BLDE

(Deemed to be University), Vijayapura

Workshop on Computational Drug Design and Molecular Simulation

Organized by

Centre for Advanced Medical Research (CAMR)
In collaboration with School of Applied Science and Technology

Dec 22 & 23, 2025

Detailed Report on the Workshop on Computational Drug Design and Molecular Simulation

Dates: 22 & 23 December 2025
Duration: Two Days
Mode: Hands-on Workshop with Expert Lectures

1. Background and Rationale

Computational drug design has emerged as a powerful approach to accelerate the discovery and development of novel therapeutic molecules. Advances in molecular docking, molecular dynamics simulations, and multi-omics integration have significantly reduced the time and cost associated with traditional drug discovery pipelines. In this context, the Workshop on Computational Drug Design and Molecular Simulation was organized to equip participants with both theoretical insights and practical skills in modern computational tools and methodologies.

The workshop was designed to bridge the gap between conceptual understanding and real-time application of computational techniques, catering to postgraduate students, research scholars, faculty members, and early-career researchers in life sciences, pharmacy, and bioinformatics.

2. Objectives of the Workshop

- To introduce fundamental concepts of computational drug discovery
- To provide hands-on training in protein and ligand preparation
- To demonstrate molecular docking using open-source tools and Flare software
- To familiarize participants with binding site prediction, ADME-Tox evaluation, and molecular dynamics simulations
- To promote interdisciplinary learning and research collaboration

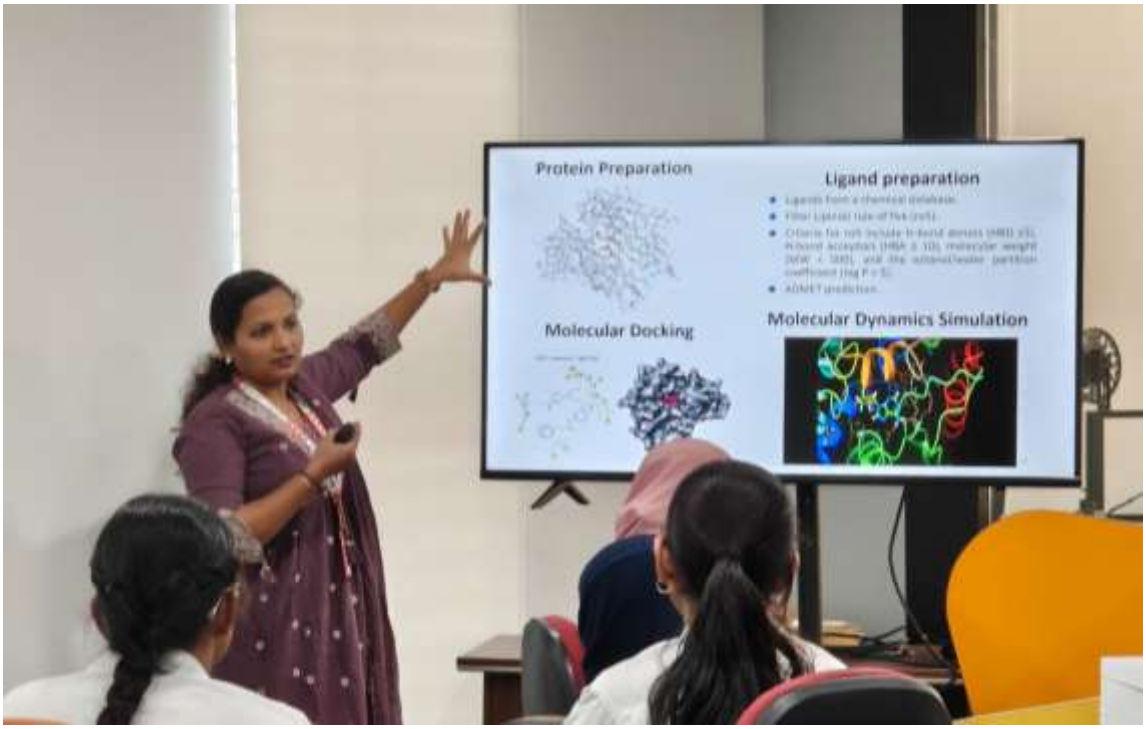
3. Day-wise Detailed Proceedings

Day 1: 22 December 2025 (Monday)

