

SCHOOL OF CHEMICAL SCIENCES

REPORT of Two-day National Crystallographic ICDD Workshop 2023

on

“Materials Characterization Using Powder X-ray Diffraction”

ICDD® Workshop on Materials Characterization Using Powder X-ray Diffraction was hosted by School of Chemical Sciences, Goa University in collaboration with Vivertana Distributors Pvt. Ltd. The workshop was organised by the Analytical Chemistry Section of SCS-GU on December 7th to 8th, 2023, at School of Chemical Sciences Auditorium. The workshop was conveyed by Dr. Digamber G. Porob and co-conveyed by Dr Savita A. Kundaikar and Dr Kiran T. Dhavskar. The organising team included Dr. Rupesh E. Patre, Dr. Hari K. Kadam and Dr. Prajesh S. Volvoikar.

Following speakers were invited as Resource persons for the workshop



Dr. Soorya N. Kabekkodu,
Editor-in-Chief, International
Centre for Diffraction Data,



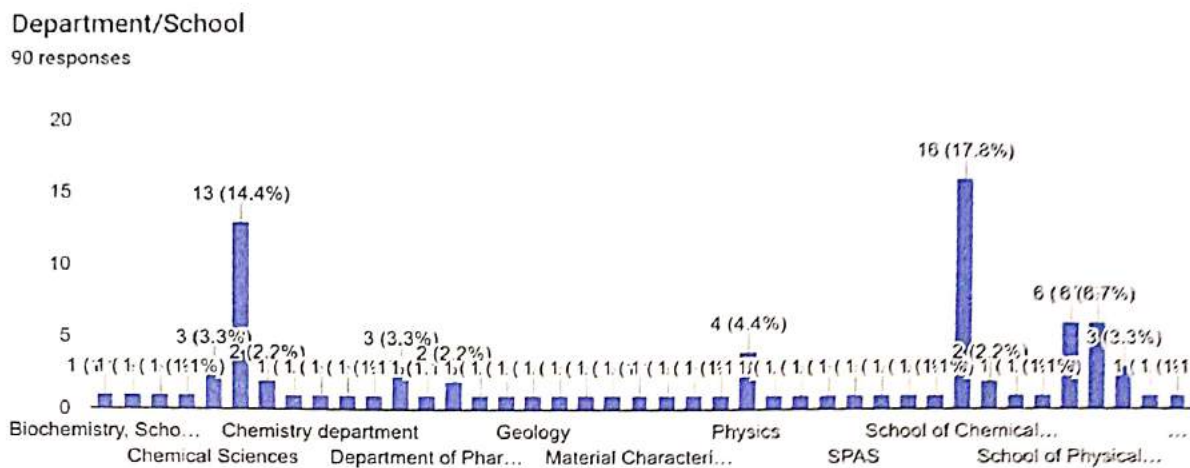
Professor Tayur N. Guru Row
Emeritus Professor, SSCU,
Indian Institute of Science,



Professor Arun M. Umarji,
Emeritus Professor, MRC,
Indian Institute of Science,

The workshop was inaugurated by the Honourable Vice Chancellor of Goa University, Prof. Harilal Menon, who was the Chief Guest of the program. The Dean of the School of Chemical Sciences, Prof. VMS Venekar, welcomed the resource speakers and participants from different institutes across India. The workshop witnessed the participation of faculties and researchers from different institutes across India like IISER Bhopal, IISER Mohali, IIT Delhi, IIT Madras, Dr Harisingh GOUR Central University, Punjab University, BITs Goa and Saint Gobin research India Pvt Ltd. The researchers of different schools of Goa University, including SCS and teachers from affiliated colleges also registered for the workshop

There were total of 66 participants across country including Goa. The MSc II students of School of Chemical Sciences volunteered and participated in this workshop showing their enthusiastic response for this workshop



The participants registered were from different disciplines of sciences like Geology, Physics, Material Chemistry, Pharmacy, Chemistry, Biochemistry and Biotechnology indicating the relevance of X-ray diffraction technique in their field emphasizing the significance of GUCW I 2023.

