. S. Bhatia



Inaugural Address by Principal Dr. H. N. More

Pharmaceutical Chemistry Department of Bharati Vidyapeeth, College of Pharmacy, Kolhapur (Maharashtra), in collaboration with **Advent Informatics Pvt. Ltd, Pune**, had organized **‘Skill Development Workshop on Computational Drug Discovery and Development’** for M. Pharm students, research scholars & faculty on **Wednesday, 2nd August, 2023**. The inaugural address by Principal, Dr. H. N. More was followed by a brief introduction of the workshop by convener of the workshop Dr. M. S. Bhatia, Vice-Principal (Academics) and Head, Pharmaceutical Chemistry Department. Resource Person of the first session, Dr. Mohsin Khan Pathan, (Junior application Scientist, Advent Informatics Pvt. Ltd., Pune) was felicitated by Principal, Dr. H. N. More and guest Mr. Amit Bedi (Sales Executive, Advent Informatics Pvt. Ltd., Pune) was felicitated by Dr. M. S. Bhatia, Vice-principal- Academics. The resource person of the second session, Dr. P. B. Choudhari (Associate Professor, Bharati Vidyapeeth College of Pharmacy, Kolhapur) was introduced by Ms. Rutika Patil. This Skill Development Workshop was co-ordinated by Dr. Mrs. S. A. Arvindekar (Assistant Professor of Pharmaceutical Chemistry) as Co-ordinator. Principal, Dr. Harinath N. More, Vice-Principal (Academics) Dr. M.S. Bhatia, Vice-Principal (Admin.) Dr. Namdeo R. Jadhav, all the faculty members, supporting staff members and students were present on the occasion. Applications of Molsoft’s ICM software suite and all freewares for drug design and development were demonstrated in the workshop.

Session 1: 11.00am to 1.30pm by Dr. Mohsin Khan Pathan



Dr. Mohsin Khan Pathan demonstrating Molsoft's ICM software package

Dr. Mohsin Khan Pathan, a NIPER post-graduate and doctorate and also a CADD expert demonstrated the Molsoft's ICM software with detailed deliberations on,

1. ICM-Pro homology modelling
2. ICM-Pro desktop modelling for protein-ligand & protein-protein docking.
3. ICM-Pro virtual ligand screening for batch docking including fragment, structure based & ligand-based docking.
4. ICM-Chemist-Pro for calculating ADME properties, QSAR studies

Session 2: 03.00pm to 5.00pm by Dr. P. B. Choudhari



Dr. P. B. Choudhai discussing about Autodock/PyRx software

Dr. P. B. Choudhari discussed about Autodock/Pyrx software demonstration which includes,

1. Basics of molecular docking

2. Visualization of protein structure
3. Molecular docking using Autodock/Pyrx
4. Visualization of interaction by Biovia Discovery studio.

Staff, research scholars & students actively participated with inquisitive questions and discussions related to applications of the demonstrated and other software packages with comparable outcomes. Concluding remarks and a Vote of thanks of First session were given by Mrs. P. B. Varne and of second session by Ms. Kajal Mohite. Both expressed sincere thanks to Dr. Mohsin Khan Pathan, Mr. Amit Bedi and Dr. P. B. Choudhari for guiding and sharing the valuable information & demonstration on applications of MolSoft ICM Software, Autodock/PyRx software, and related freewares.