

CIRCULAR



SCHOOL OF PHARMACY NOTICE

No: AJU/SOHAS/007/26

Date 08.01.2026

It is hereby notified to all the students of B. Pharm that Team MakeIntern, E-Cell IIT Hyderabad, invited you to participate in the National Zonal Championship 2025-26, along with a certification-based training program. The workshop will be hosted by School of Pharmacy in association with Industry Institute Interaction Cell, ARKA JAIN University.

Event Structure

The championship consists of two rounds:

Round 1: Training & Certification Program

Venue: At your College Campus

Minimum Batch Size- 45

Duration Options:

- 3 Days (18 Hours) – ₹1750 + 18% GST per participant
- 5 Days (30 Hours) – ₹3000 + 18% GST per participant

Note: The 5-day certification program aligns with NAAC guidelines for certified training programs.

Training Topic

Computer-Aided Drug Design & Discovery

Deliverable:

Industry-led hands-on training

Certification from MakeIntern & E-Cell IIT Hyderabad

LMS access for content revision

Internship assurance (via MakeIntern internship portal)

Evaluation test at the end of the workshop

Top 5 students (based on mock test + GD) will be shortlisted to represent your college in the Final

Round at IIT Hyderabad/Delhi.

Benefits of Participation:

Training by industry experts

National-level certification

Assured internship assistance

Enhanced campus visibility

Representation at IIT Hyderabad/Delhi

Prize pool worth ₹50,000

Zonal Center Status for your institution

Faculty Development Program (7 days Virtual FDP offered free for the college)

Excellence Award & Certificate for the College

10% of the total amount will be refunded towards the college welfare fund

Free LMS access for revision and reference

MoU along with NAAC Report

Students are encouraged to participate.

Dean

School of Pharmacy



Dean
School of Pharmacy
ARKA JAIN University Jharkhand

Copy to

Vice Chancellor

IQAC

Office of the Registrar

Class Coordinator Academic

Coordinator

ERP Coordinator

IIC Members

In-charge Website Office file

Student WhatsApp group

भारतीय भेषजी परिषद् (स्वास्थ्य एवं परिवार कल्याण मंत्रालय के अंतर्गत सांख्यिक निकाय) भारत सरकार आई-300, नौरोजी मंजिल, टावर-1, वर्ल्ड ट्रेड सेंटर, नौरोजी नगर, नई दिल्ली-110029 टेलीफोन नंबर 011-65218900-01 E-mail: registrar@pci.nic.in		PHARMACY COUNCIL OF INDIA (Statutory body under Ministry of Health & Family Welfare) Government of India I-300, 3rd floor, Tower-I, World Trade Centre, Nauroji Nagar, New Delhi-110029 Telephone No. 011-65218900-01 E-mail: registrar@pci.nic.in
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Circular**Ref. No. 14-449/2025-PCI**

To,
All State Pharmacy Councils
All the Institutions approved by PCI-
- u/s 12 of the Pharmacy Act, 1948
- for conduct of course
All the Pharmacy Teachers, Researchers, and Leading Pharma
Industry Officials

Sub.: Celebration of Pharma Anveshan 2026 - Theme
Announcement - reg.
for National Pharmacy Education Day', on 6th March 2026.

-----Ref.: Our Circular No. 14-449/2025-PCI, dt.
13.02.2026

Sir/Madam,

With reference to the subject cited above, In continuation to the Council's circular dated 13.02.2026, we are pleased to inform that PCI urges to all Pharmacy institutions to celebrate national Pharmacy Education Day', on 6th March 2026 to commemorate the birth anniversary of long-time unsung hero of pharmacy education in India and thus making a deep mark on the various aspects of Pharmacy Education.

In view of above, I am directed to inform that the Theme for **Pharma Anveshan 2026** has been finalized as:

"Future Pharma Ecosystem: Fostering Synergy among Academia, Industry, Research, Regulatory and Practice."

