Workshop on Materials Characterization Using Powder X-Ray Diffraction (WMC-PXRD)

Venue: CSIR-National Chemical Laboratory, Pune
November 27-28, 2025

The Central Analytical Facility at CSIR-National Chemical Laboratory, Pune
In collaboration with

International Center for Diffraction data (ICDD), Philadelphia, USA
and
Vivertana Distributors Pvt. Ltd., Bangalore, India

This workshop will emphasize the techniques and applications of powder X-ray diffraction (PXRD), a powerful method for structural analysis and material characterization. Special focus will be placed on its applications in pharmaceutical research, including phase identification, polymorphism studies, and quality control. Participants will develop a comprehensive understanding of PXRD principles, data acquisition, and data interpretation, making the workshop particularly valuable for researchers in pharmaceutical sciences, crystallography, and materials science. The WMC-PXRD workshop will be highly interactive, featuring a blend of lectures and hands-on sessions. Participants will work through problem sets ranging from basic to advanced levels, reinforcing essential concepts. The program will also cover data mining using the ICDD PDF-5+® database and analytical methods implemented in ICDD PDF-5+® Sieve+ and ICDD MDI JADE® Pro software. Hands-on access to PDF-5+® and JADE Pro® will be provided via a remote desktop server through web access. Participants are required to bring their own laptops equipped with wireless internet access (Edge, Chrome, or Firefox browsers recommended).

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

First day (Nov 27): Demonstration of *the PDF-5+® databases, database overview, features, datamining capabilities and Sieve+ for phase identification and quantification (RIR method).*

Second day (Nov 28): Demonstration of q*ualitative and quantitative XRD analyses (Rietveld) using MDI JADE Pro® software. In addition, materials characterization using the JADE Pro Toolkit features. The PDF-5+® database and JADE Pro software will be accessible through a remote desktop server for a period of 3 weeks after the workshop.*

Speakers:

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

Organizers:

- **The Central Analytical Facility (CAF), CSIR-National Chemical Laboratory, Pune.**
- **The Skill Development Program (SDP) Center, CSIR-National Chemical Laboratory, Pune.**

WMC-PXRD Information

The online application for workshop registration will be open from 6th October to 6th November 2025. After submission, up to 50 applicants will be shortlisted based on their CVs. Details regarding registration and fee payment will be communicated to the selected candidates. The maximum number of participants (with access to the software) is 50.

Participants are required to bring their own laptops for the hands-on training sessions using crystallography software. Mac (macOS) users should ensure that a Windows emulator is installed on their system prior to the workshop.

Important Dates:

- **6th October 2025 – Start of Online application to Register for the workshop**
- **6th November 2025 – Last day to submit the online application**
- **10th November 2025 – Selected participant will be informed to pay the fees**
- **15th November 2025 – Last day to make payment.**
- **17th November 2025 – Confirmation Registration**
- **27th and 28th November 2025 – Workshop**

Registration Fees:

- **Rs. 1000/- for the Master students**
- **Rs. 2000/- for the Research Students**
- **Rs. 5000/- for the faculty members**
- **Rs. 10000/- for participants from Industry**

Email id: **ncl.sdtc.ncl@csir.res.in (+912025902641/ 7007225052)**

Registration link: https://nclsdp.ncl.res.in/Course/Default.aspx

Note:

1. Refreshments and meals will be provided on 27–28 November 2025.
2. Limited on-campus accommodation may be available for students, subject to availability. Please contact us in advance. Participants who are not allotted campus accommodation are requested to make their own arrangements.
3. Participants are expected to strictly follow the workshop schedule.
4. Attendance in all sessions is mandatory to be eligible for the participation certificate.
5. Participants must carry a valid ID card for gate entry and verification.

PROGRAMME SCHEDULE

Day 1:	27th November 2025 (Thursday)
09:30 - 10:00 AM	Inaugural Function, SSBLT Hall, CSIR-NCL, Pune
10:00 - 10:30 AM	High Tea
10:30 - 11:00 AM	Powder Xray Diffraction Method and Application
11:00 - 12:30 PM	Diffraction Geometry, Systematic Angular Errors and Calibration Procedures, Sample Preparation
12:30 - 01:00 PM	Setting up PDF-5 + and JADEPro access
01:00 - 02:00 PM	Lunch Break
02:00 - 03:30 PM	Hands- on Session: Introduction to Search/ Match Procedures with PDF-5/ Sieve+, PDF-5+ Database and Features Overview, Data mining
03:30 - 04:00 PM	Tea Break
04:00 - 05:30 PM	Phase Identification Method, Qualitative and Semi-quantitative Phase Analysis, Advanced Phase Identification (With Amorphous Component, Trace Phases), Additional Problem Solving, Q&A

Day 2 :	28th November 2025 (Friday)
09:30 - 10:00 AM	Data collection strategies for materials characterization
10:00 - 11:00 AM	Introduction to PXRD indexing
11:00 - 11:30 AM	Tea break
11:30 - 01:00 PM	Introduction to profile functions, Fitting And quantity phase analysis using Rietveld method
01:00 - 02:00 PM	Lunch break
02:00 - 03:30 PM	JADEpro hands-on sessions, JADEpro features overview, Angular Calibration (Instrument Profile Curve, IPC), Pattern indexing Using JADE
03:30 - 04:00 PM	Tea Break
04:00 - 05:00 PM	JADEpro hands-on sessions Whole Pattern Fitting (WPF) and Rietveld Refinement, Phase Identification and Quantitative Phase Analysis (Rietveld), Crystallinity Measurement, Crystallite size and Micro-strain Analysis
05:00 - 05:30 PM	Q&A, Concluding Remarks and Feedback from Participants