

3rd OIST-CCP4 Workshop on Structure Solution

The structure of the workshop is that there are generally lectures in the morning starting from 9am, with problem solving and tutorials in the afternoon and evenings. Students are encouraged to bring their own data and problems. Monday afternoon has 2 hours set aside for “student presentations”, Wednesday afternoon is reserved for a visit to the Okinawa aquarium.

Day 1 (Mon. 2 Nov) Welcome and Data Processing		
9:20 – 9:45	Welcome to the workshop	F. Samatey/C. Ballard
9:45 – 10:30	Data Collection at Spring 8	K. Hasegawa
10:30 – 11:00	Coffee break	
11:00 – 11:45	The Diffraction Experiment	P. Evans
11:45 – 12:30	Data Processing with iMosflm	P. Evans
12:30 – 14:00	Lunch	
14:00 – 16:00	Student Stories	Students
16:00 – 16:30	Coffee	
16:30 – 18:30	Tutorial: data processing (imosflm)	
18:30 – 19:30	Dinner	
19:30 -	Tutorial and problem solving	
Day 2 (Tue. 3 Nov.) More Data Processing and Data Analysis		
9:00 – 9:45	TBC	T. Tomizaki
9:45 – 10:30	Data Processing with DIALS	D. Waterman
10:30 – 11:00	Coffee	
11:00 – 11:45	Data Scaling and Quality	P. Evans
11:45 – 12:30	Introduction to the Tools (Hands on)	C. Ballard/A.Lebedev
12:30 – 14:00	Lunch	
14:00 – 16:00	Tutorials on dataprocessing and scaling	
16:00 – 16:30	Coffee	
16:30 – 18:30	Tutorials and problem solving	
18:30 – 19:30	Dinner	
19:30 -	Tutorials and problem solving	
Day 3 (Wed. 4 Nov.) Experimental Phasing		
9:00 – 9:45	Introduction to Experimental Phasing and Density Modification	R. Pannu
9:45 – 10:30	Experimental Phasing with Shelx	S. Sammito
10:30 – 11:00	Coffee	
11:00 – 11:45	Automatic Experimental Phasing with CRANK2	R. Pannu
11:45 – 12:15	Phaser in CCP4	C. Ballard/ A.Lebedev
12:15 -	Trip to Aquarium	
Day 4 (Thur. 5 Nov.) Molecular Replacement		
9:00 – 9:45	Introduction to Molecular Replacement	A. Lebedev
9:45 – 10:30	Automatic Molecular Replacement (I) – BALBES, MRBump, AMPLE, ARCIMBOLDO	R. Keegan/G. Murshudov/M. Sammito
10:30 – 11:00	Coffee	
11:00 – 12:00	Automatic Molecular Replacement (II) – BALBES, MRBump, AMPLE,	R. Keegan/G. Murshudov/M. Sammito

	ARCIMBOLDO	
12:00 – 12:30	Combining MR and EP	R. Pannu
12:30 – 14:00	Lunch	
14:00 – 16:00	Tutorials on Experimental Phasing	
16:00 – 16:30	Coffee	
16:30 – 18:30	Tutorials on Molecular Replacement	
18:30 – 19:30	Dinner	
19:30 -	Problem solving	
Day 5 (Fri. 6 Nov.)	Model Building and Refinement	
9:00 – 9:45	Refinement with Refmac	G. Murshudov
9:45 – 10:30	Dictionary Usage in Refinement	G. Murshudov
10:30 – 11:00	Coffee	
11:00 – 11:45	Model Building with ARP/wARP	J. Pereria
11:45 – 12:30	Manual Model Building with COOT	B. Lohkamp
12:30 – 14:00	Lunch	
14:00 – 16:00	Tutorials on Model Building and Refinement	
16:00 – 16:30	Coffee	
16:30 – 18:30	Tutorials on Model Building and Refinement	
18:30 – 19:30	Dinner	
19:30 -	Problem solving	
Day 6 (Sat. 7 Nov)	Ligands, model completion and Validation	
9:00 – 9:45	Ligands in Coot	B. Lohkamp
9:45 – 10:30	Ligands in ARP/wARP	J. Pereira
10:30 – 11:00	Coffee	
11:00 – 11:45	PDB_REDO	R. Joosten
11:45 – 12:30	Is my protein and Oligomer	E. Krissinel
12:30 – 14:00	Lunch	
14:00 – 16:00	Tutorials	
16:00 – 16:30	Coffee	
16:30 – 18:30	Problem solving and Tidy up	
18:30 – 19:30	Dinner	