

# CCP4 workshop on Computational Crystallography

*February 15<sup>th</sup> -19<sup>th</sup> , 2010*

**All India Institute of Medical Sciences**

Course Tutors: Charles Ballard (Daresbury Laboratory)  
Randy Read (Cambridge)  
Garib Murshudov (York)  
Andrew Turnbull (Oxford)  
Phil Evans (MRC-LMB)  
Eleanor Dodson (York)  
Victor Lamzin (EMBL Hamburg)  
Gerrit Langer (EMBL, Hamburg)  
Raj Pannu (Leiden)  
Santosh Panjekar(EMBL Hamburg)

Lectures ~ 30 mins – 45mins

Lectures will be in the morning and tuotirails in the afternoon. Evening sessions will be problem solving. All tutors will be available to help with particular problems participants may have.

<b>Day 1: Data processing</b>		
9:00-9:30	All	Introduction of Students and tutors
9:30-10:00	Charles Ballard	Introduction to CCP4
10:00-10:45	Phil Evans	Data Processing with MOSLFM
10:45-11:15	Coffee Break	
11:15-12:00	Phil Evans	SCALA
12:00-12:45	Hasan	Data collection using synchrotron
<b>Day 2: Experimental Phasing and Introduction to Coot</b>		
9:00 – 9:45	Murthy	Auto indexing methods, pitfalls and cell transformations
9:00 – 9:45	Raj Pannu	Introduction to Experimental Phasing and CRANK
9:45-10:30	Santosh Panjekar	AutoRickshaw
10:30 – 11:00	Coffee	

11:00-11:45	Eleanor Dodson	Phase Improvement: Pirate and Buccaneer
11:45-12:30	Andrew Turnbull	Introduction to Coot
<b>Day 3: Molecular replacement I and experimental Phasing</b>		
9:00 - 9:40	Gopal	Practical uses of crystallography
9:45– 10:20	Eleanor Dodson	Introduction to Molecular Replacement
10:20-11:00	Shekhar C. Mande	Bioinformatics for model selection and model analysis
11:00 - 11:15	Coffee break	
11:15-11:45	Garib Murshudov	Automatic Molecular Replacement with BALBES
11:45-12:15	Charles Ballard	Automatic Molecular Replacement with MrBump
12:15-13:00	Victor Lamzin	Introduction to Arp/Warp
<b>Day 4: Molecular Replacement II and Refinement</b>		
9:00 – 9:45	Randy Read	Phaser for Molecular replacement
9:45 – 10:30	Randy Read	Phaser for combined Molecular replacement and experimental Phasing
10:30 - 10:45	Coffee break	
11:00-11:45	Garib Murshudov	Refinement with Refmac
11:45-12:15	Garib Murshudov	Data Peculiarities: Twinning and all that
<b>Day 5: Ligands and validation</b>		
9:00 - 9:30	Garib Murshudov	Ligand chemistry and description
9:30 – 10:00	Andrew Turnbull	Locating ligands with Coot
10:00-10:45	Sankaranarayanan	Crystallography and Enzymology
10:45 – 11:15	Coffee Break	
11:15-12:00	Gerrit Langer	Automatic Ligand building in ARP/warp
12:00-12:45	Andrew Turnbull	Validation with Coot

All are invited to the lectures

Tutorials and problem solving sessions are limited to invited participants only.

**Important: This schedule is a rough indicator and will, in all likelihood, change from day to day. We would update you on the schedule a day in advance.**