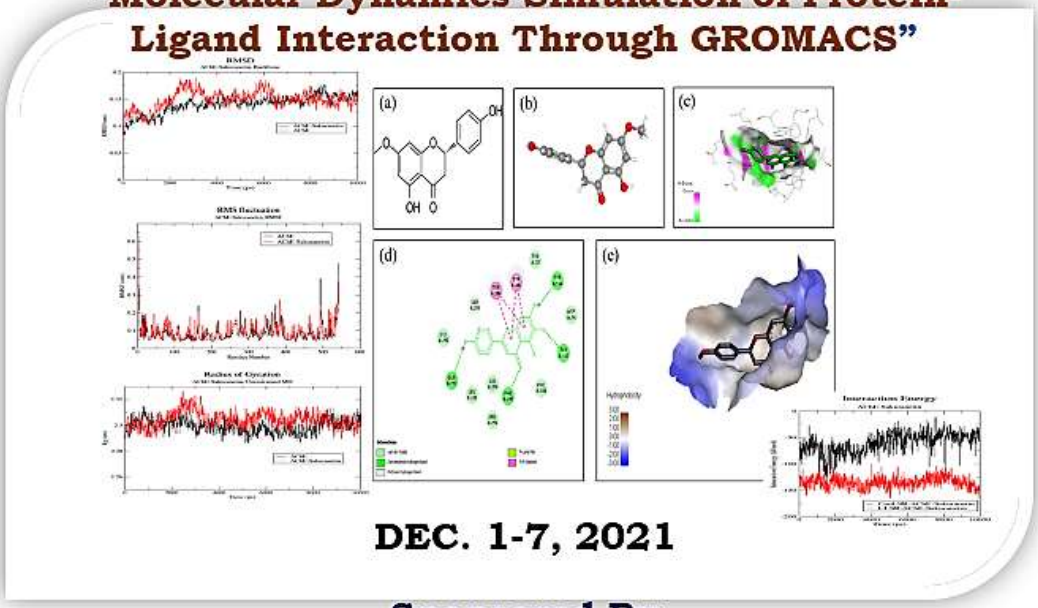
Seven-Days Online Bioinformatics Skill Development Training Program On

"Molecular Dynamics Simulation of Protein-Ligand Interaction Through GROMACS"



DEC. 1-7, 2021

Sponsored By

Council of Scientific & Industrial Research, New Delhi (Govt. of India)

Organized By

CSIR-Central Institute of Medicinal & Aromatic Plants, Lucknow

Training program contents:

- Introduction to MD Simulation
- Installation set up for GROMACS (Linux)
- Prepare the protein topology
- Prepare the ligand topology
- Define box, Solvate & Add Ions
- Energy Minimization (Steepest Descent)
- Equilibration
- Applying restraints to the ligand
- Treatment of temperature coupling groups
- NVT & NPT equilibration
- Production of MD simulation (10 ns)
- Recentering and Rewrapping coordinates
- Analyzing protein-ligand interaction
- Ligand Dynamic
- Protein-Ligand Interaction Energy
- Demo exercise
- Practicals/Hands-on (Online Live)
- Trouble-shooting: During setup & MD simulation

Convenor
Dr. Feroz Khan

Coordinator
Dr. Laiq-ur Rahman

Chairman
Dr. Prabodh Kumar Trivedi
Director, CSIR-CIMAP

About CSIR-CIMAP, Lucknow

CSIR-Central Institute of Medicinal & Aromatic Plants (CSIR-CIMAP) is a premiear multidisciplinary research institute of Council of Scientific & Industrial Research (CSIR), New Delhi, India with its major focus on exploiting the potential of medicinal and aromatic plants (MAPs) by cultivation, bioprospection, chemical characterization, extraction, and formulation of bioactive phytomolecules. With a strenght of 100 scientists, 162 technical officers, 129 support staff and nearly 300 doctoral and post-doc scholars at its head-quarter in Lucknow and research centers at Bengalure, Hyderabad, Pantnagar, and Purara. CSIR-CIMAP has played a key role in positioning India as a global leader in production of mints, vetiver and other aromatic grasses, and in ensuring indigenous production of artemisinin – a WHO approved antimalarial. CSIR-CIMAP houses a National Gene Bank on MAPs, which is one of the three of its kind in India. CSIR-CIMAP has played a key role in successfully commercializing an ayurvedic herbs based antidiabetic formulation, which has now benefitted millions. The institute is presently accredited by ICS-UNIDO and Indian-Ocean Rim Association (IORA) as a focal point for research and training on Medicinal Plants among 21 participating member countries. For more details please see the CSIR-CIMAP website www.cimap.res.in

