KARPAGAM ACADEMY OF HIGHER EDUCATION
COIMBATORE-21

DEPARTMENT OF CHEMISTRY

A brief Report on the Training Programme on "Molecular Docking" conducted on 20-09-2018 in Karpagam Academy of Higher Education.

Department of Chemistry has organized and conducted a training programme on "Molecular Docking" on 20-9-2018. About 52 students of I-M.Sc., Chemistry participated in the programme. Dr. S. Ravi, Professor & Head, Department of Chemistry, conducted the Programme. Structure-based drug design seeks to identify and optimize specific attractive interactions between two partner molecules in biological systems between ligands and their host molecules, typically proteins. The simple answer to what's holding the industry back in terms of adoption of latest drug discovery techniques is Education. There simply aren't enough individuals trained on the use of Proteomics, Virtual Screening, Molecular Docking, Simulations, Dynamics and ADMET-multidisciplinary approaches, which is why we conducted this training programme.

In this one day training programme we have focused the use of efficient technologies used in the discovery & designing of Drugs on the basis of the biological targets critical to the disease condition. The basic principles of Rational Drug Design along with Proteomics in Drug Discovery was introduced.

Training was provided in the following areas.

1. Drawing of chemical structures using computer softwares.
2. Downloading of 3D protein structure from Protein Data Bank.
3. Optimization of the ligand and the protein (Energy minimization)
4. Molecular docking using Autodock software.

The deliberations of the programme was well received by the participants. They enthusiastically interacted with the Faculty Member to clarify their doubt. The programme went on well.

Students watching the Molecular docking process during a training session

Dr. S. Ravi, demonstrates the process of molecular docking during the training session