The workshop commenced at 10:30 AM with the Inauguration, Welcome Address, and Workshop Overview, conducted by the organizing team. The inaugural session highlighted the importance of computational approaches in current biomedical research and outlined the structure, learning outcomes, and expectations of the two-day program.

Following the inaugural session, participants attended a Keynote Lecture titled “Role of Multi-omics and Simulations in Accelerating Drug Discovery Process”, delivered by Dr. Joy Hoskeri from 11:45 AM to 12:45 PM, under the moderation of Dr. G. S. Kadakol. The speaker elaborated on how genomics, proteomics, and metabolomics data can be integrated with molecular simulations to improve target identification and lead optimization, supported by real-world research examples.

The next session, held from 12:45 PM to 01:45 PM, focused on Protein and Ligand Preparation using Open-Source Tools. This hands-on and demonstration-based session was conducted by Dr. Shivaleela B, moderated by Dr. Prachi P. Participants were trained in preparing biomolecular structures, cleaning protein files, optimizing ligand geometries, and setting up molecules for docking studies using freely available computational resources.



After the lunch break, the session on Binding Site Prediction and ADME-Tox Evaluation was conducted from 02:45 PM to 04:15 PM by Dr. Shivaleela B. This session emphasized the identification of active sites in target proteins and the evaluation of pharmacokinetic and toxicity parameters, enabling participants to assess the drug-likeness of candidate molecules.

The post tea break session from 04:30 PM to 05:15 PM involved a hands-on demonstration of molecular docking using AutoDock, followed by docking result analysis, conducted by Dr. Shivaleela B. Participants learned how to interpret docking scores, binding poses, and protein ligand interactions.

The first day concluded with an interactive Q&A and discussion session from 05:15 PM to 05:30 PM, where participants actively engaged with the resource persons, clarifying doubts and discussing practical challenges encountered during docking studies.

Day 2: 23 December 2025 (Tuesday)

The second day began at 10:00 AM with a Keynote Lecture titled “The Intelligent Molecule: Where Chemistry Meets Computation”, delivered by Dr. Dakshinamurthy Sivakumar and moderated by Dr. Prachi P. The lecture focused on intelligent molecular design, highlighting the role of computational intelligence, scoring functions, and predictive models in modern drug discovery.

From 11:00 AM to 11:30 AM, a hands-on session on Protein and Ligand Preparation and Structure-Based Docking using Flare was conducted by Mr. Ali A. Participants were introduced to the Flare interface, workflow setup, and docking protocols. This session was followed by a short tea break.

The subsequent session from 11:45 AM to 12:45 PM focused on Interaction Analysis, Scoring, and Optimization Using Flare, again conducted by Mr. Ali A and moderated by Dr. Prachi P.

Participants learned how to analyze binding interactions, evaluate docking scores, and optimize ligand conformations for improved binding affinity.

After lunch, the Molecular Dynamic Simulation with Flare session was conducted from 01:45 PM to 02:45 PM. This session provided participants with an understanding of molecular dynamics concepts, system setup, simulation parameters, and trajectory analysis to assess the stability of protein–ligand complexes.

From 02:45 PM to 03:45 PM, a session on Institution's Innovation Council (IIC) was delivered by Mr. Ajith B, focusing on innovation, entrepreneurship, and opportunities for translating research ideas into impactful outcomes.