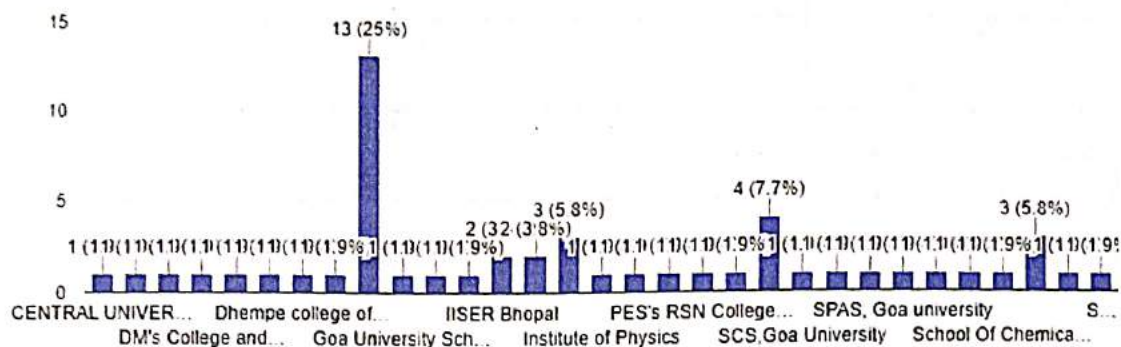
The workshop began with a lecture by Prof. Guru Row, who briefly introduced Crystallography. Dr. Kabekkodu gave information on PDF databases, database overview, and features, and explained data mining capabilities and Sieve+ for phase identification.

On the second day of the workshop, the first talk was delivered by Prof. A. Umarji, who gave information about Vivertana Distributors Pvt. Ltd and explained powder XRD data collection strategies for good quality data. The second day involved qualitative and quantitative XRD analyses using MDI JADE Pro software. In addition, materials characterization using the JADE Pro Toolkit features was also demonstrated by Dr. Kabekkodu after Prof. Umarji's lecture.

Very good feedback was received from participants of the workshop during the valedictory function, which was chaired by Prof. Dhuri, Vice Dean Academic of the School of Chemical Sciences. The valedictory function was graced by Prof. Priolkar, Dean of the School of Physical and Applied Sciences. He appreciated the efforts of the Organising team for such an informative workshop. Further, Prof. Dhuri expressed help and cooperation to all the participants in future. The workshop ended with a vote of thanks and conclusive remarks by the convenor, Dr. Porob. The feedback form showed excellent participant responses, as directed in the following data from Google feedback.

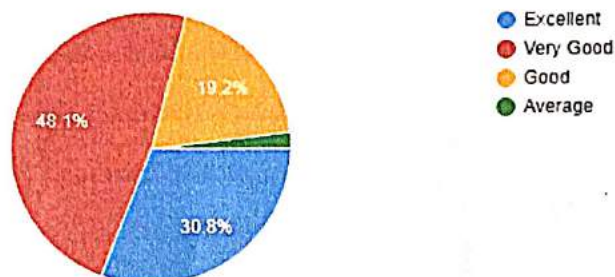
Name of the Institution

52 responses



How would you rate the workshop?

52 responses



The majority participants found the workshop informative to recommend the same for their friends in future. The positive feedback has motivated organising team to conduct more workshop on X-ray diffraction techniques at Goa University so that maximum number of researchers and faculties take benefit of knowledge on the applications of X-ray Diffraction in their respective field.

REPORTED BY:

Dr. Kiran T. Dhavskar (Co-Convenor GUCW I 2023)

Dr. Savita A. Kundaikar (Co-Convenor GUCW I 2023)

