About Electronics & ICT Academy at PDPM IIITDM Jabalpur

The Ministry of Electronics and Information Technology (MeitY), Government of India has instituted Electronics and ICT Academies in the year 2015. In the second phase, the academy at PDPM IIITDM Jabalpur aims at scalable training programmes in niche areas of Electronics and ICT for the development of the required knowledge base, skills and tools to unleash the talent of the Indian population. In addition to the faculty development programmes (FDPs) on fundamental and advanced topics in electronics, information and communication technologies, the Academy conducts customized training programmes for students, corporate sectors and research promotion workshops in emerging areas. The Academy is identified by the MeitY as the central hub of activities on training, internships, research, and consultancy programmes.

About PDPM IIITDM Jabalpur

PDPM IIITDM Jabalpur was established in 2005 with a focus on education and research in IT-enabled Design and Manufacturing. Since its inception, PDPM IIITDM Jabalpur has been playing a vital role in producing quality human resources for contribution to India's mission of inclusive and sustainable growth. The Institute offers undergraduate, postgraduate and PhD programmes in Computer Science and Engineering, Electronics and Communication Engineering, Mechanical Engineering, Design and PhD programmes in Mathematics, Physics and Literature. Further, the Institute offers an undergraduate programme in Smart Manufacturing. Under IIIT act, the Institute has been declared as an Institute of National Importance. The Institute campus is developed on 250 acres of land close to Dumna Airport, Jabalpur. The Institute is 10 kms from the main railway station and 5.5 kms from Dumna Airport, Jabalpur.

Faculty Development Programme

on Artificial Intelligence-based Drug Design

The course is designed to provide fundamental knowledge on the recent developments in artificial intelligence (AI)-based drug design. The primary aim is to train future generations to use computer-based algorithms and methods to promptly identify lead molecules without wasting time and money synthesizing random molecules against a known or unknown target.

Who can attend: The Programme is open to faculty from all colleges, universities, and technical and professional institutes. Students, fresh graduates, researchers, and industry personnel working in allied disciplines can also attend.

Important Dates:

Last Date of Online Registration: Feb 28, 2025 FDP Dates: March 17-22, 2025 Coordinators: Dr. Nihar R. Jena, Discipline of Natural Sciences PDPM IIITDM Jabalpur

Contact us:

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Faculty Development Programme on Artificial Intelligence-based Drug Design

March 17-22, 2025 (Hybrid mode)



Electronics and ICT Academy, Phase II



An Initiative of Ministry of Electronics and Information Technology, Government of India



PDPM Indian Institute of Information Technology, Design and Manufacturing, Jabalpur

Dumna Airport Road, Jabalpur 482005

Faculty Development Programme on Artificial Intelligence-based Drug Design

March 17-22, 2025 (Hybrid mode)

RESOURCE PERSONS

- Prof. G.N. Sastry, IIT Hyderabad
- Prof. Anshuman Dixit, ILS, Bhubaneswar
- Prof. G.P.S. Raghava, IIIT Delhi
- Prof. Mukesh Doble, IIT Madras
- Prof. N.S. Gandhi, MIT, Karnataka
- Prof. S.K. Singh, Alagappa University, Tamilnadu
- Prof. Manjari Gupta, IIT BHU
- Dr. Rajnish Kumar, IIT BHU
- Dr. N.R. Jena, IIITDM Jabalpur
- Dr. Suyash Pant, Schrodinger, Hyderabad
- Dr. Ashutosh Shandilya, IIT Delhi
- Dr. Rupesh Chikhale, CCDC UK

COURSE COORDINATOR

Dr. Nihar Ranjan Jena, Discipline of Natural Sciences PDPM IIITDM Jabalpur Email: <u>nrjena@iiitdmj.ac.in</u> Phone: +91-761-2794347

Course Contents

Fundamentals of

- Artificial intelligence
- Machine learning
- Virtual screening
- Docking
- Molecular dynamics simulations.
- Free energy methods.
- Structure-activity relationships
- Drug toxicity measurements.

Hands-On Sessions

- Visualization of target (protein or DNA) structure and drug-target interactions by using Pymol
- Drug designing by using artificial intelligence algorithms
- Docking and virtual screening by using Autodock, CCDC's GOLD and other programs
- Molecular dynamics simulations by using the Desmond program of Schrodinger
- Free-energy calculations
- Big data analysis
- Quantitative structure-activity relationship (QSAR)
- Computer-aided drug toxicity measurements

Programme Features

- To gain theoretical and practical knowledge on drug design
- Opportunities to connect with experts in the field.
- Instructor-led rigorous hands-on sessions with online (live streaming) sessions.
- Certificate on successful completion with full access to the course material.

Registration Details

- Registration link Please fill out registration using the following link: <u>https://docs.google.com/forms/d/e/1FAIpQLSe</u> <u>HrVs968Fd9JEAN1-</u> <u>jZ9ppiqGyNPhuPFuMZbUsKjz1alVcsA/closed</u> form
- Registration fee: 1000/- INR for offline participation and 500/ for online participation
- Last Date for Registration: Feb 28, 2025

Online Payment Details

• Internet banking

Beneficiary	PDPM	IIITDM
Name	Jabalpur	
Bank Name	ne INDIAN BANK	
A/C No.	50018692852	
IFSC Code	IDIB000M694	

• UPI ID: iiitdmj@indianbk