In this regard, you are requested to organize and celebrate **Pharma Anveshan 2026** in alignment with the above theme. The event should aim to promote meaningful collaboration among academic institutions, pharmaceutical industries, research organizations, regulatory bodies, and pharmacy practitioners, thereby strengthening the future pharmaceutical ecosystem of the country.

CIRCULAR ISSUED BY PCI

**ZONAL CHAMPIONSHIP & CERTIFICATION BASED TRAINING PROGRAM TO
CELEBRATE PHARMA ANVESHAN 2026
NATIONAL PHARMACY EDUCATION DAY 2026**

Date of Event	16.03.2026 to 18.03.2026
Name of the Event	Zonal Championship & Certification Based Training Program To Celebrate Pharma Anveshan 2026, National Pharmacy Education Day 2026
Type of the Event	Celebration/ Organizing National commemorative days Experiential Learning/ Participative Learning/ Problem Solving Methodologies
Conducted by	School of Pharmacy in association with Industry Institute Interaction Cell, ARKA JAIN University and MakeIntern, E-Cell IIT Hyderabad
No. Of Participants	45

OBJECTIVE:

The program was organized with the objective of commemorating National Pharmacy Education Day and honoring the contributions of Professor M. L. Schroff to pharmacy education in India. It also aimed to introduce students to Computer Aided Drug Design and Discovery (CADD) and its role in modern pharmaceutical research and development. Furthermore, the program focused on providing practical training on scientific databases and computational tools used in drug discovery. It sought to enhance students' technical knowledge and research orientation in pharmaceutical sciences, as well as to promote innovation and interdisciplinary thinking through interactive sessions and idea-pitching activities.

DETAILS:

The School of Pharmacy, Arka Jain University, in collaboration with from 16th to 18th March 2026 to celebrate Pharma Anveshan 2026 – National Pharmacy Education Day. The event was conducted to commemorate the birth anniversary of Professor M. L. Schroff, regarded as the Father of Pharmacy Education in India.

The three-day program focused on Computer Aided Drug Design and Discovery (CADD) and aimed to provide students with exposure to modern computational techniques used in pharmaceutical research and drug development.

Day 1: Inaugural Session and Conceptual Learning

The program began with an inaugural session welcoming the participants and the resource person. The speaker introduced the concept of Computer Aided Drug Design (CADD) and discussed its significance in modern drug discovery. The session covered topics such as the drug discovery process, identification of lead compounds, due diligence in pharmaceutical research, and the importance of global research collaborations.

Participants were also introduced to drug design approaches such as ligand-based and target-based drug discovery along with the Rule of Five, which is an important principle in evaluating drug-like molecules.

Day 2: Practical Training and Skill Development

The second day focused on hands-on training and practical exposure. Participants were introduced to important scientific databases and tools such as ChEMBL, Protein Data Bank (PDB), PubChem, Data Warrior, and IUPHAR.

Students learned how to retrieve chemical and biological data and perform molecular docking simulations using software such as Argus Lab. The session also explored the applications of CADD in various sectors including pharmaceuticals, veterinary science, and agrochemical industries.

Additionally, a session on Artificial Intelligence in pharmaceutical research was conducted where participants learned about generative AI and prompt engineering. The day also included an activity on professional branding and LinkedIn profile optimization, highlighting the importance of networking and career development.

Day 3: Innovation Activity and Valedictory Session

The final day focused on evaluation and innovation-based learning. Participants were trained to analyze molecular interactions, toxicity profiles, and compatibility of compounds, which are critical aspects of drug development.

An interactive “Shark Tank” style idea pitching session was organized where students presented innovative ideas on the use of Artificial Intelligence in healthcare and medical devices. The ideas were evaluated based on creativity, feasibility, and presentation.

An assessment test was conducted to evaluate participants’ learning outcomes. Based on their performance, five top candidates were selected for the next challenge round of the zonal competition. The program concluded with a valedictory session and vote of thanks. The event was coordinated by Mr. Subha Pramanik, Mr. Sumanta Sen, & Dr. Shweta.

