Guest Lecture: Computational Biology – A Gateway to Drug Design

Speaker: Dr. Basha
Date: 8th April, 2025
Venue: Webinar hall
Organized by: Department of Zoology

A guest lecture was conducted on the topic "Computational Biology and Its Impact on Drug Discovery" by the esteemed speaker Dr. Basha, who brought valuable insights into the emerging field of computational biology and its revolutionary impact on life sciences, particularly drug development. He began by defining computational biology as an interdisciplinary field that applies computational techniques and tools to understand and model biological systems. According to him, this discipline merges biology, computer science, mathematics, and statistics to analyse complex biological data, especially at the molecular and genetic levels. He elaborated on its vast scope, highlighting areas such as Genomics and Proteomics, Systems Biology, Structural Biology, Molecular Modelling, Bioinformatics and Personalized Medicine

He emphasized that computational biology is rapidly transforming the landscape of life sciences, enabling researchers to derive insights from large biological datasets, identify potential drug targets, and predict the outcomes of experimental interventions. He explained that traditional drug discovery methods are time-consuming and expensive, but computational approaches have made it more cost-effective and faster. He particularly emphasized the significance of molecular docking, a crucial computational technique in drug discovery. According to Dr. Basha, molecular docking involves predicting the interaction between a drug molecule and its biological target (usually a protein) to identify how well they bind. This technique plays a pivotal role in lead identification, optimization, and screening of drug candidates. Dr. Basha shared insights on popular molecular docking tools and their applications in research. Some of the tools mentioned include AutoDock and AutoDock Vina, Schrödinger Suite, Molecular Operating Environment (MOE), PyMOL, SwissDock and Chimera

In the concluding part of his lecture, Dr. Basha highlighted how skills in computational biology and molecular docking open up numerous career opportunities in pharmaceutical industries, biotech companies, research institutions, and academia. He encouraged students to gain handson experience in these tools, as they are highly valued in research and industrial settings.

The lecture concluded with a Q&A session, where attendees interacted with Dr. Basha and clarified their doubts. Overall, the guest lecture was a great success and left a lasting impact on all participants.