

Macromolecular Crystallography School

MCS2019 22 - 28 April 2019

Mon. 22nd will be fully dedicated to *Fundamentals of Crystallography*, by **Dr. C. Giacovazzo**, starting at 11:00h and finishing at 18:00h (with the corresponding breaks). **Presentations:** *Symmetry - X-ray diffraction - The phase problem*

Instituto de Química-Física "Rocasolano, CSIC, Madrid (Spain), 22-28 April 2019

	Tue. 23rd	Wed. 24th	Thu. 25th	Fri. 26th	Sat. 27th	Sun. 28th
08:30-09:00h	Data collection. Considerations and compromises. Data quality. Noise, errors, and mistakes Dr. K. Diederichs	AUTO-RICKSHAW: New automated procedures for Multidata sets processing/phasing Dr. S. Panjekar	PHENIX: Structure solution Dr. P. Adams	PHENIX: Ensemble, ligand and low resolution refinement. Validation and map calculation Dr. P. Afonine	REFMAC and tools for low resolution refinement Dr. G. Murshudov	<i>Perspectives in cryo-Electron Tomography</i> Dr. A.J. McCoy
09:00-09:30h						
09:30-10:00h						
10:00-10:30h						
10:30-11:00h	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
11:00-11:30h	Principles of data processing with XDS. Serial Crystallography at Synchrotron Dr. K. Diederichs	New phasing approaches from the <i>Bari Factory</i> Dr. C. Giacovazzo	Density modification in PHENIX Dr. P. Adams	Workshop on refinement and validation in PHENIX Dr. P. Adams Dr. P. Afonine	Workshop on REFMAC Dr. G. Murshudov / Dr. R. Nicholls	Fundamentals on <i>cryo-EM</i> Dr. J.M. Carazo
11:30-12:00h						
12:00-12:30h						
12:30-13:00h	Free-time for lunch	Free-time for lunch	Free-time for lunch	Free-time for lunch	Free-time for lunch	Free-time for lunch
13:00-13:30h	Workshop on XDS Dr. K. Diederichs	Automated pipelines for protein crystallography and fragment screening Dr. J. Marquez	Workshop on MR and phasing in PHENIX Dr. P. Adams Dr. P. Afonine	Production of protein samples for crystallization and other biophysical techniques Dr. M. Solá	Refinement and manual model building using COOT Dr. P. Emsley	Sample preparation, initial screening and optimization for <i>cryo-EM</i> Dr. R. Fernández-Leiro
13:30-14:00h						
14:00-14:30h						
14:30-15:00h						
15:00-15:30h	Break	Break	Break	Break	Break	Break
15:30-16:00h						
16:00-16:30h						
16:30-17:00h						
17:00-17:30h	General overview about SHELX , PHASER and ARCIMBOLDO Dr. I. Usón	PHENIX: General introduction and general overview of automated structure solution Dr. P. Adams	General introduction to structure refinement and <i>phenix.refine</i> Dr. P. Afonine	CCP4: General introduction Dr. E. Krissinel / Dr. R. Nicholls	Workshop on COOT Dr. P. Emsley	From micrographs to atomic model: Data processing overview in <i>cryo-EM</i> Dr. R. Fernández-Leiro
17:30-18:00h						
18:00-18:30h						
18:30-19:00h	Student's presentations (*)	Student's presentations (*)	Discussions, questions and time for student's projects (*)	FIESTA !		FAREWELL
19:00-19:30h		Discussions, questions and time for student's projects (*)				
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At the end of each day, discussion sections will be moderated by Drs. J.A. Hermoso, A. Albert, I. Usón, and M. Solá, with the participation of remaining teachers.

(*) Students will be requested to prepare a short introductory presentation (max. 3 PowerPoint slides in pdf format) on their group, current stage of their project, personal motivation and/or their crystallographic problems. At the same time, they should feel free to bring their own data to discuss with the teachers and the rest of students.