Assistant Professors in Analytical Chemistry, SCS

Dr Digamber G. Porob
Convenor GUCW I 2023



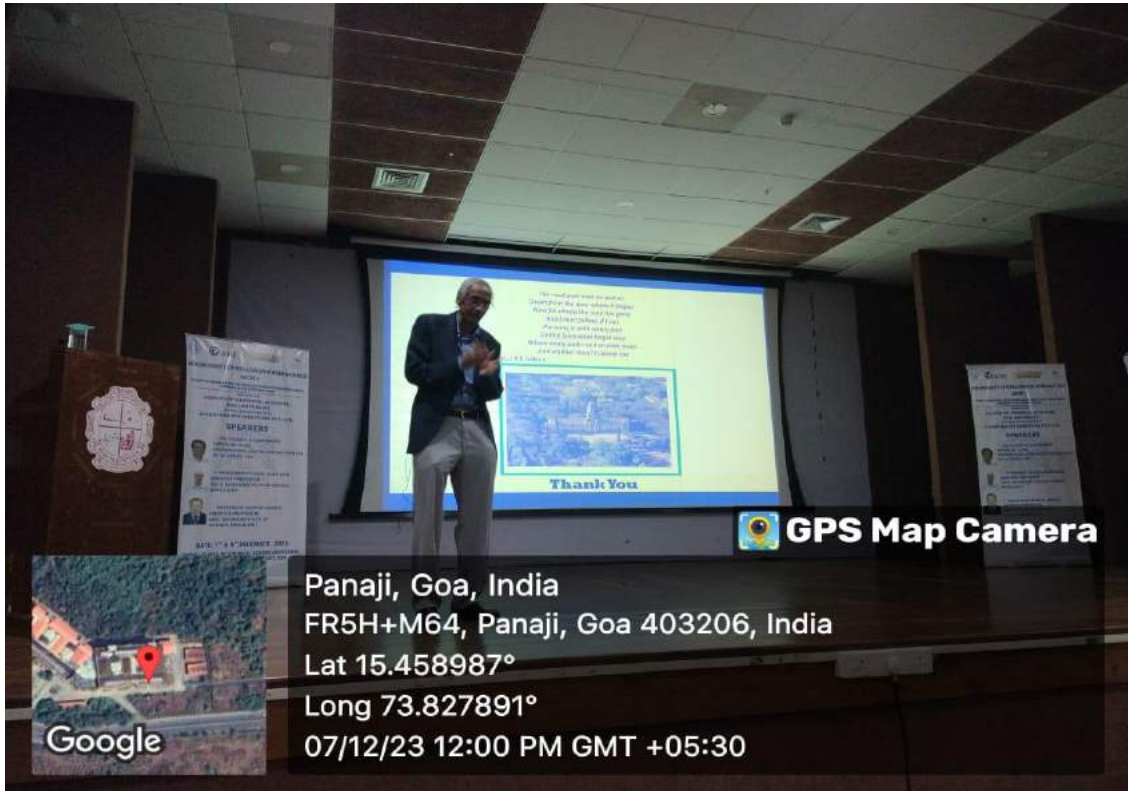
Prof. VMS Verenkar,
Dean, School of Chemical Sciences

Following are some of the glimpses of the workshops





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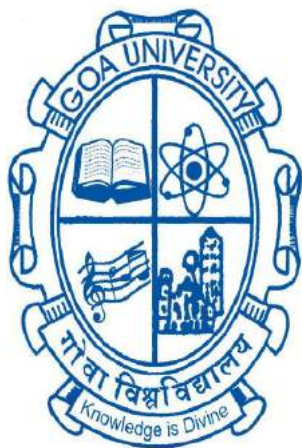






Goa University Crystallography Workshop 2023 – GUCW-I
**ICDD® Workshop on Materials Characterization Using
Powder X-ray Diffraction**

Hosted by School of Chemical Sciences, Goa University in
collaboration with Vivertana Distributors Pvt. Ltd.



Date: December 7th to 8th, 2023
Venue: School of Chemical Sciences Auditorium,
Science Block E, Goa University, Goa

The structure of the workshop is intended to be very interactive with lectures followed by (or along with) hands-on sessions. Hands-on sessions are designed to learn the concepts by solving problems of different complexity levels (simple to advanced)

This workshop will describe both data mining using the ICDD PDF-5+® database and methods of analysis embodied in ICDD PDF-5+® Sieve+ and ICDD MDI JADEPro® software.

Hands-on access to PDF-5+® and JADEPro® will be available through a remote desktop server via web access. Attendees should bring their laptop computer with wireless web access (Edge, Chrome, Firefox).

Note: Mac laptop (macOS) users should have Windows emulator installed

The first day of the workshop will present the PDF databases, database overview, features, datamining capabilities and Sieve+ for phase identification.

The second day will be qualitative and quantitative XRD analyses using MDI JADEPro software. In addition, materials characterization using the JADEPro Toolkit features will be demonstrated.

Attendees will have two-week (December 15th to 30th, 2023) post meeting access to PDF-5+® and JADEPro®.

