

Target Audience:

Faculty members, Research Scholars, UG and PG students

Registration: The participants are requested to register for the workshop through the following link

<https://events.vit.ac.in/>

**Registration fee (Including GST):
Rs. 500**

**Last date for registration:
17.04.2026**

**For further details contact:
ssajithalulu@vit.ac.in
9944807641**

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VIT[®]
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(Deemed to be University under section 3 of the UGC Act, 1956)

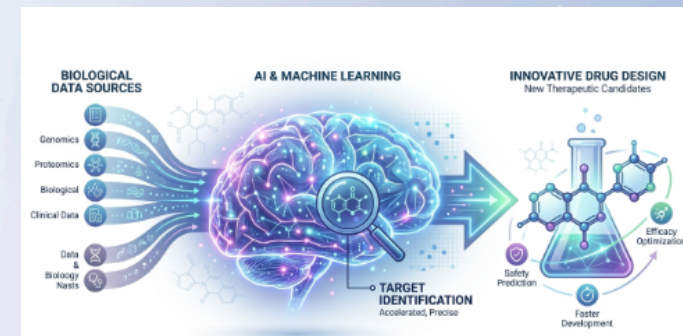


Hands-on Workshop
On

Drug Discovery and AI Applications

Date : 27.04.2026 to 28.04.2026

Venue: SMV G15



Organized by
School of Bio Sciences and Technology (SBST)
Vellore Institute of Technology,
Vellore - 632014

About VIT

VIT was established with the aim of providing quality higher education on par with international standards. It persistently seeks and adopts innovative methods to improve the quality of higher education on a consistent basis. The campus has a cosmopolitan atmosphere with students from all corners of the globe. Experienced and learned teachers are strongly encouraged to nurture the students. The global standards set at VIT in the field of teaching and research spur us on in our relentless pursuit of excellence. In fact, it has become a way of life for us. The highly motivated youngsters on the campus are a constant source of pride. Our Memoranda of Understanding with various international universities are our major strength. They provide for an exchange of students and faculty and encourage joint research projects for the mutual benefit of these universities. Many of our students, who pursue their research projects in foreign universities, bring high quality to their work and esteem to India and have done us proud. With steady steps, we continue our march forward. We look forward to meeting you here at VIT.

About SBST

The School of Bio Sciences and Technology (SBST) comprises four departments: Biotechnology, Integrative Biology, Biosciences, and Biomedical Sciences. The School offers one undergraduate programme (B.Tech. Biotechnology), four postgraduate programmes (M.Sc. and M.Tech.), two integrated M.Sc. programmes, and Ph.D. programmes. In alignment with the National Education Policy (NEP), flexible entry and exit options are available in integrated programmes, along with specialized tracks in emerging areas.

SBST provides a dynamic academic and research environment, offering students exposure to current scientific advancements and industry requirements. Faculty members are actively involved in both fundamental and translational research, contributing to sustainable solutions and offering consultancy services to industries. The school has published over 6,000 research articles, achieved an h-index of 97, and secured 55 patents. It is internationally recognized and ranked in the 301-350 range in Biological Sciences (world Ranking) and 7 in India by the QS World University Rankings by Subject 2026.

About Workshop

AI in drug discovery is revolutionising how new therapeutics are designed by combining biological data with intelligent algorithms to rapidly identify targets, screen compounds, and optimise drug candidates. Using advanced platforms like Flare software, participants can perform structure-based drug design, molecular modelling, and binding affinity analysis in a hands-on environment, bridging theory with real-world application. This practical exposure not only enhances research capabilities but also opens pathways for high-impact publications and potential patent development through novel molecule design and computational insights. This workshop uniquely empowers registrants with training licence access to Flare, enabling them to continue their research beyond the session, transforming ideas into publishable results and innovative intellectual property.

Contents of the Programme

Date	Time	Topic	Speaker	Software / Theory
27th April 2026	10:00 AM - 10:45 AM	Making "undruggable" targets "druggable"	Girinath G Pillai, PhD	Session
27th April 2026	11:00 AM - 1:00 PM	Mastering Flare: From Overview to Hands-On session Molecular Docking, Electrostatic Complementarity (EC)	Mr. Gopukrishnan	Flare
27th April 2026	2:00 PM - 4:30 PM	Molecular Dynamics in Flare: Setup, Execution, and Analysis	Mr. Gopukrishnan	Flare
27th April 2026	4:30 PM - 5:00 PM	Q & A session	Mr. Gopukrishnan	
DAY - 2				
28th April 2026	10:00 AM - 11:00 AM	Exploring Ligand-Based Drug Design: Theory and Applications.	Ms. Aradhana	Flare
28th April 2026	11:00 AM - 3:30 PM	Fundamentals of QSAR and Machine Learning Approaches : Hands-On session	Ms. Aradhana	Flare
28th April 2026	3:30 PM - 4:30 PM	Demonstration of Chemical Space Exploration: Hit Expansion and Library Enumeration in Flare	Ms. Aradhana	Flare
28th April 2026	4:30 PM - 5:00 PM	Q & A session	Ms. Aradhana	

Resource Persons



Girinath G. Pillai, PhD,
Lead Scientist, Computational Chemistry, Sygnature Discovery Ltd, United Kingdom



Aradhana Varughese
Senior Scientist (Applications) - Medicinal Chemistry, Zastra Innovations Pvt. Ltd, Indira Nagar, Bengaluru, Karnataka



Gopukrishnan R
Senior Scientist (Applications) - Life Science, Zastra Innovations Pvt. Ltd, Indira Nagar, Bengaluru, Karnataka