The workshop concluded with the Valedictory Function from 04:00 PM to 05:00 PM, organized by the organizing team. During this session, participants shared feedback, the overall outcomes of the workshop were summarized, and certificates were distributed.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4. Outcomes and Impact

- Participants acquired hands-on experience in computational drug design workflows
- Improved understanding of molecular docking, ADME-Tox analysis, and molecular dynamics
- Exposure to both open-source tools and commercial software (Flare)
- Encouraged interdisciplinary research and collaboration
- Positive feedback indicating high relevance and practical utility

5. Conclusion

The Workshop on Computational Drug Design and Molecular Simulation was successfully conducted and achieved its intended objectives. The combination of expert lectures and practical sessions provided a comprehensive learning experience. The workshop significantly enhanced participants confidence in applying computational techniques to real-world drug discovery problems.

Total number of participants

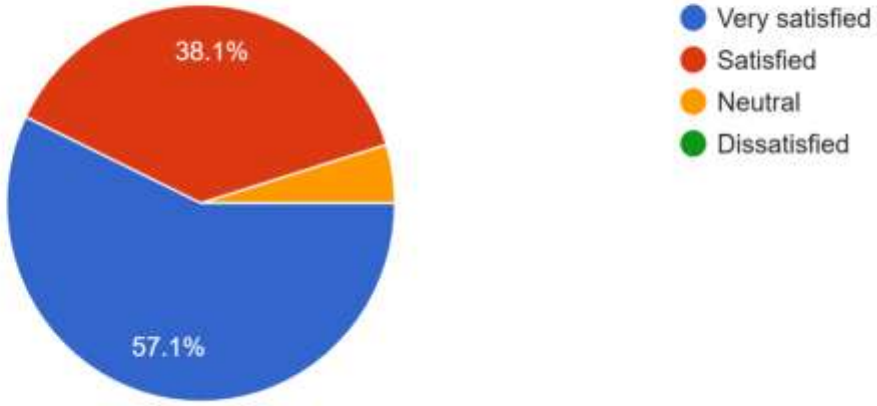
Sl.No.	Name	Designation	Institute	Contact
1	Dr. Damodar Naik	Associate professor	BLDEA's Avs Ayurveda Mahavidyalaya, Vijayapur	8792121755
2	Dr. Mallamma H Biradar	Professor	BLDEA's AVS Ayurveda Mahavidyalaya Hospital And Research Centre Vijayapura	8951001964
3	Dr Shweta Nidagundi	Assistant Professor	BLDE AVS Ayurveda Mahavidyalaya Hospital And Research Centre	8951192664
4	Dr. Manjunatha H Mathada	Assistant professor	BLDEA'S SB Arts And KCP Science College Vijayapura	7259500065
5	Ms. Shravya S Savalasang	Student	BLDE (Deemed To Be University) Vijayapura.	9964693772
6	Ms. Shruti phadke	M pharmacy	BLDEA's Ssm College Of Pharmacy And Research Centre Vijayapura	9591743705
7	Ms. Pavitra R Patil	Student	BLDEA'S SSM College Of Pharmacy And Research Centre Vijayapura	7975811233
8	Ms. Kavya Chandrakant Pujari	M Pharmacy	BLDE	9148645741
9	Ms. Rajeshwari Patrot	Assistant Professor	Smt.I.S Yadawad Government First Grade College Ramadurg	9606654434
10	Dr. Manjula badami	Lecture	Smt I. S. Yadawad Gfgc Ramdurg	9901956045
11	Ms. Shilpa Bhagavant muchhandi	M.pharmacy	BLDEA'S SSM College Of Pharmacy & Research Center Vijayapura - 586103	7795820129
12	Ms. Birajdar Savita Shivanand	PG scholar	BLDEA's Ssm College Of Pharmacy , Vijaypura	7414974424
13	Dr. Ahelam Tikotikar	Assistant Professor	KBN University	8147182300
14	Dr. Jarnain R. Naik	Assistant Professor	Khaja Bandanawaz University	8073246891
15	Dr. Ajmal Nasim	JUNIOR RESIDENT	Shri. B. M. Patil Medical College Hospital And Research Centre	9544677301