Speakers:

Dr. Soorya N. Kabekkodu, Editor-in-Chief, International Centre for Diffraction Data (ICDD), USA

Professor Tayur N. Guru Row, Emeritus Professor, SSCU, Indian Institute of Science, Bangalore

Professor Arun M. Umarji, Emeritus Professor, MRC, Indian Institute of Science, Bangalore

Convener:
Dr. Digamber G. Porob

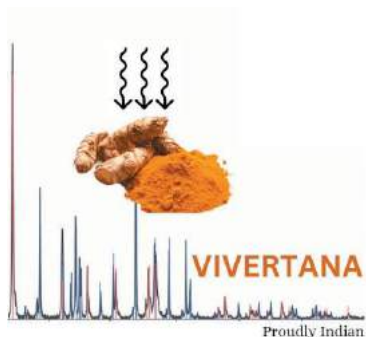
Dean,SCS:
Prof. Vidhyadatta M. Shet Verenkar

Co-Conveners:
Dr. Savita A. Kundaikar and Dr. Kiran T. Dhavskar

Members:
Dr. Rupesh E. Patre, Dr. Hari K. Kadam and Dr. Prajesh S. Volvoikar

Registration link: <https://forms.gle/5vTiqfVgHo8KgCL86>

Email:
gucw@unigoa.ac.in



Goa University Crystallography Workshop 2023 – GUCW-I

ICDD® Workshop on Materials Characterization Using Powder X-ray Diffraction
hosted by School of Chemical Sciences, Goa University in collaboration with
Vivertana Distributors Pvt. Ltd.

Venue: School of Chemical Sciences Auditorium, Science Block E, Goa University, Goa
7th and 8th, December 2023

Programme Schedule

Day 1: 7th December 2023 (9:30 am to 5:30 pm)

9:30 – 10:00am	Inaugural function
10:00 – 10:30am	High Tea
10:30 – 11:00am	Powder X-ray Diffraction Method and Applications (TNG)
11:00 – 12:30pm	Diffraction Geometry, Systematic Angular errors and calibration procedures, sample preparation (SNK)
12:30 – 1:00pm	Setting up PDF-5+ and JADEPro access
1:00 – 2:00pm	Lunch Break
2:00 – 3:30pm	Hands-on sessions: Introduction to Search/Match Procedure with PDF-5+/Sieve+, PDF-5+ Database and features overview, Data mining (SNK)
3:30 – 4:00pm	Tea Break
4:00 – 5:30pm	Phase identification methods (SNK) Qualitative and semi-quantitative (RIR) phase analysis, Advanced phase identification (with amorphous components, Trace phases), Additional problem solving, Q&A

Day 2: 8th December 2023 (9:30 am to 5:30 pm)

9:30 – 10:00am	Data collection strategies for materials characterization (AMU)
10:00 – 11:00am	Introduction to PXRd indexing (SNK)
11:00 – 11:30am	Tea Break
11:30 – 1:00pm	Introduction to profile functions, fitting, and Quantitative Phase Analysis (QPA) using Rietveld method (SNK)
1:00 to 2:00pm	Lunch Break
2:00 to 3:30pm	JADEPro hands-on sessions (SNK) JADEPro features overview, Angular Calibration (Instrument Profile Curve, IPC) Pattern Indexing using JADE
3:30 to 4:00pm	Tea Break
4:00 to 5:00pm	JADEPro hands-on sessions (SNK) Whole pattern fitting (WPF) and Rietveld refinement, Phase identification and Quantitative Phase Analysis (Rietveld), Crystallinity measurement, Crystallite Size and Micro-Strain Analysis
5:00 to 5:30pm	Q&A, concluding remarks and feedback from participants

Speakers:

SNK – Dr. Soorya N. Kabekkodu, Editor-in-Chief, International Centre for Diffraction Data, USA
TNG – Prof. Tayur N. Guru Row, Emeritus Professor, SSCU, Indian Institute of Science, Bangalore
AMU – Prof. Arun M. Umarji, Emeritus Professor, MRC, Indian Institute of Science, Bangalore

Convener:

Dr. Digamber G. Porob

Dean, SCS:

Prof. Vidhyadatta M. Shet Verenkar

Co-Conveners:

Dr. Savita A. Kundaikar and Dr. Kiran T. Dhavskar

Members:

Dr. Rupesh E. Patre, Dr. Hari K. Kadam and Dr. Prajesh S. Volvoikar

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Venue: School of Chemical Sciences Auditorium, Science Block E, Goa University, Goa
7th and 8th, December 2023

Workshop Information

Online application to Register for the workshop will be available from 16th till 30th October 2023. After the application is submitted, the first 50 applicant will be shortlisted for registration and details for the payment of fees will be communicated. Selection will be based on first come first basis. Maximum number of participants (with access to software) is 50.

Participants **must carry their own laptops** which will be required for hands on training on crystallography software's. Mac laptop (macOS) users should have Windows emulator installed.

Important Dates:

16th October 2023 - Online application to Register for the workshop will be available

30th October 2023 – Last day to submit the application

3rd November 2023 – Selected participant will be informed to pay the fees

8th November 2023 – Last day to make payment.