TAKEAWAY (OUTCOMES):

The program achieved the following outcomes:

- Students gained knowledge about modern computational methods used in drug discovery.
- Participants developed hands-on skills in molecular docking and database analysis.
- The program enhanced awareness about Artificial Intelligence applications in pharmaceutical research.
- Students improved their analytical thinking, research skills, and problem-solving abilities.
- Participants gained exposure to industry practices, networking strategies, and career opportunities in the pharmaceutical sector.

Shortlisted Candidates:

1. Kashish Kumari (AJU/230795)
2. Riya Modi (AJU/241934)
3. Sourish Nanda (AJU/230067)
4. Khushi Sharma (AJU/230563)
5. Nirupam Jana (AJU/241844)

Back-up Candidates:

1. Vivek Kumar (AJU/251525)
2. Kuldeep Mahto (AJU/230645)

POSTER OF THE EVENT

JGI ARKA JAIN University Jharkhand NAAC GRADE A ACCREDITED UNIVERSITY THE WEEK RANKED 38TH ALL INDIA UNIVERSITY RANKING (PRIVATE UNIVERSITY CATEGORY) ISO

School of Pharmacy
Organizes
in association with
Makeintern & E-Cell (IIT Hyderabad)
Conducts
Zonal Championship & Certification
Based Training Program
To Celebrate
PHARMA ANVESHAN 2026
NATIONAL PHARMACY EDUCATION DAY
16th -18th March 2026 | Time : 10:00 AM
To Commemorate the Birth anniversary of
Professor M. L. Schroff
Coordinated by Mr. S. K. Mishra (Makeintern & E-Cell (IIT Hyderabad))
A National Commemorative Day Celebration

INDUSTRY INSTITUTE|INTERACTION CELL, AJU

PHOTOS OF THE EVENT



Fig.1- Dr. Punnet Kacker, Trainer from Makeintern and E-Cell, IIT Hyderabad, interacting with the participant regarding Zonal Championship and Certification Based Training Program



Fig. 2- Dr. Punnet Kacker delivered introductory remarks on Computer-Aided Drug Design and Discovery



Fig. 3- Dignitaries, faculty members and students paying tribute to Professor M. L. Schroff on the occasion of National Pharmacy Education Day during Pharma Anveshan 2026.



Fig. 4- Participants engaged in hands-on training on Computer-Aided Drug Design Simulations

