

**Macromolecular Crystallography School - 6th edition
MX2017**
**“Structural Biology to enhance high impact research in
health and disease”**

Institut Pasteur de Montevideo, Uruguay

November 13-23, 2017

- *Lectures will mainly be delivered in the mornings, with tutorials and hands-on practical classes in the afternoons*
- *Practical classes will be aimed at solving genuine problems brought in by the students (starting from the students' X ray diffraction data)*
- *“Burning questions” sessions as well as poster presentations (based on students' work), will reinforce active discussion times.*
- *Note that most of the computational programs to be used – many of them are widely used in the international macromolecular crystallography community – are planned to be taught directly by the program developers themselves, constituting a unique opportunity for the students.*

Color code:

Meal or Coffee break

Lecture session

Practical session

Tutorial session

Other

Monday, 13th November

Day 1: Introductory Concepts - (attempting a more homogenous theory level for all students)

08:30 – 09:00	Registration	
09:00 – 09:30	Overview of the workshop	A. Buschiazzo
09:30 – 10:30	Basic math of crystallography	A. Buschiazzo
10:30 - 11:00	Coffee	
11:00 – 12:00	Theory of X-ray diffraction	A. Buschiazzo
12:00 – 13:30	Lunch	
13:30 – 14:30	Reciprocal Space	J. Holton
14:30 – 15:30	Symmetry and Space groups	J. Holton
15:30 – 16:00	Coffee	
16:00 – 17:00	CCP4 Suite - A Roadmap	E. Krissinel
17:00 – 18:00	Discussion and questions session: based on material provided via Moodle	A. Buschiazzo / R. Keegan / J. Holton (moderators)

Tuesday, 14th November

Day 2: Data processing

09:00 – 10:00	Data collection and diffraction geometry	J. Holton
10:00 – 10:45	Data Processing with Mosflm	A. Leslie
10:45 - 11:00	Coffee	
11:00 – 11:45	Data processing with autoPROC/XDS	C. Vonrhein
11:45 – 12:30	Data processing with DIALS	J. Parkhurst
12:30 – 13:30	Lunch	
13:30 – 14:15	Scaling and Merging	A. Leslie
14:15 – 14:45	Student Introduction	All Students
14:45 – 16:00	Mosflm/Scaling Tutorial	A. Leslie
16:00 – 16:30	Coffee	
16:30 – 17:45	autoPROC/XDS Tutorial	C. Vonrhein
17:45 – 19:00	DIALS Tutorial	J. Parkhurst
19:00 – 20:30	Data processing problem solving 1	All participants
20:30 –	Welcome gathering, all invited!	

Wednesday, 15th November

Day 3: Data Processing and Phasing 1: Introduction

9:00 – 9:45	Examples of data pathologies	A. Lebedev
9:45 – 10:30	Twinning (and Pseudo-symmetry)	J. Holton
10:30 – 10:45	Coffee	
10:45 – 12:30	Data processing problem solving 3	All relevant speakers
12:30 – 13:30	Lunch	
13:30 – 14:15	Phases and the phase problem	J. Holton
14:15 – 15:00	Introduction to Experimental Phasing	R. Read
15:00 – 15:30	Introduction to Molecular Replacement	A. Lebedev
15:30 – 15:45	Coffee	
15:45 – 16:30	Introduction to CCP4i2: Project Demo	E. Krissinel
16:30 – 17:30	Introduction to Coot	P. Emsley
17:30 – 20:00	Posters & Beer session	

Thursday, 16th November

Day 4: Phasing 2: Basics

09:00 – 09:45	Expt. Phasing SHELX	I. Uson
09:45 – 10:30	Expt. Phasing with SHARP and autoSHARP	C. Vonrhein
10:30 – 10:45	Coffee	
10:45 – 11:20	SHELX Tutorial	I. Uson
11:20 – 11:55	Expt. Phasing with Phaser Tutorial	R. Read
11:55 – 12:30	SHARP/autoSHARP Tutorial	C. Vonrhein
12:30 – 13:30	Lunch	
13:30 – 14:15	Density Modification	TBA
14:15 – 15:00	MR with Phaser	R. Read
15:00 – 15:45	MR search models and assessing the solution	R. Keegan
15:45 – 16:15	Coffee	
16:15 – 17:00	MR with Phaser Tutorial	R. Read
17:00 – 20:30	Hands on problem solving	All participants