10th November 2023 – Confirmation of Registration

7th and 8th December 2023 – Workshop

Registration fees:

The registration is free for all the research students and teachers of School of Chemical Sciences, Goa University.

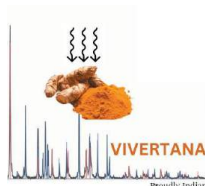
- (i) Rs. 500/- for the research students of other Schools of Goa University and affiliated colleges.
- (ii) Rs. 1000/- for the teachers of other Schools of Goa University and affiliated colleges.
- (iii) Rs. 1000/- for the research students of all other institutes not affiliated to Goa University.
- (iv) Rs. 2000/- for the teachers of all other institutes not affiliated to Goa University.
- (v) Rs. 5000/- for participants from Industry.

Email id: gucw@unigoa.ac.in

Registration link: <https://forms.gle/5vTiqfVgHo8KgCL86>

Note:

- Refreshments and lunch will be provided on both the days.
- Outstation participants will have to make their own arrangements for accommodation and travel.
- Participants must strictly adhere to the workshop timings.
- Attendance for all sessions is mandatory to receive the certificate of participation.





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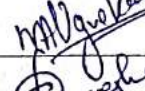
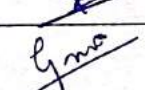
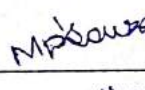


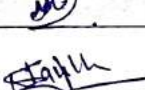
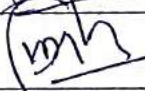

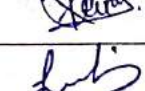
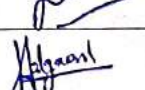
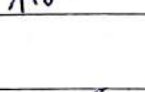

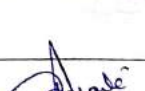
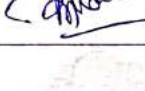

Programme Schedule

Day 1: 7th December 2023






Time	Inaugural Programme
9:30 to 9.35 am	Welcome Song
9:35 to 9.40 am	Welcome Address by Prof. Vidyadatta M. S. Verenkar, Dean, School of Chemical Sciences, Goa University.
9:40 to 9.45 am	Inauguration by lighting traditional lamp
9:45 to 9.50 am	Address by Guest of Honour Prof. Vishnu S. Nadkarni, Registrar of Goa University.
9:50 to 9.55 am	Address by Chief Guest Prof. Harilal B. Menon, Hon'ble Vice Chancellor of Goa University.
9:55 to 10.00 am	Vote of Thanks by Dr. Digamber G. Porob

**REGISTRATION FOR GOA UNIVERSITY CRYSTALLOGRAPHY WORKSHOP-
GUCW-I 2023**

DATE: 7th December 2023

serial number	Name of the participants	Name of the institution	Name of the department	Signature
1	Samantha Da Costa	Goa University	School of Chemical Science	
2	Namrata Kumari	Goa University	School of Chemical Sciences	
3	Manasi Ugvekar	Goa University	School of Chemical sciences	
4	Sarvesha S. Shetgaonkar	Goa University	School of Chemical Sciences	
5	Sonam kumari	Goa University	School of Chemical Sciences	
6	Dipika Gosavi	Goa University	School of Chemical Sciences	
7	Nikita N. Harmalkar	Goa University	School of Chemical Sciences	
8	Milagrina Dsouza	Goa University	School of Chemical Sciences	
9	Samidha Narvekar	Goa University	School of Chemical Sciences	
10	Jeffrey L. Viegas	Goa university	School of Chemical sciences	
11	Ms. Mangala U. Sawal	Goa University	School of Chemical Sciences	
12	Sanjali Navelkar	Goa University	School of chemical sciences	
13	Vipul Mangesh Ghare	Goa University	School of Chemical Sciences	
14	Pritesh khobrekar	Goa University	School of Chemical Sciences	
15	Apeksha Hiru Naik	Goa University	School of chemical sciences	
16	Sonali Gaonkar	Goa University	School of chemical sciences	
17	Pranav Valvaikar	Goa University	School of chemical sciences	
18	Siddhi K Salgaonkar	Goa University	School of Chemical Science	
19	Rohan Keshav Kunkalekar	Goa University	School of chemical sciences	
20	Disha Gauns	Goa University	School of Chemical Sciences	
21	Priyanka P. Kavalekar	Goa University	School of chemical sciences	
22	Ms. Anuja B. Naik	Goa University	School of Chemical Sciences	