About the Bioinformatics Skill Development Program

Molecular dynamics (MD) is a computational simulation method for analyzing the physical movements of atoms and molecules. Atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic "evolution" of the system. The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles, where forces between the particles and their potential energies are often calculated using interatomic potentials or molecular mechanics force fields (Wikipedia; Salmaso, 2018). It was developed to simulate simple systems, with the first application to study collisions among hard spheres, in 1957 (Alder and Wainwright, 1957). The first MD simulation of a biomolecule was accomplished in 1977 with 9.2 ps simulation on 58 residues long Bovine Pancreatic Trypsin Inhibitor (BPTI) (McCammon et al., 1977). Now, MD simulations have evolved into a mature technique that can be used effectively to understand macromolecular structure-to-function relationships and protein-ligand binding stability. Keeping in mind the importance of MD simulation, in this bioinformatics skill development training program, we will describe the key steps of protein MD simulation and protein-ligand MD simulation. Through this training participants may know how to perform (i) 3D structure preparation of target protein and small molecule, (ii) Energy plot generation for potential energy, pressure, temperature and density for NVT, NPT and MD simulation, also to determine average value for each graph, (iii) RMSD (Root-Mean Square Displacement) analysis to study stability based on atoms position, (iv) RMSF (Root-Mean Square Fluctuation) – overall flexibility detection of protein and complex, it will also help to detect the most flexible residue in the system, (v) Radius of Gyration (Rg) evaluation (stability study based on compactness), it will give answer whether target protein is in sphere form or not?

The Aim of Bioinformatics Skill Development Training Program

To familiarize students/researchers/academicians/industry experts with the basics of MD simulation of protein and protein-ligand complex structure or docked complex. Participants may understand the role of MD simulation in the assessment of molecular interaction, stability assessment, docking results evaluation and its interpretation. In parallel, practical exercises/example demo for technical skill development will be scheduled online after introductory lectures. Participants need to follow the instructions and perform the different steps. Live trouble shooting will assist the participants in smooth learning of tools and techniques of machine learning. The training program will cover an invited lecture from in-house/external experts utilizing the in-silico tools and techniques in their research work, a training program theme based lecture and demo presentation by lead expert (Bioinformatics), and online live practical exercise session. The training program would cover the following aspects:

- Installation set up for GROMACS and associated tools e.g., Avogadro program in Linux (Ubuntu) OS system (64 bit; 4-8 core or more core with multithreading feature CPU, 8-64 GB RAM, 1-2 TB HDD/SSD)
- Generate Topology -
    - Prepare the protein topology
    - Prepare the ligand topology – (AMBER/CHARMM/OPLS force field may be used)
- Define box and Solvate –Defining the Unit Cell and Adding Solvent
- Add Ions – Neutralize the system
- Energy Minimization – Steepest Descent method use, calculate Potential energy, Maximum force and Normalized force
- Equilibration –
    - applying restraints to the ligand
    - treatment of temperature coupling groups
    - NVT equilibration
    - NPT equilibration
- Production of MD simulation – run 10 ns MD simulation of protein and complex/docked complex
- Analysis –
    - Recentering and Rewrapping coordinates
    - Analyzing protein-ligand interactions
    - Ligand Dynamics
    - Protein-Ligand Interaction Energy
- Example demo
- Practicals/Hands-on exercise (online)
- Home work: Learn free energy calculations & non-equilibrium MD

The participants may get important web resources links, research papers, tutorials information and example hands-on practicals by faculty related to protein/protein-ligand MD simulation during the training. The online skill development training gained through this program may help in making the career in structural bioinformatics, especially studying receptor-ligand interactions or binding mode conformation of proteins and inhibitors and entrepreneurship in bioinformatics/biotechnology/ biomedical research domains. Trouble shooting may be done through remote login through AnyDesk app, especially in installation part and running MD simulation during practicals.

