



# YENEPOYA

Homoeopathic Medical  
College & Hospital



AYUSH Campus, Naringana, Mangaluru-575018

A CONSTITUENT COLLEGE OF YENEPOYA (DEEMED TO BE UNIVERSITY)

## Workshop on **MOLECULAR DOCKING**



**8<sup>th</sup> March 2025**

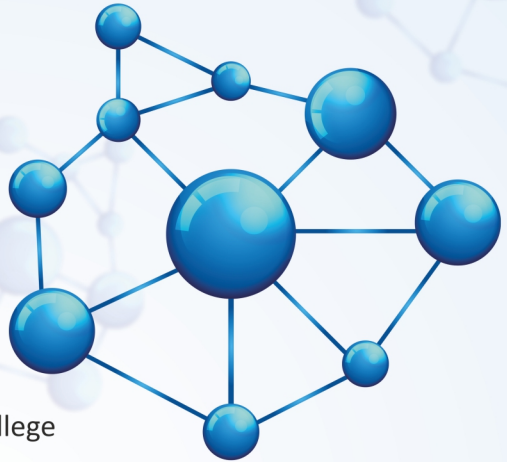


**9:30 AM - 5.00 PM**



**Board Room**

**Yenepoya Homoeopathic Medical College  
AYUSH Campus**



### About the Workshop

Unlock the Future of Homeopathic Research: Hands-on Molecular Docking Workshop! Homeopathy stands at a crucial juncture - its mechanism of action at the molecular level remains one of the most debated scientific frontiers. It is time for homeopaths to take charge and bridge this gap with cutting-edge research tools. To empower homeopaths with the skills to explore homeopathy at the molecular level, the Research and Development Cell of Yenepoya Homeopathic Medical College, in collaboration with the Centre for Integrative Omics Data Sciences, presents an exclusive Workshop on Molecular Docking - a revolutionary technique in computational drug discovery. This hands-on workshop will introduce participants to the power of Molecular Docking, enabling them to visualize and analyze interactions between medicinal molecules and biological targets. The carefully designed sessions will cover:

- Fundamentals of Molecular Docking - Understanding how homeopathic remedies may interact at the molecular level.
- Protein & Ligand Extraction - Preparing structures for docking studies.
- Molecular Docking with Open-Source Tools - Mastering free yet powerful software for research.
- Result Analysis & Interpretation - Making sense of docking scores and binding affinities.
- Interactive Hands-on Session - Apply your learning by performing docking on your own computer.

*Join us in this transformative journey and gain practical skills that can open new dimensions in homeopathic research. Let's take homeopathy into the era of computational biology!*

Register now and be part of this groundbreaking initiative!

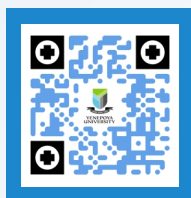
Only 25 participants will be trained for the molecular docking.

Instruction: The participants are requested to bring their laptops/notebooks for the workshop

*Registration Details:*

**Fee: ₹750/-**

**Registration Link: <https://rzp.io/rzp/oGwqfcR>** 



**QR CODE  
for registration and  
fee payment.**

**Lunch, Tea, and Snacks will be provided**

Accommodation: Participants have to arrange their accommodation. However, we recommend the following sites for stay.

**Hotel Comfort Inn: Contact - 7090940330**

**Aurelia Comforts: Contact - 0824 - 6637199**

Transportation: We are happy to provide transportation from the main entrance of the Yenepoya (Deemed to be University) on 8th March at 8:45 am to the venue located at the AYUSH campus (approximately 8km from the University campus).

*Contact :*

**Dr Harinarayanan: 9738508386**

*or*

**Dr. Arun K John: 9844131030**

for the details.



## We wish to introduce the following Resource Persons



**Dr. Abhithaj J**  
MSc, PhD

**Dr. Abhithaj J** is an esteemed researcher in computational biology, specializing in molecular docking, drug discovery, and structural biology. He holds a PhD in Life Sciences from Kannur University, with extensive research in **in silico assessment of inflammatory marker antagonists and their in vitro and in vivo validation**.

Currently serving as an **Assistant Professor at the Center for Integrative Omics Data Sciences**, Dr. Abhithaj has contributed significantly to the field through multiple high-impact publications, book chapters, and international conference presentations. His expertise spans **virtual screening, molecular dynamics, and computational drug design**, with a strong focus on phytomedicine and ethnopharmacology.

Dr. Abhithaj has also held faculty positions and actively participates in peer-reviewing for prestigious journals. As an invited speaker and workshop trainer, he brings hands-on experience in cutting-edge computational techniques for **molecular docking and drug discovery**.

Mr. Levin John is a **Bioinformatician and Data Scientist** specializing in **molecular docking, molecular dynamics, protein modeling, and drug repurposing**. He holds a Master's degree in Bioinformatics from Mar Athanasios College for Advanced Studies (MACFAST), Kerala.

Currently serving as a **Data Scientist at the Center for Integrative Omics Data Sciences (CIODS), Yenepoya (Deemed to be University)**, Mr. Levin applies **deep learning and computational biology techniques to analyze large-scale biological datasets, particularly in phosphoproteomics and structural biology**. His expertise includes **machine learning applications in bioinformatics, high-throughput data analysis, and computational drug discovery**.

With multiple high-impact research publications, Mr. Levin is actively involved in **training and mentoring interns**, leading data visualization initiatives, and reviewing for reputed journals. His hands-on expertise in **Autodock, Schrodinger Suite, and molecular modeling tools** makes him a valuable resource person in the field of **molecular docking and computational drug design**.



**Mr. Levin John**  
MSc



**Mrs. Fathimath Henna**  
MSc

Mrs. Fathimath Henna is a **Computational Biologist** with expertise in applying artificial intelligence techniques to homeopathy and molecular research. She holds a **Bachelor's degree in Chemistry from Pondicherry University** and a **Master's degree in Computational Biology from Kannur University**.

She previously served as a **Junior Research Fellow at Yenepoya Homeopathic Medical College**, where she played a key role in developing **HomoeOmics** - the first Omics Database for Homeopathy. Her work has significantly contributed to integrating computational biology with homeopathic research.

Currently, she is a **Research Assistant at Yenepoya Homeopathic Medical College**, focusing on **leveraging AI-driven approaches to advance homeopathic medicine**. Her research involves **computational modeling, data analysis, and AI applications in alternative medicine**, making her a valuable contributor to the field of **molecular docking and computational biology**.

She is actively involved in Data analysis, manuscript writing and submitted 4 peer reviewed papers in reputed International Journal.

*Organizing Chairman:*

**Dr. Vijayendra V Itagi**

Principal, Yenepoya Homoeopathic Medical College

*Joint Organizing chairman:*

**Dr. Rajesh Raju**

Director, Centre for Integrative Omics Data Sciences

**Dr. Shivaprasad K**

Medical Superintendent, Yenepoya Homoeopathic Medical College

*Organizing Secretary:*

**Dr. Kurian P J**

Phone : 9740935383