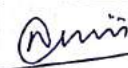
SCS

23	Vanita S. Kunkalkar	Goa University	School of Chemical Sciences	
24	Vignesh R Naidu	Goa University	School of Chemical Sciences	
25	Shefali Santosh Ainkar	Goa University	School of Chemical Science	
26	Leo Francisco Blaise DSouza	Goa University	School of Chemical Sciences	
27	Dr. Kanchanmala Deshpande	Goa University	School Of chemical sciences	
28	Snehal Chandekar	Goa University	Biochemistry, School of chemical sciences	

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Nitesh Venji



Goa University, School of Chemical Sciences

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**REGISTRATION FOR FOR GOA UNIVERSITY CRYSTALLOGRAPHY
WORKSHOP- GUCW-I 2023**

DATE: 7th December 2023

Serial number	Name of the participant	Name of the institution	Department/School	signature
1	Diksha	Goa University	School of physical and applied sciences	
2	Myren Azavedo	Goa University	School of Physical and Applied Sciences	
3	Mahendra Choudhary	Goa University	School of physical and applied sciences	
4	Shaikh Irshad Ahamad	Goa University	School of Physical and Applied Sciences	
5	Nandesh Nandakishore Kinlekar	Goa University	School of physical and applied sciences	
6 X	Bholanath Pahari	Goa University	School of Physical and Applied Sciences	—
7	Samiksha Malik	Goa University	School of Physical and Applied Sciences	
8	Shatakshi jakhi	Goa university	School of Physical and Applied Sciences	
9	Sujay Shivaji Rane	Goa University	School of Physical Sciences	
10	Nafea Manea Bhlos	Goa University	SPAS	
11	Shilpa R. Amonkar	Goa University	School of Physical & Applied Sciences	
12	Avani Anil Talkatkar	Goa University	School of Physical and Applied Sciences	

13.

Elaine Dias


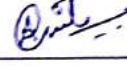
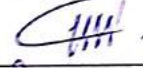




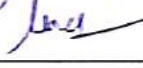
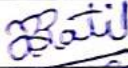

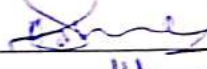

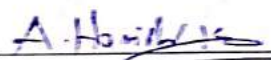
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**REGISTRATION FOR GOA UNIVERSITY CRYSTALLOGRAPHY WORKSHOP-
GUCW-I 2023**

DATE: 7th December 2023

Serial number	Name of the participant	Name of the institution/College	Signature
✓ 1	Sakshi	IISER MOHALI	
✓ 2	Vandana Vishwakarma	IISER Mohali	Vandana
✓ 3	Sunanada	IISER Mohali	Sunanada
4 ✓	Koushik Mandal	IISER Bhopal	Kan
✓ 5	Anila M Menon	IISER Bhopal	
* 6 ✓	Archisha Sharma		
✓ 7	Dr. Pratik Asogekar	PES ASN College of Arts & Science	
✓ 8	Dr. Harsha P. Uskaikar	PES KRVN College of Arts & Science	
✓ 9	Bishnupriya Swain	IIT Roorkee	
10	Mrs Deepa M Audi	Dharmapriya College of Arts & Science Mhamburda, Panaji Goa	
✓ 11	Mukul Nawani	IISER Mohali	Mukul
✓ 12	Aditya Kumar Prajapati	IIT Delhi	Aditya
✓ 13	Nevin Noble	ICP, Bhuvaneswar	
✓ 14	Dr. Miskil Naik	DCU'S Dharmapriya College of Arts & Science	
✓ 15	Malisetty Ravi Teja	IIT Delhi	M. Ravi Teja
✓ 16	Arjun Kumar Sah	IISER Mohali	Arjun Kumar Sah
✓ 17	Anagha Baburao Patil	BITS Pilani (Goa Campus)	 21/12/23
✓ 18	Naveena S Veerangaiah	Central University of Karnataka	
✓ 19	Akash Sinha	MAU College, Raipur	
✓ 20	Dr. Sudesh M Morajkar	DM'S College & Research Centre	
21 ✓	Dr. Adigilli Harish Kumar		

✓22	Nivatha E		
✓23	Mohan Kumar M		MS E
✓24	Ms. Pradnya Suresh Sawant	Govt. college Khemdola	Pradnya
✓25	Dr. Chandan Naik	Dhempur college	Dr. Chandan Naik
✓26	Ms. Manisha Mhalsekar	Dhempur college	MS