Friday, 17th November

Day 5: Phasing 3: Advanced Phasing

09:00 – 09:45	Phaser EP and Log Likelihood Gain Maps	R. Read
09:45 – 10:30	EP with ARCIMBOLDO	I. Uson
10:30 – 10:45	Coffee	
10:45 – 11:45	Advanced EP with Phaser Tutorial	R. Read
11:45 – 12:45	ARCIMBOLDO Tutorial	I. Uson
12:45 – 13:30	Lunch	
13:30 – 14:00	SHELXE for MR	I. Uson
14:00 – 15:00	CCP4mg MR Tutorial	R. Keegan
15:00 – 16:15	Hands on problem solving	All participants
16:15 – 16:30	Coffee	
16:30 – 17:30	“Burning Questions” session 1	All participants
17:30 – 20:30	Hands on problem solving	All participants

Saturday, 18th November

Day 6: Refinement and Model Building 1

09:00 – 10:00	Refinement with Global Phasing/Buster	C. Vonrhein
10:00 – 11:00	Refinement with Refmac	G. Murshudov
11:00 – 11:15	Coffee	
11:15 – 12:30	Refinement Tutorials	C. Vonrhein and G. Murshudov
12:30 – 13:30	Lunch	
13:30 – 14:30	Building with ARP/wARP	G. Chojnowski
14:30 – 15:30	Building with Buccaneer/Nautilus	TBA
15:30 – 16:00	Coffee	
16:00 – 17:00	ARP/wARP Tutorial	G. Chojnowski
17:00 – 18:00	Buccaneer/Nautilus Tutorial	TBA
18:00 – 20:30	Hands on problem solving	All participants

Sunday, 19th November

Day 7: Free Day

Free Time - (tour activity : alternative proposals by the organizers, at the expense of each attendee)

Monday, 20th November

Day 8: Refinement and Model Building 2

09:00 – 09:45	Advanced Model Building with Coot	P. Emsley
09:45 – 10:30	ProSMART & LORESTR- restraints for refinement	G. Murshudov
10:30 – 10:45	Coffee	
10:45 – 11:45	Advanced Coot Tutorial	P. Emsley
11:45 – 12:30	ProSMART & LORESTR Tutorial	G. Murshudov
12:30 – 13:30	Lunch	
13:30 – 14:00	Is the SG correct? - Zanuda	A. Lebedev
14:00 – 14:45	Ligand Building with ARP/wARP	G. Chojnowski
14:45 – 15:30	AceDrg	G. Murshudov
15:30 – 16:00	Coffee	
16:00 – 16:45	ARP/wARP ligand tutorial	G. Chojnowski
16:45 – 17:30	AceDrg tutorial	G. Murshudov
17:30 – 20:30	Hands on problem solving	All participants

Tuesday, 21st November

Day 9: Validation & Structure Analysis

09:00 – 10:00	Cryo-EM - 3D Electron Microscopy	C. Palmer
10:00 – 11:00	Refinement CryoEM structures	G. Murshudov
11:00 – 11:30	Coffee	
11:30 – 12:30	Fitting models to CryoEM maps	P. Emsley
12:30 – 13:30	Lunch	
13:30 – 16:00	CryoEM Refinement and Building Tutorial	P. Emsley & G. Murshudov & C. Palmer
16:00 – 16:30	Coffee	
16:30 – 20:30	Hands on problem solving	All participants

Wednesday, 22nd November

Day 10: Integrative Structural Biology

09:00 – 09:45	Coot Ligands and Validation	P. Emsley
09:45 – 10:30	CCP4 Beyond Structure Solution	E. Krissinel
10:30 – 11:00	Coffee	
11:00 – 11:45	Analysis of Macromolecular Complexes (PISA)	E. Krissinel
11:45 – 12:30	TBA	TBA
12:30 – 13:30	Lunch	
13:30 – 16:00	Hands on problem solving	All participants
16:00 – 16:30	Coffee	
16:30 – 20:30	Hands on problem solving	All participants

Thursday, 23rd November

Day 11: 3D models from a user's perspective

09:00 – 10:00	Model Quality: Concepts & Statistics	A. Buschiazzo
10:00 – 11:00	Structure Analysis: What information can be drawn from an atomic model	R. Garrat
11:00 – 11:30	Coffee	
11:30 – 12:30	“Burning Questions” session 2	All Participants
12:30 – 13:30	Lunch	
14:00 – 16:30	Students Presentations	All Students
16:30 – 17:00	Final conclusions & Evaluation Form	A. Buschiazzo