

Invited Lecture on "X-ray Crystallography, Molecular Structures and Structure Based Drug Design" 19 December 2022

Speaker: Prof. D. Velmurgan, Former Head, CAS in Crystallography and Biophysics, IIT-Madras

Organized by: School of Biotechnology, Gautam Buddha University
Greater NOIDA, Gautam Budh Nagar, Uttar Pradesh

Coordinator: Dr. Nagendra Singh, Head SoBT

Summary: X-ray Crystallography is a versatile tool in unraveling the three dimensional structures of biomolecules. Single crystals of dimensions 0.2mm x 0.2mm x 0.2mm can be subjected to X-ray diffraction. From the measured Bragg intensities, atomic sites which are the electron density maxima can be computed once one knows the phase angles of these Bragg reflections which are missing in the outcome of the diffraction experiment. This bottleneck called Phase Problem can be overcome by Direct Methods in the case of small molecules and by methods like MR, SIR, MIR, SAD and MAD in the case of Macromolecules. More than thirty five Nobel Prizes were awarded to the pioneers in this field so far. Knowledge of three dimensional structures of molecules is needed not only to understand the Structure- Function relationships but also to modulate the function of the macromolecule. This has emerged as the new discipline Structure Based Drug Design. More than 11 lakhs small molecular structures are deposited in the Cambridge Structural Database and more than 1.8 lakhs Macromolecular structures are deposited in the Protein Data Bank so far. The presentation will cover the above aspects along with the novel use of herbs or natural products in overcoming various human ailments.

Details of Participants: M.Tech., M.Sc., Ph.D. Research Scholars and Faculty members, SoBT

Photo Gallery

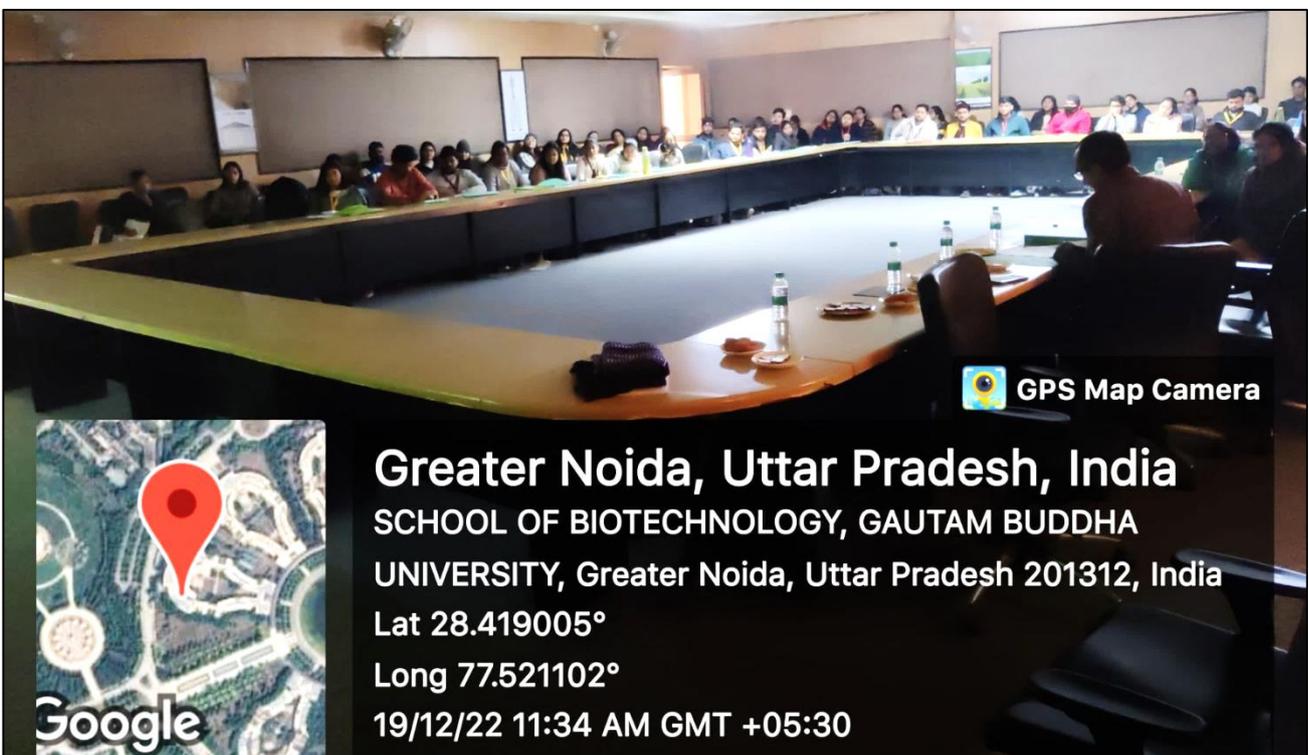


Photo Gallery