16	Ms. Deepa Mallappa Korawar	PG Scholar(department of Pharmaceutical Chemistry)	BLDEA's Ssm College Of Pharmacy And Research Centre Vijayapur	9591743273
17	Ms. Shraddha Patil	PG scholar (pharmacognasy)	BLDEA's SSM College Of Pharmacy And Research Centre Vijaypur	8310893991
18	Ms. Muskan Bammanhalli	Student	BLDE DU	8310558297
19	Ms. Tanzeem Patel	Student	BLDE DU	7019665499
20	Ms. Shreelekha pattanashetti	M pharm	BLDE SSM College Of Pharmacy And Research Centre Vijayapura	8867534778
21	Dr. Shridharkumaer S Biradar	Associate Professor	BLDEA's SSM College Of Pharmacy And Research Center Vijayapur	8867135309
22	Dr. Anand Vibhute	Assistant Professor	BLDEA'S Avs Ayurveda Mahavidyalaya, Vijaypura	7758034704
23	Dr. Vidyalaxmi Pujari	Associate professor	BLDEA'S Avs Ayurveda Mahavidyalaya, Vijaypura	7899683167
24	Dr. Kashinath H	Associate Professor	BLDEA'S Avs Ayurveda Mahavidyalaya, Vijaypura	7204483843
25	Dr GANGADHARAT ARALELIMATH	Professor	Shri Jagadguru Gavisiddheshwara Ayurveda Medical College Hospital and P G Research Centre, Koppal	9480207969
26	Dr. Manjushree.H.D	Assistant Professor	Shri Jagadguru Gavisiddheshwara Ayurveda Medical College Hospital and P G Research Centre, Koppal	8660342795

Feedback

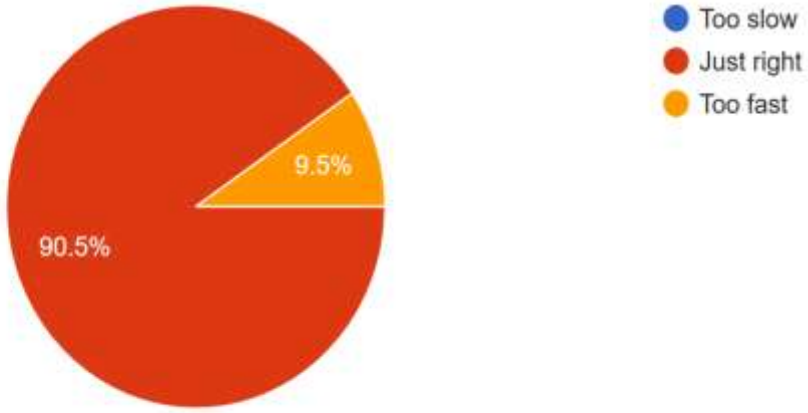
Overall, how satisfied were you with the workshop?

21 responses



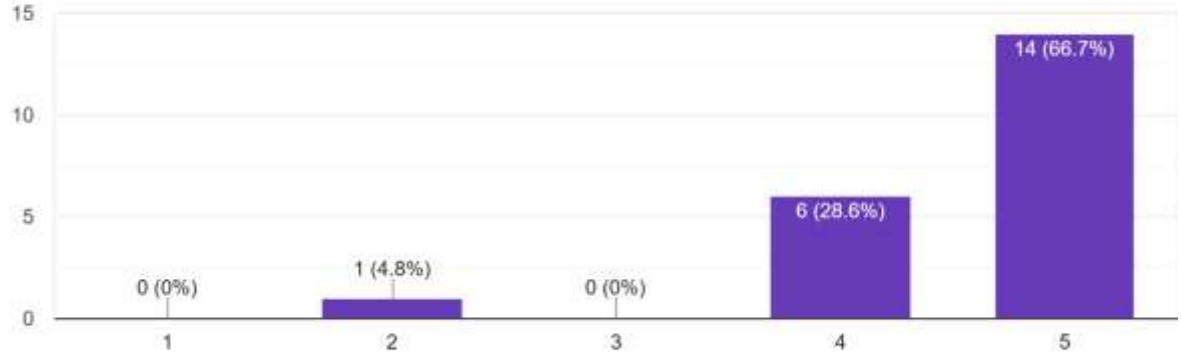
The pace of the workshop was appropriate.