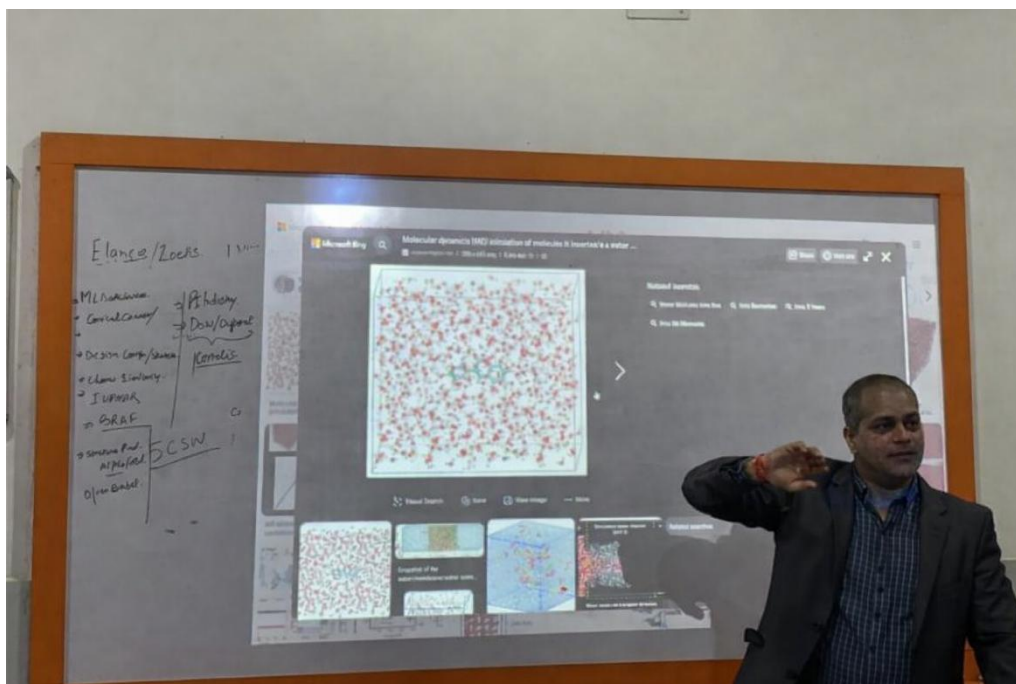


Fig. 5- Dr. Punnet Kacker demonstrates molecular modeling concepts



Fig. 6- Prof. (Dr.) Jyotirmaya Sahoo, Dean, School of Pharmacy highlighting key outcomes and learnings of the training session during the valedictory session



Fig. 7- Felicitation of Dr. Punnet Kacker by Prof. (Dr.) Jyotirmaya Sahoo, Dean School of Pharmacy during the valedictory session



Fig. 8- Group photograph of dignitaries, faculty members, and students after valedictory session of Zonal Championship & Certification Based Training Program organized on the occasion of National Pharmacy Education Day at the School of Pharmacy, Arka Jain University, Jharkhand.



E-Cell
IIT Hyderabad



**E-Cell 2K26-27
(IIT Hyderabad Event)**

in association with www.makeintern.com

Certificate of Excellence

Awarded To

**School of Pharmacy
ARKA JAIN University, Jharkhand**

In recognition of being Training Center for a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.

Mr. Srijan Shahi
Overall Coordinator
E-Cell, IIT Hyderabad

Mr. Hardeep Singh Puri
Director
Makeintern

Certificate of Excellence by Makeintern & E-Cell IIT Hyderabad

LIST OF PARTICIPANTS


**ARKA JAIN
University**
Jharkhand


SCHOOL OF PHARMACY

Event Registration cum
Attendance Form

Name of the Event: Zonal championship & 3-day workshop & certification based Training Programme on Computer-Aided Drug Design & Discovery Date of the Event: 16-03-26 to 18-03-26

Sl. No.	Name of the Candidate	Enrolment No	Signature of the Candidate	Feedback								Attendance				
				How would you like this session/event	The speaker explained the topic clearly				Would you like to attend this type of event/session in future	D1	D2	D3	D4	D5		
															E	V
1	Nirupam Jana	AJU/241844	Nirupam	✓						✓			P	P	P	
2	Sneha Mandal	AJU/240812	Sneha Mandal	✓						✓			P	P	P	
3	Bobby Jhapa	AJU/230026	Bobby Jhapa	✓						✓			P	P	P	
4	Aashna Singh	AJU/230016	Aashna Singh		✓					✓			P	P	P	
5	Khushi Kumari	AJU/230160	Khushi		✓					✓			P	P	P	
6	Deepak K. Pandit	AJU/241234	Deepak	✓						✓			P	P	P	
7	Manu Kumar	AJU/230211	Manu	✓						✓			P	P	P	
8	Anant Kumar	AJU/230007	Anant	✓						✓			P	P	P	
9	Kuldip Mahita	AJU/230645	Kuldip Mahita	✓						✓			P	P	P	
10	Rohit RAJ	AJU/230550	Rohit RAJ	✓						✓			P	P	P	

