

CCP4 Workshop and Computational Crystallography School

October 22 – October 26, 2018

Institute of Microbial Technology, CISR, Chandigarh, India.

Course Tutors:

Santosh Panjikar, Melbourne, Aus.

Charles Ballard, CCP4, UK

Harry Powell, UK

Luis Fuentes-Montero, DLS, UK

Rob Nichols, MRC-LMB, UK

Roberto Steiner, KCL, UK

Udupi A. Ramagopal, Poornaprajna Institute of Scientific Research, Bengaluru, India

B. Gopal, Indian Institute of Science, Bengaluru, India

Eugene Krissinel, CCP4, UK

Eleanor Dodson, York, UK

Gregorz Chojnowski, EMBL, Germany

Paul Bond, York, UK

Pravinda Kumar, Indian Institute of Technology, Roorkee, India

Bichitra K. Biswal, National Institute of Immunology, New Delhi, India

Abhik Mukhopadhyay, EBI, UK

Lectures are timetabled to take place, with the afternoons dedicated to tutorials and problem solving.

Day 1 Data Collection and Processing		
9:00 – 9:15	Welcome and overview	Director, IMTECH Dr. Charles Ballard
9:15 – 10:30	Data collection	Dr. U. A. Ramagopal
	Coffee break	
11:00 – 11:45	Data processing theory	Dr. Harry Powell
11:45 – 12:30	Introduction to DIALS	Dr. Luis Fuentes-Montero
	Lunch Break	
14:00 – 15:00	Student Posters	

14:00 onwards	Data processing tutorial Problem solving	
Day 2 Still processing data		
9:00 – 9:45	Scaling of data and data quality	Dr. B. Gopal
9:45 – 10:30	Spacegroups and twinning	Dr. Charles Ballard
	Coffee Break	
11:00 – 11:45	Introduction to CCP4	Dr. Charles Ballard/Dr. Eugene Krissinel
11:45 – 12:30	Introduction to COOT	TBC
	Lunch Break	
14:00 - onwards	I2 and COOT tutorials, data processing Problem solving	
Day 3 Phasing		
9:00 – 9:45	Phasing problem	Dr. B. K. Biswal
9:45 – 10:30	Experimental Phasing	Dr. Santhosh Panjekar
	Coffee Break	
11:00 – 11:45	Manual Molecular Replacement	Prof. Eleanor Dodson
11:45 – 12:30	Automated MR	Dr. Pravindra Kumar
	Lunch Break	
14:00 – onwards	Phasing Tutorials, Problem Solving	
Day 4 Model Building and Refinement		
9:00 – 9:45	Dictionaries for refinement	Dr. Rob. Nichols

9:45 – 10:30	Refinement	Dr. Rob Nichols
	Coffee Break	
11:00 – 11:45	Arp/Warp automatic building	Dr. Gregorz Chojnowski
11:45 – 12:30	Buccaneer model building	Dr. Paul Bond
	Lunch Break	
14:00 - onwards	Model building and Refinement tutorial Problem solving	
Day 5 Ligands and analysis		
9:00 – 9:45	Automatic completion	Prof. Roberto Steiner
9:45 – 10:30	Model metrics	Dr. Abhik Mukhopadhyay/ Roberto Steiner
	Coffee Break	
11:00 – 11:45	Oligomeric states	Dr. E. Krissinel
11:45 – 12:30	Deposition	Dr. Abhik Mukhopadhyay
	Lunch Break	
14:00 – 15:30	What I learned	Students
14:00 - onwards	Problem solving Tidy up	

The lectures are open.

The tutorial and problem solving sessions are limited to participants only.

Important: This schedule is a rough indicator, and will, in all likelihood, change from day to day.