Eligibility

UG/PG Science/Engg. students (Bioinformatics/ Biotechnology/ Pharmacy/ Biochemistry/ Microbiology/Life Science/BioPhysics/Chemistry/Medicinal Chemistry/Pharma. Chemistry/Botany/Zoology/Plant Sciences/BioMedical Sciences; Ph.D. fellows/Post-Doc scholars/RA/Young Scientist/Women Scientist/Pool Scientist fellow/Technical Officers; Project fellows/Technical Officers/Company Professionals/Entrepreneurs/Academicians can attend. Basic knowledge of Biology, Chemistry, Physics, and working experience of Linux OS (Ubuntu) on terminal command line is required. For fresher's, tutorial will be provided for basics commands of Linux. Applicants should have desktop PC/Linux system/Laptop with Linux OS (Ubuntu) installed or sub-system Linux Ubuntu terminal app installed on Windows 10 prof. (64 bit) or installed through virtual machine.

Certification

Training program's participants will receive a digital certificate of participation from the CSIR-CIMAP, Lucknow after successful completion of the skill development program. The digital certificate will be emailed after the successful completion of training program.

Feedback

After training program, participants may be asked to submit the given feed-back form. Participants may be asked to express their training experiences and suggestions for further improvement.

Technical requirements

Participants may have Laptop/Desktop PC with Windows 10 OS with Linux Ubuntu sub-system app, knowledge of DOS commands, Scripting knowledge on any text editor e.g., Notepad, Notepad++, and working experience of MS Office. A working version of Windows, MS Office software is necessary to follow the practical examples/training sessions online. Knowledge of basic cell biology and biostatistics will be will be beneficial.

Training mode

Online mode through MS Team/Google Meet or similar online app.

Registration Fee

Rs. 5,000/- for a student (UG/PG), **Rs. 6000/-** for a Ph.D. Research Scholars/Project Assistant(PA), **Rs.8000/-** for an Academic faculty/Teacher, Technical Officer (TO) /Scientist/Young Scientist fellow/Research Associate (RA), and **Rs.10,000/-** for an Industry candidate/Entrepreneurs/Sponsored candidate. The registration fee includes digital Registration kit which includes Training brochure, program schedule, tutorials, training lectures (provided during training or completion of training program), practicals exercise, feed-back form and a certificate (digital copy will be emailed, while offline collection option of certificate hard copy will be there for the participants) after successful completion of training.

Registration fee can be pay through online mode to SBI bank A/c No. 00000030267691783, SBI Main branch, Hazratganj, Lucknow (IFSC code: SBIN0000125) or through Demand Draft in favor of '**Director, CIMAP**', payable to Lucknow. Complete registration form along with the fee details should reach us on or before deadline i.e., Nov. 29, 2021 upto 5:00 PM. Registration to the skill development training program will be on 'First-come-First-serve' basis. Seats are limited.

For any query related to this skill development training program, kindly contact:

Dr. Feroz Khan (f.khan@cimap.res.in)

Dr. Laiq-Ur Rahman (l.rahman@cimap.res.in).

For any further details please contact:

Director

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E-mail: director@cimap.res.in , Website: www.cimap.res.in

Application/Registration Form

Candidate Full Name: _____

Designation/Position: _____

Affiliation (Institute/Univ.):_____

Address:_____

_____

Locality Type (Urban/Rural):_____

Category (Gen/OBC/SC/ST):_____

Gender (Male/Female):_____

Area of Interest: _____

E-mail: _____

Contact No.: (+91) _____

Payment Details:

Registration Fee Amount: Rs. _____

Mode of payment (Online/DD): _____

Online Transaction/DD No._____ Date _____

Bank Name: _____

Name _____Signature_____