*E-Excellent, V-Very good, G-good, A-Average, P-Poor

Signature of the Head

School of Pharmacy
ARKA JAIN University Jharkhand

Signature of the Event Coordinator


**ARKA JAIN
University**
Jharkhand


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					E	V	G	A	P	Y		N					D1	D2	D3	D4	D5	D6	D7				
11	Ujjwal K. Harabo	AJU/230146	Ujjwal	✓						✓			Y	N					P	P	P						
12	Rishav Kumar Chaurasia	AJU/230019	Rishav	✓						✓			✓						P	P	P						
13	Anish Choudhary	AJU/230035	Anish	✓						✓			✓						P	P	P						
14	Soorav Nanda	AJU/230067	Soorav Nanda	✓						✓			✓						P	P	P						
15	Ashutosh Raju	AJU/230007	Ashutosh	✓						✓			✓						P	P	P						
16	GAURAN BHATTACHARJEE	AJU/231758	Gauran B	✓						✓			✓						P	P	P						
17	Pratima Kumari	AJU/232328	Pratima Kumari	✓						✓			✓						P	P	P						
18	Udhav Mandal	AJU/230014	Udhav	✓						✓			✓						P	P	P						
19	Deepak Anand	AJU/230079	Deepak	✓						✓			✓						P	P	P						
20	Bibhu Biju Mandal	AJU/230025	Bibhu Biju	✓						✓			✓						P	P	P						

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Signature of the Head

School of Pharmacy
ARKA JAIN University Jharkhand

Signature of the Event Coordinator



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Jharkhand



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				E	V	G	A	P	Y	N			
21	Rajivathkr. Saha	AJU/230545	<i>Rajivathkr. Saha</i>	✓					✓			P	P
22	Isha Shakun	AJU/230331	<i>Isha Shakun</i>	✓					✓			P	P
23	Khuski sharma	AJU/230513	<i>Khuski sharma</i>	✓					✓			P	P
24	Akshita Saha	AJU/230649	<i>Akshita Saha</i>	✓					✓			P	P
25	Keshish Kumar	AJU/230795	<i>Keshish Kumar</i>	✓					✓			P	P
26	Bikes Kr. Bala	AJU/230174	<i>Bikes Kr. Bala</i>	✓					✓			P	P
27	Anamika Kumari	AJU/230434	<i>Anamika Kumari</i>	✓					✓			P	P
28	Priya Kumari	AJU/230410	<i>Priya Kumari</i>	✓					✓			P	P
29	Dnyanesh Saha	AJU/240214	<i>Dnyanesh Saha</i>	✓					✓			P	P
30	Amit Gupta	AJU/240964	<i>Amit Gupta</i>	✓					✓			P	P

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Chakra
Signature of the Head
Sch. Pharmacy
ARKA JAIN University Jharkhand

Shweta
Signature of the Event Coordinator



**ARKA JAIN
University**
Jharkhand



SCHOOL OF PHARMACY
Event Registration cum
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				E	V	G	A	P	Y	N			
31	Riya Nodi	AJU/241034	<i>Riya Nodi</i>	✓					✓			P	P
32	Champa Kumari	AJU/230642	<i>Champa Kumari</i>	✓					✓			P	P
33	Kritika Pramanik	AJU/240034	<i>Kritika Pramanik</i>	✓					✓			P	P
34	Shikha Jha	AJU/230009	<i>Shikha Jha</i>	✓					✓			P	P
35	Vivek Kumar	AJU/251525	<i>Vivek Kumar</i>	✓					✓			P	P
36	Chitransh Koley	AJU/251855	<i>Chitransh Koley</i>	✓					✓			P	P
37	Rajkumar Mahata	AJU/251572	<i>Rajkumar Mahata</i>	✓					✓			P	P
38	Aditya Kumar	AJU/230162	<i>Aditya Kumar</i>	✓					✓			P	P
39	Satish Pati	AJU/230008	<i>Satish Pati</i>	✓					✓			P	P
40	Beegata Mandal	AJU/240404	<i>Beegata Mandal</i>	✓					✓			P	P

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Chakra
Signature of the Head
School of Pharmacy
ARKA JAIN University Jharkhand