21 responses



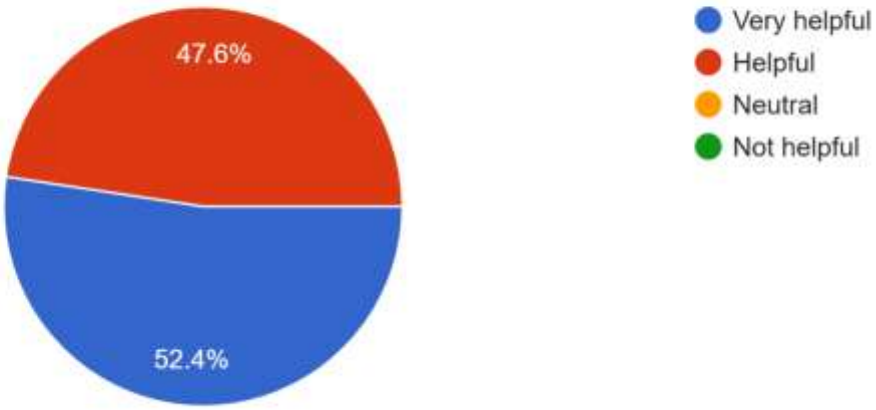
The facilitator(s) explained concepts clearly.

21 responses



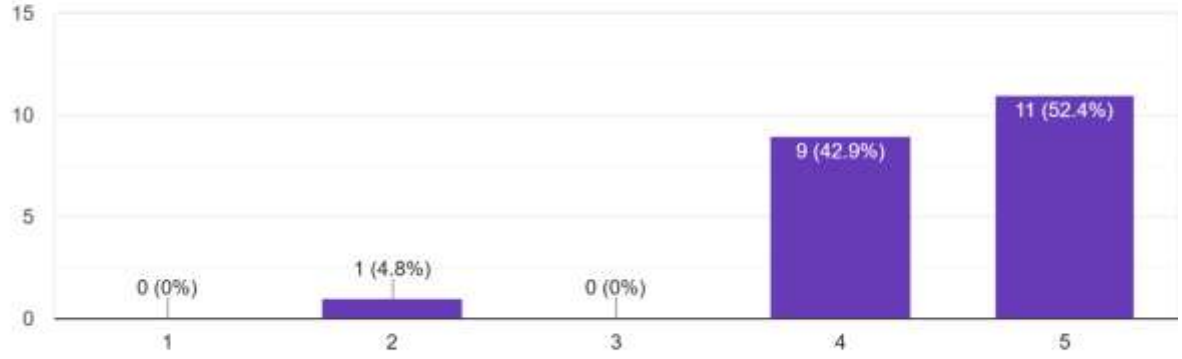
The materials/resources provided were helpful.

