MANIPAL UNIVERSITY JAIPUR

International Summer School-Manipal University Jaipur [ISSMUJ]-2024

[Hybrid Mode]

Course Overview

Name of Course- Molecular Modelling and Bioinformatics

Name of Instructor: Dr. Saurabh Srivastava/ Dr. Sandeep Kumar Srivastava/Dr. Shubhandra Tripathi

Session: June-July 2024

Language of instruction: English

Number of contact hours: 36

Credit awarded: 03

Pre-requisite: Chemistry/Biology at UG level and Mathematics up to 10+2 level

Objective of Course/Project

The objective of the course is to train students in the field of molecular modelling and computational chemistry/biology and to develop skills in tackling problems related to drug enzyme interactions as well as studying reaction mechanisms using Quantum Mechanical/Molecular Mechanical methods.

Syllabus:

Cheminformatics/Bioinformatics: SMILES, SMARTS, InChI notations, database, structure representations; *Molecular Modelling*: Molecular force field, force field parameters, energy minimization, simulation set up in GROMACS, AMBER, CHARMM GUI, Free Energy calculation, QM/MM simulations, Geometry optimizations, Umbrella Sampling, Metadynamics.

Organization of Course

Total contact Hours: 36		
1st week:	9 hrs (classes)	9 hrs (self-study/project/Mid-term)
2nd week:	9 hrs (classes)	9 hrs (End-term exam/assessment/discussion)

Mode of lectures: Hybrid mode lecture/videos/case study/ discussion/ workshop/ hands-on

MANIPAL UNIVERSITY
JAIPUR

Course/Project Plan

Lecture no.	Topic	Lecture mode	Instructor
L: 1-2	Cheminformatics: SMILES, SMART, InChI, Tanimoto Similarity, Small Molecule Database Zinc, PubChem etc. Structure representation PDB, MOL2, SDF etc.	Theory	Dr. Saurabh Srivastava
L: 3-4	Practical Application and practice of database search, File formation and conversion, simple Linux commands for file manipulations, Avogadro Software	Practical/Hands-on	Dr. Saurabh Srivastava
L: 5-6	Force Fields, Force field parameters, Velocity verlet algorithm, Molecular dynamics Calculation using AMBER force fields.	Theory	Dr. Saurabh Srivastava
L: 7-8	Simulation of water in a box, Visualization in VMD, Force field parameter manipulation.	Practical/Hands-on	Dr. Saurabh Srivastava
L: 9-10	Energy minimization, Steepest decent method, Various ensembles, NVT, NPT, NVE, Potential Energy, Kinetic Energy, Density	Theory	Dr. Saurabh Srivastava
L:11-12	Simulation of water box in various ensembles, plotting using xmgrace, gnuplot, plots of energy, density, temperature, pressure, volume, in various ensembles	Practical/Hands-on	Dr. Saurabh Srivastava
L:13-14	Molecular Dynamics Simulations using GROMACS, input file parameters, Various steps involved in MD Simulation. RMSD, RMSF, Rg, SASA, Hydrogen Bonding in MD Simulations	Theory	Dr. Shubhandra Tripathi
L: 15-16	Learning MD Simulation of TRPCage Protein and the properties calculation studied in theory.	Practical/Hands-on	Dr. Shubhandra Tripathi
L:17-18	Mid-Term Examination/Assignments/Quizzes	Examination	Dr. Saurabh Srivastava
L: 19-20	Free energy Calculation, Timescale, Sampling Techniques, Probability distribution	Theory	Dr. Saurabh Srivastava
L: 21-22	Practicing all the theory simulations on Alanine Di Peptide, Ramachandran Plot	Practical/Hands-on	Dr. Saurabh Srivastava
L: 23-24	Drug-enzyme Interactions and Screening	Case Studies	Dr. Sandeep Kumar Srivastava
L: 25-26	Protein Folding and Unfolding	Case Study	Dr. Shubhandra Tripathi
L: 27-28	QM Geometry Optimizations, QM/MM Simulation	Theory	Dr. Saurabh Srivastava
L: 29-30	QM/MM Simulation and Reaction Mechanism	Practical/Hands-on	Dr. Saurabh Srivastava
L: 31-32	Enhanced Sampling Methods, Umbrella Sampling, Metadynamics	Theory	Dr. Saurabh Srivastava
L: 33-34	Enhanced Sampling Methods, Umbrella Sampling, Metadynamics	Practical/Hands-on	Dr. Shubhandra Tripathi
L: 35-36	End Term Examination/Assignments/Quizzes	Examination	Dr. Saurabh Srivastava

MANIPAL UNIVERSITY
JAIPUR

Brief profile of the instructor with Photograph

Dr. Saurabh Srivastava
Assistant Professor (Senior Scale)
Department of Chemistry, Faculty of Science
Manipal University Jaipur

Dr. Saurabh Srivastava is working as an assistant professor (senior scale) in the department of chemistry at Manipal University Jaipur (MUJ). He has obtained his Ph. D from Indian Institute of Technology Kanpur (IITK) in 2013 under the supervision of Professor N Sathyamurthy. After graduating from IITK he moved to the WPI-MANA centre of National Institute for Materials Science (NIMS), Tsukuba, Japan to work as a post-doctoral researcher till 2016 where he worked on the electron transport calculations for Molecular Electronics. Dr. Saurabh then moved to CEMES, CNRS lab at Toulouse France as a senior post-doctoral researcher where he worked till 2019 on the various nano materials to study the molecular gears. He has published 15 articles in the various high impact journals. Dr. Saurabh joined the Manipal University Jaipur in 2021 as an assistant professor and has fetched the start-up research grant of 25 Lakh from the DST-SERB. His current research is focused on the covalent organic frameworks to work as molecular gears and molecular electronics. His group at MUJ is also working to study the reaction mechanism in the drug-enzyme, of the cancer proteins and HIV virus. Dr. Saurabh has presented papers at various national and international conferences and given invited talks and have peer reviewed for many journal articles.

Dr. Shubhandra Tripathi
Scientist, Computational Chemistry,
Aganitha Cognitive Solutions, Hyderabad

Dr. Shubhandra earned his Ph.D. from CSIR−Central Institute of Medicinal and Aromatic Plants, Lucknow, where his research focused on molecular interaction studies of targets and drugs associated with breast cancer.

He has three years of postdoctoral research experience from the His research interests lie in the intersection of chemistry, biology, and computational science, aiming to identify and optimize lead molecules for drug Indian Institute of Technology, Kanpur, and two years of postdoctoral experience from the University of New Hampshire. In his postdoctoral research, he implemented the temperature-accelerated sliced sampling (TASS) method for ligand unbinding studies. His expertise extends to various computational techniques such as molecular dynamics simulations, alchemical methods (free energy perturbation), and enhanced sampling techniques like umbrella sampling and metadynamics. His research

interests lie in the intersection of chemistry, biology, and computational science, aiming to identify and optimize lead molecules for drug discovery, protein conformational dynamics studies, and ligand unbinding studies from protein.