Shweta
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				How would you like this session/event					The speaker explained the topic clearly			Would you like to attend this type of event/session in future		D1	D2	D3	D4	D5	D6		
				E	V	G	A	P	Y	N		Y	N								
41	Anika Sharma	AJU/230476	Anika	✓					✓			✓				P	P	P			
42	Nandin Kumar Pandey	AJU/230527	Nandin Pandey	✓					✓			✓				P	P	P			
43	MD SAEWAE KHAN	AJU/232182	SANWAE KHAN	✓					✓			✓				P	P	P			
44	Sourav Kumar Singh	AJU/232201	Sourav Kumar Singh	✓					✓			✓				P	P	P			
45	Samy Kishor	AJU/232103	Samy Kishor	✓					✓			✓				P	P	P			
6																					
7																					
8																					
9																					
10																					

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Signature of the Head
Dean

School of Pharmacy
ARKA JAIN University Jharkhand

Signature of the Event Coordinator

CERTIFICATES OF APPRECIATION



CERTIFICATES OF MERIT


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IIT Hyderabad



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(IIT Hyderabad Event)
in association with www.makeintern.com

Certificate of Merit

This is to congratulate

KA SHESH KUMAR (AJU/230795)

for his/her exemplary performance during a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.


 Prof. (Dr.) Jyotirmaya Sahoo
Dean, School of Pharmacy
ARKA JAIN University, Jharkhand


 Mr. Srijan Shahi
Overall Coordinator
E-Cell, IIT Hyderabad


 Mr. Hardeep Singh Puri
Director
Makeintern


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Certificate of Merit

This is to congratulate

KHUSHI SHARMA (AJU/230563)

for his/her exemplary performance during a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.


 Prof. (Dr.) Jyotirmaya Sahoo
Dean, School of Pharmacy
ARKA JAIN University, Jharkhand


 Mr. Srijan Shahi
Overall Coordinator
E-Cell, IIT Hyderabad


 Mr. Hardeep Singh Puri
Director
Makeintern

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IIT Hyderabad**E-Cell 2K26-27
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This is to congratulate

NIRUPAM JANA (AJU/241844)

for his/her exemplary performance during a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.

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ARKA JAIN University, Jharkhand

Mr. Srijan Shahi
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E-Cell, IIT Hyderabad

Mr. Hardeep Singh Puri
Director
Makeintern

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(IIT Hyderabad Event)**in association with www.makeintern.com**Certificate of Merit**

This is to congratulate

REYA MODE (AJU/241934)

for his/her exemplary performance during a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.

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Dean, School of Pharmacy
ARKA JAIN University, Jharkhand

Mr. Srijan Shahi
Overall Coordinator
E-Cell, IIT Hyderabad

Mr. Hardeep Singh Puri
Director
Makeintern

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(IIT Hyderabad Event)**in association with www.makeintern.com**Certificate of Merit**

This is to congratulate

SOURISH NANDA (AJU)230067)

for his/her exemplary performance during a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.

Prof. (Dr.) Jyotirmaya Sahoo
Dean, School of Pharmacy
ARKA JAIN University, Jharkhand

Mr. Srijan Shahi
Overall Coordinator
E-Cell, IIT Hyderabad

Mr. Hardeep Singh Puri
Director
Makeintern

CERTIFICATES OF COMPLETION


ARKA JAIN
University
Jharkhand


 E-Cell
IIT Hyderabad



E-Cell 2K26-27
(IIT Hyderabad Event)
in association with www.makeintern.com

Certificate of Completion

This is to certify that

CHAMPA KUMARJ (AJU/230642)

has successfully completed a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.


 Prof. (Dr.) Jyotirmaya Sahoo
 Dean, School of Pharmacy
 ARKA JAIN University, Jharkhand


 Mr. Srijan Shahi
 Overall Coordinator
 E-Cell, IIT Hyderabad


 Mr. Hardeep Singh Puri
 Director
 Makeintern


ARKA JAIN
University
Jharkhand


 E-Cell
IIT Hyderabad



E-Cell 2K26-27
(IIT Hyderabad Event)
in association with www.makeintern.com

Certificate of Completion

This is to certify that

CHITRANSH KASHYAP (AJU/251855)

has successfully completed a Three-Day On-Campus Training Programme on "Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026, organized by School of Pharmacy, ARKA JAIN University, Jharkhand in association with the National Zonal Championship, Makeintern and E-Cell IIT Hyderabad.


