A 3-Day National Workshop on Molecular Modeling Using Open Source Software (Sponsored by UGC-SAP-DRS II) during 29th - 31st October 2018 had an overwhelming response with about 105 participants. The workshop went on with scientific deliberations involving lectures and hands-on-sessions in an interactive manner.

The workshop got initiated on first day with key note lecture of Bhatnagar Awardee, Dr Narahari sastry followed by Prof Lalitha Guru Prasad’s, Dr Girinath Pillai, on second day by Prof Vijjyullatha and on third day with Prof. Devapriya Kumar on various topics like Computational studies on protein structure and function correlation, the role of computational methods and data for drug candidate selection and Understanding Bimolecular Interactions using Quantum Mechanical Calculations. The hands on sessions started with 2D QSAR continued with 3D QSAR using py-COMFA software. Docking analysis was explained using iGEM dock and Autodock softwares. It was followed by Molecular Modeling and Structural Elucidation of Molecules mainly using ARGUSLAB and Homology modelling was explained using Modeller software.
Department of Chemistry, Osmania University
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