21 responses



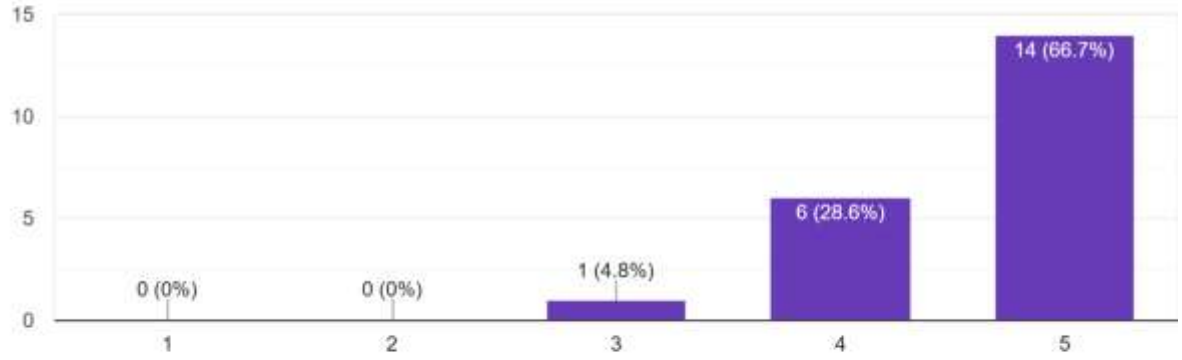
I gained useful knowledge or skills from this workshop.

21 responses



How would you rate the overall arrangements for the workshop?

21 responses



Flyer

BLDE (Deemed to be University)

Accredited with 'A' Grade by NAAC (Cycle-2)
Declared as Deemed to be University u/s 3 of UGC Act, 1956

Workshop on

Computational Drug Design and Molecular Simulation

Organized by Centre for Advanced Medical Research in Collaboration with School of Applied Science and Technology

BLDE(Deemed to be University), Vijayapura, is a premier institution committed to excellence in education, research, and healthcare. With a strong focus on advancing scientific knowledge and fostering innovation, the University continues to support high-impact research across medical and allied health sciences. The Centre for Advanced Medical Research (CAMR) is a well-equipped research facility under BLDE (DU), dedicated to promoting advanced scientific investigation, interdisciplinary collaboration, and skill development in emerging scientific domains.

In line with this vision, CAMR is organizing a workshop on Docking and Simulation Studies, aimed at providing participants with hands-on exposure to computational tools used in modern drug discovery. This program will enable students and researchers to understand molecular interactions, perform virtual screening, and explore simulation-based approaches essential for biomedical research.

Workshop Content

- Introduction to Computer-Aided Drug Design (CADD)
- Protein and Ligand Preparation Techniques
- Binding Site Prediction and Molecular Docking using Flare and freely available tools.
- Docking Result Analysis, Drug-likeness, and ADME-Tox Evaluation
- Molecular Dynamics Simulation for Protein-Ligand Complex Stability

Date: Dec 22 & 23, 2025
Time: 10:00 AM
Venue: Centre for Advanced Medical Research

Participation charges:
Student/Research Scholar/Postdoc/Faculty/Others : **Rs. 500/-**
Registration form: https://forms.gle/2JiosykWhxqbwqrXA

Limited seats are available. Registration will be on a first come first serve basis. Hurry up

Contact: +91 7507436576, **Email:** office.camr@bldedu.ac.in

Certificate

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Centre for Advanced Medical Research
Collaboration with School of Applied Science and Technology

CERTIFICATE OF PARTICIPATION

THIS IS TO CERTIFY THAT

has actively participated in the **Two Days**
"Workshop on Computational Drug Design and Molecular Simulation", held at the Centre for Advanced Medical Research (CAMR), BLDE (DU), Vijayapura, from **22nd & 23rd December 2025.**

Dr. R. V. Kulkarni — Registrar, BLDE (Deemed to be University)
Dr. M. M. Patil — Director Research & Development
Dr. S. V. Patil — Dean FoS & AHS
Prof. Kusal K. Das — Director, CAMR

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CERTIFICATE OF APPRECIATION

THIS IS TO CERTIFY THAT

served as a **Resource Person** and actively contributed to the **Two Days**
"Workshop on Computational Drug Design and Molecular Simulation", held at the Centre for Advanced Medical Research (CAMR), BLDE (DU), Vijayapura, from **22nd & 23rd December 2025.**

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