 Prof. (Dr.) Jyotirmaya Sahoo
 Dean, School of Pharmacy
 ARKA JAIN University, Jharkhand


 Mr. Srijan Shahi
 Overall Coordinator
 E-Cell, IIT Hyderabad


 Mr. Hardeep Singh Puri
 Director
 Makeintern

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(IIT Hyderabad Event)**in association with www.makeintern.com**Certificate of Completion**

This is to certify that

SHIKHA KUMARI (AJU/230009)

has successfully completed a **Three-Day On-Campus Training Programme** on
"Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026,
organized by **School of Pharmacy, ARKA JAIN University, Jharkhand** in
association with the **National Zonal Championship, Makeintern and E-Cell IIT
Hyderabad.**

Prof. (Dr.) Jyotirmaya Sahoo
Dean, School of Pharmacy
ARKA JAIN University, JharkhandMr. Srijan Shahi
Overall Coordinator
E-Cell, IIT HyderabadMr. Hardeep Singh Puri
Director
MakeinternARKA JAIN
University
JharkhandE-Cell
IIT Hyderabad**E-Cell 2K26-27
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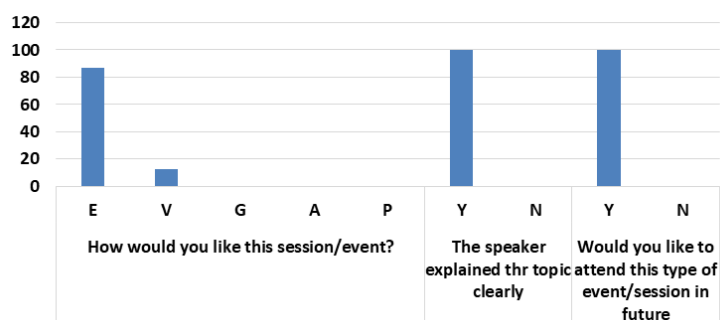
SANNY KASERA (AJU/241109)

has successfully completed a **Three-Day On-Campus Training Programme** on
"Computer-Aided Drug Design & Discovery" held from 16th to 18th March 2026,
organized by **School of Pharmacy, ARKA JAIN University, Jharkhand** in
association with the **National Zonal Championship, Makeintern and E-Cell IIT
Hyderabad.**

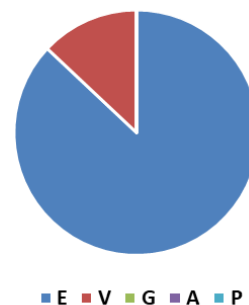
Prof. (Dr.) Jyotirmaya Sahoo
Dean, School of Pharmacy
ARKA JAIN University, JharkhandMr. Srijan Shahi
Overall Coordinator
E-Cell, IIT HyderabadMr. Hardeep Singh Puri
Director
Makeintern

FEEDBACK

FEEDBACK ANALYSIS OF ZONAL CHAMPIONSHIP & CERTIFICATION BASED TRAINING PROGRAM



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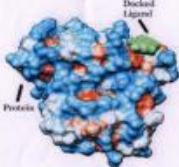
WRITE-UP

JGI **ARKA JAIN University** **NAAC GRADE A**
Jharkhand

A Report
On
THREE DAYS WORKSHOP ON COMPUTER AIDED DRUG DESIGN & DISCOVERY
(MAKEINTERN IN COLLABORATION WITH E-CELL IIT HYDERABAD)

SUBMITTED BY:

NAME: SOURISH NANDA
ENROL. NO.: AJU/230067
3rd year, 6th Semester
Batch-(2023-27)



School of Pharmacy, ARKA JAIN UNIVERSITY

REPORT ON 3-DAY WORKSHOP ON COMPUTER AIDED DRUG DESIGN AND DISCOVERY (CADD)

Organized by: MakeIntern & E-Cell (IIT Hyderabad)

Speaker: Mr. Puneet Kaushen

Duration: 3-days

A three-day workshop on Computer Aided Drug Design (CADD) was organized by IIT Hyderabad to provide participants with knowledge about modern computational approaches used in drug discovery. The workshop sessions were conducted by Mr. Puneet Kaushen, who shared valuable insights into the application of computational tools in pharmaceutical research & development.

