

Structural Biology 2.0: Integrating X-ray diffraction and modern computational tools
Institut Pasteur Montevideo - April 21 -30, 2025

	Day 1 - Monday 21		Day 2 - Tuesday 22		Day 3 - Wednesday 23		Day 4 - Thursday 24		Day 5 - Friday 25		Day 6 - Saturday 26		
08.30-09.00	Registration												08.30-09.00
09.00-09.30	Overview of the workshop	AB	About symmetry and space groups	MNL	Phases and the phase problem	BG	Introduction to Coot	LC/PE	Advanced Model Building with Coot	LC/PE	Automatic approaches for model building	JP	09.00-09.30
09.30-10.00	A historic perspective of Structural Biology: integrating crystallography, cryoEM and computational methods	AB				AI-based approaches for 3D structure prediction							MF
10.00-10.30			Data collection and diffraction geometry	BG	Model quality and validation: concepts & statistics	AB	ProSMART and other tools to generate/handle restraints	LC/PE	Coot Ligands and Validation	LC/PE	10.00-10.30		
10.30-11.00			Coffee break								Coffee break		10.30-11.00
11.00-11.30	Sequences, alignments, phylogeny: why does it matter to start with this?	MG	Coffee break		Introduction to Molecular Replacement	FT	Coffee break		Coffee break		Coffee break		11.00-11.30
11.30-12.00			Data Processing: from indexing to scaling	MNL			Why do we need to take care about biomolecules' dynamics?	MM	Advanced Coot Tutorial I	LC/PE & staff	Advanced Coot Tutorial II	LC/PE & staff	11.30-12.00
12.00-12.30	Lunch		Lunch		Lunch								Lunch
12.30-13.00							12.30-13.00						
13.00-13.30							13.00-13.30						
13.30-14.00	Basic X-ray crystallography in a nutshell	BG	autoPROC Tutorial	NL & staff	AlphaFold: advanced uses, hands-on tutorial	MF & staff	Xtallographic model refinement: why we need it? Main approaches	DL	The very basics of molecular dynamics, proteins on the move	AZ	Lunch	13.30-14.00	
14.00-14.30												14.00-14.30	
14.30-15.00	Computational approaches for structural analysis	AZ			Refine in Phenix tutorial	DL & staff	Molecular dynamics tutorial I	AZ, MM	Molecular dynamics tutorial II	AZ, MM	14.30-15.00		
15.00-15.30											15.00-15.30		
15.30-16.00	Coffee break		Coffee break		Molecular replacement and AlphaFold talk to each other	DL	Coffee break		Coffee break		Molecular dynamics tutorial II	AZ, MM	15.30-16.00
							While refining: using validation tools in Phenix						
16.00-16.30	Working roadmaps in Structural Biology: experimental and computational approaches combined all the way	AB	Hands-on problem solving. All participants; working with students' own data		Phaser in Phenix tutorial	DL & staff	Coffee break		Coffee break		Coffee break		16.00-16.30
16.30-17.00									Coot intro tutorial I		LC/PE & staff	Hands-on problem solving. All participants; working with students' own data	Hands-on problem solving. All participants; working with students' own data
17.00-17.30	Discussion and questions session: based on material provided via Moodle - All participants								17.00-17.30				
17.30-18.00									17.30-18.00				

	Day 7 - Sunday 27	Day 8 - Monday 28		Day 9 - Tuesday 29		Day 10 - Wednesday 30		
09:00-09:30	Free Time - (tour activity: alternative proposals by the organizers, at the expense of each attendee)	Empowering deep phylogenetics with structural information	MG / DM	Integrative methods in Structural Biology	JK	Structure Analysis: What information can be drawn from an atomic model	AB	09:00-09:30
09:30-10:00								09:30-10:00
10:00-10:30		Probing evolutionary relationships with 3D structures	DM	Artificial intelligence for protein design	MM	In-cell structural biology	JK	10:00-10:30
10:30-11:00								10:30-11:00
11:00-11:30		Coffee break		Coffee break		Coffee break		11:00-11:30
11:30-12:00		Structural phylogenetics: a hands-on tutorial	DM & staff	Large protein complexes: structure prediction & analysis, hands-on tutorial	DiM / JK	Engineering new protein functions for Synthetic Biology	FT	11:30-12:00
12:00-12:30								12:00-12:30
12:30-13:00		Lunch		Lunch		Lunch		12:30-13:00
13:00-13:30		Lunch		Lunch		Lunch		13:00-13:30
13:30-14:00		Lunch		Lunch		Lunch		13:30-14:00
14:00-14:30		Modern methods to study conformational ensembles	DA	Protein design hands-on tutorial	MM / FT	“Burning Questions” session - All Participants		14:00-14:30
14:30-15:00								14:30-15:00
15:00-15:30		Introduction to protein design	FT	Coffee break		Final conclusions & Evaluation Form		15:00-15:30
15:30-16:00								15:30-16:00
16:00-16:30		Coffee break		Hands-on problem solving. All participants; working with students’ own data				16:00-16:30
16:30-18:00		High-throughput AI-based structure prediction using AlphaPulldown	DiM / JK					16:30-18:00

Teaching Staff

AB, Alejandro Buschiazso (Inst Pasteur Montevideo, Uruguay)
AZ, Ari Zeida (Univ de la Republica, Uruguay)
BG, Beatriz Guimarães (Fiocruz, Brazil)
DA, Diego del Alamo (GSK Basel, Switzerland)
DiM, Dmitry Molodenski (EMBL Hamburg, Germany)
DL, Dorothee Liebschner (Lawrence Berkeley National Lab, USA)
DM, David Moi (Univ of Lausanne, Switzerland)
FT, Felipe Trajtenberg (Inst Pasteur Montevideo, Uruguay)

JK, Jan Kosinski (EMBL Hamburg, Germany)
LC, Lucrezia Catapano (Lab of Mol Biology / MRC, United Kingdom)
MF, Matheus Ferraz (NEC Bio Therapeutics, Mannheim, Germany)
MG, Martin Graña (Inst Pasteur Montevideo, Uruguay)
MM, Matias Machado (Inst Pasteur Montevideo, Uruguay)
MNL, Maria Natalia Lisa (Inst Biol Mol y Celular de Rosario, Argentina)
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PE, Paul Emsley (Lab of Mol Biology / MRC, United Kingdom)