



Bon Secours College for Women (Autonomous)

NAAC Accredited with A++ Grade in cycle II

UGC recognized 2(f) and 12(B) Institution

Affiliated to Bharathidasan University, Tiruchirappalli

Vilar Bypass, Thanjavur- 613 006, Tamil Nadu

DBT STAR SCHEME: Strengthening UG Programmes

(Science Departments – Biotechnology, Botany, Physics and Chemistry)

Programme Report

A Workshop on **Computer-Aided Drug Discovery** was organised on July 13, 2024, at 10:00 AM in St. Joseph's Auditorium. **Dr. S. Gayathri**, Principal and Chairperson of the DBT Star Scheme, presided over the program. The resource person was **Dr.R.R.Saravanan.** , Assistant Professor in Physics, Bon Secours College for Women (Autonomous), Thanjavur was a resource person.

Expertise of Dr.R.R.Saravanan:

- He has published 20 research papers in the field of Molecular Docking.
- The Fields of Interest and Specialisations are Crystal Growth, Crystallography, Spectroscopy, and Bioinformatics.
- The Research profile includes h-index: 6, i10-index: 6, No. of Citation: 129, Total Impact factor: 45.94.
- He was an expert in Structure Solving using Crystallography Data, Spectroscopic simulations, and Bioinformatics tools.

Dr. R.R. Saravanan emphasized the development of the COVID-19 vaccine, discussing its rationale and significance. He explained the steps involved in drug discovery and provided a timeline for the process. Additionally, he introduced terminologies used in Computer-Aided Drug Discovery (CADD), covering key concepts such as protein, ligand, Protein Data Bank, Lipinski's rule of five, ADME toxicity, binding affinity, molecular docking, and molecular dynamics.

He detailed the steps involved in molecular docking, which include protein selection and preparation, ligand selection and preparation, docking calculation, selection of the best pose, and binding and visualization. He demonstrated the use of tools such as Auto Dock, ChemBioDraw, PyMOL, PASS database, and CASP.

He also discussed how to conduct **interdisciplinary research** using molecular docking and how to publish research articles in reputable journals. The session saw participation from 35 faculty members from the departments of Biotechnology, Botany, Physics, and Chemistry, who actively engaged and clarified their doubts.

Photo Gallery