The sessions combined theoretical explanations with practical demonstrations to help participants understand how computational methods accelerate the drug discovery process.

First Day of the Workshop:-

The 1st day of the workshop was an introductory session by Puneet Kaushen who was the one conducting the workshop. The session revolved around CADD that revolutionized the pharmaceutical industry by enabling faster, cost-effective & more accurate drug discovery. Traditional drug discovery methods were time-consuming & expensive whereas CADD integrates computational tools to predict drug behaviour, optimize lead compounds & minimize experimental failures.

Objectives of the workshop:-

- 1) To introduce the principles & application of CADD
- 2) To familiarize participants with computational tools & software
- 3) To understand molecular docking & ligand-receptor interactions & to gain insight into molecular dynamics simulation.
- 4) To bridge theoretical knowledge with practical implementation

The first day focused on building a strong foundation in Computer Aided Drug Design. The session began with an overview of drug discovery processes & the role of computational techniques in

modern pharmaceutical research.

CADD was classified into two main approaches: 1) Structure-Based Drug Design that uses 3D structure of target proteins & relies on molecular docking & simulations whereas ligand based drug design uses known active compounds.

Introduction to key databases includes the Protein Data Bank (PDB) that is the source of 3D protein structures whereas Pubchem & Drugbank relies on providing the pharmacological & chemical data. DataWarrior is an open-source tool that integrates data visualization, chemical structure analysis & property prediction in a single platform.

Hands on session:-

Participants performed:-

- # Downloading protein structures from databases
- # Visualizing proteins & identifying active sites
- # Preparing ligands & proteins for docking.
- # Arguslab in CADD was used for building, visualizing, & analyzing molecular structures. During the workshop, Arguslab was introduced as an easy to use tool for beginners to understand molecular modeling & basic docking concepts.

Day 2 :-Introduction to Molecular Docking & Docking Process

The second day focused on molecular docking, a technique used to predict the interaction between a drug (ligand) & its target (protein). Docking helps in predicting binding affinity, identifying binding mode & screening potential drug candidates.

Puneet Gargen Sir described the below steps in molecular docking:-

- 1) Protein preparation
- 2) Ligand preparation
- 3) Grid generation to define the active site.
- 4) Docking simulation
- 5) Scoring & analysis of interactions

Hands on Practical :- Docking of a ligand into a target protein
 ⇒ Analysis of binding interactions
 ⇒ Visualization of hydrogen bonds.

Day 3 :- Molecular Dynamics (MD) Simulations :-

The final day focused on molecular dynamics simulations, which study the physical movements of atoms & molecules over time.

MD simulations provide dynamic behaviour of molecule, stability of protein-ligand complex, real-time interaction analysis.

Principles of MD simulations - are based on Newton's laws of motion & force fields (mathematical models describing interactions).

Hands on Training :-

- 1) Running a short MD simulation
- 2) Plotting RMSD graphs
- 3) Interpreting simulation results

Overall Learning & Experience :-

The workshop provided a comprehensive understanding of CADD, progressing from basic concepts to advanced simulation techniques, the learning became more interesting because of day-to-day unique practical exercises given by the speaker to the participants like creating infection headshots, dashboards just like powerBI.

Key Takeaways :-

- 1) Practical exposure enhanced conceptual clarity.
- 2) Docking helps to identify potential drug candidates.
- 3) Integration of computational tools accelerates drug discovery.
- 4) Use of Artificial Intelligence, breaks the overall steps in identifying a potential drug candidate.