Macromolecular Crystallography School 2014

"From data processing to structure refinement and beyond"

April 8th -- 16th, 2014

Instituto de Física de São Carlos, USP, São Carlos, SP, Brasil

Day 1: Data processing Tuesday 8th April

08:30--09:00 *Registration*
09:00--09:10 **Welcome** E. Horjales; R. Garratt
09:10--10:00 **Data collection: considerations and compromises** (L) K. Diederichs
10:00--10:15 *Coffee Break*
10:15--11:00 **Data processing with Mosflm** (L) A. Leslie
11:00--11:45 **Scaling (SCALA , aimless and pointless, truncate)** (L) A. Leslie
11:45--12:30 **Principles of data processing with XDS** (L) K. Diederichs
12:30--13:30 *Lunch*
13:30--14:00 **Student Introduction** Students
14:30--16:00 **Mosflm/Scaling**(T) A. Leslie; with help from other available Speakers
16:00--16:30 *Coffee Break*
16:30--18:00 **XDS** (T) K. Diederichs; with help from other available Speakers
18:00--18:45 **Twinning** (L) A. Thorn
18:45--20:30 **Data Processing Problem Solving 1** (P) A. Leslie; K. Diederichs; others
20:30 *Posters installation + Cocktail*

Day 2: Data Processing & Phasing I: Introduction Wednesday 9th April

09:00--09:40 **Data quality: noise, errors, and mistakes** (L) K. Diederichs
09:40--10:30 **Data Processing Problem Solving 2** (P) A. Leslie; K. Diederichs; others
10:30--10:45 *Coffee Break*
10:45--12:30 **Data Processing Problem Solving 2** (P) A. Leslie; K. Diederichs; others
12:30--13:30 *Lunch*
13:30--14:30 **Introduction to Experimental Phasing (EP)** (L) R. Read
14:30--15:30 **Molecular Replacement (MR) Basics** (L) A. Lebedev
15:30--15:45 *Coffee Break*
15:45--16:30 **Density Modification** (L) P. Skubak
16:30--17:30 **Introduction to Coot** (L) P. Emsley
17:30--20:00 *Posters session*

Day 3: Phasing II. Basic and Automation Thursday10th April

09:00--10:00 **Automation with CRANK** (L) P. Skubak
10:00--10:30 **Basic EP tutorial** (T) P. Skubak; other available speakers
10:30--10:45 *Coffee Break*
10:45--12:30 **Basic EP tutorial ctd.** (T) P. Skubak; other available speakers
12:30--13:30 *Lunch*
13:30--14:15 **Automation I. Balbes** (L) G. Murshudov
14:15--15:00 **Automation II. MrBUMP/AMPLE** (L) R. Keegan

15:00--17:00 **Basic MR Tutorial** (T) R. Keegan; A. Lebedev
17:00--17:30 *Coffee Break*
17:30--20:30 **EP+MR Problem Solving** (P) available speakers

Day 4: Phasing III. Advanced Phasing Friday 11th April

09:00--09:45 **Phaser EP and Log Likelihood Gain maps** (L) R. Read
09:45--10:30 **EP with SHELX**(L) A. Thorn
10:30--10:45 *Coffee Break*
10:45--12:30 **EP advanced tutorial** (T) R. Read, A. Thorn; other available speakers
12:30--13:30 *Lunch*
13:30--14:15 **Phaser MR** (L) R.Read
14:15--15:00 **MR with ARCIMBOLDO** (L) I. Uson
15:00--16:15 **Phaser MR + Molrep advanced tutorial** (T) R. Read; A. Lebedev; R. Keegan
16:15--16:45 *Coffee Break*
16:45--19:15 **MR problem solving** (P) R. Read; I. Uson; A. Lebedev; R. Keegan
19:15--20:15 **"Burning questions" Session** E. Horjales; R. Garratt; available speakers

Day 5: Refinement & Model Building Saturday 12th April

09:00--10:00 **Refinement with Refmac** (L) G. Murshudov
10:00--10:45 **Refinement Tutorials** (T) G. Murshudov
10:45--11:00 *Coffee Break*
11:00--12:30 **Refinement Tutorials ctd.** (T) G. Murshudov
12:30--13:30 *Lunch*
13:30--14:30 **Building with ARP/wARP** (L) V. Lamzin
14:30--15:15 **Building with Buccaneer** (L) P. Skubak
15:15--16:15 **ARP/wARP tutorial** (T) V. Lamzin; others available speakers
16:15--16:45 *Coffee Break*
16:45--17:45 **Buccaneer/Nautilus tutorial** (T) P. Skubak; R. Keegan; others available speakers
17:45--20:15 **Model Building and Refinement/Problem Solving** (P) All available speakers

Day 6: Free Day Sunday 13th April

Free Time--(tour activity offered)

Day 7: Refinement & Model Building II Monday14th April

09:00--09:45 **Advanced Model Building with Coot** (L) P. Emsley
09:45--10:45 **Advanced Coot Tutorial** (T) P. Emsley
10:45--11:00 *Coffee Break*
11:00--11:45 **ProSMART–generating restraints for refinement** (L) R. Nichols
11:45--12:30 **ProSMART tutorial** (T) R. Nichols
12:30--13:30 *Lunch*
13:30--14:00 **Jligand/Prodrg** (L) A. Lebedev
14:00--14:45 **Ligand building with ARP/wARP** V. Lamzin

14:45--16:15 **Jligand and ARP/wARP ligand building tutorials**(T) A. Lebedev; G. Murshudov; R.Keegan
16:15--16:45 *Coffee Break*
16:45--20:30 **Problem Solving** (P) available speakers

Day 8: Finalising and Analysis of structural data Tuesday15th April

09:00--09:45 **Coot ligands and validation** (L) P. Emsley
09:45--10:00 **DIMPLE** (L) R. Keegan
10:00--10:15 **Zanuda** (L) A. Lebedev
10:15--10:45 *Coffee Break*
10:45--11:30 **CCP4 beyond structure solution** (L) E. Krissinel
11:30--12:15 **Oligomers and analysis** (L) E. Krissinel
12:15--13:30 *Lunch.*
13:30--16:00 **Problem Solving** (P) available speakers
16:00--16:30 *Coffee Break*
16:30--20:30 **Problem Solving** (P) available speakers

Day 9: 3D models from a user's perspective Wednesday16th April

09:00--10:00 **Model quality: concepts statistics**(L) A. Buschiazzo
10:00--11:00 **Structure analysis: what information can be drawn from an atomic model?** (L) A. Buschiazzo
11:00--11:15 *Coffee Break*
11:15--12:30 **"Burning questions" Session II** E. Horjales; R. Garrat; available speakers
12:30--13:30 *Lunch*
13:30--16:30 **Student's presentations**
16:30--17:00 **Final conclusions filling out meeting evaluation form** E. Horjales; R. Garrat

(L)=Lecture

(T)=Tutorial

(P)=Problem solving