

# Macromolecular Crystallography School

## MCS2018 20 - 26 May 2018

Instituto de Química-Física "Rocasolano, CSIC, Madrid (Spain), 21-26 May 2017

	Mon. 21st	Tue. 22nd	Wed. 23rd	Thr. 24th	Fri. 25th	Sat. 26th
08:30-9:00h	Production of protein samples for crystallization and other biophysical techniques  <b>Dr. M. Solá</b>	General overview about <i>SHELX</i> , <i>PHASER</i> and <i>ARCIMBOLDO</i>  <b>Dr. I. Usón</b>	<i>PHENIX</i> : General introduction and general overview of automated structure solution  <b>Dr. P. Adams</b>	General introduction to structure refinement and <i>phenix.refine</i>  <b>Dr. P. Afonine</b>	<i>REFMAC</i> and tools for low resolution refinement  <b>Dr. R. Nicholls</b>	Fundamentals on <i>cryo-EM</i>  <b>Dr. J.M. Carazo</b>
9:00-9:30h						
9:30-10:00h						
10:00-10:30h						
10:30-11:00h	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	
11:00-11:30h	Data collection. Considerations and compromises. Data quality. Noise, errors, and mistakes  <b>Dr. K. Diederichs</b>	New phasing approaches from the <i>Bari Factory</i>  <b>Dr. C. Giacovazzo</b>	<i>PHENIX</i> : Structure solution  <b>Dr. P. Adams</b>	<i>PHENIX</i> : Ensemble, ligand and low resolution refinement. Validation and map calculation  <b>Dr. P. Afonine</b>	Workshop on <i>REFMAC</i>  <b>Dr. E. Krissinel</b> <b>Dr. R. Nicholls</b>	Coffee break
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	Sample preparation, initial screening and optimization for <i>cryo-EM</i> <b>Dr. R. Fernández-Leiro</b>
13:00-13:30h						
13:30-14:00h	Principles of data processing with <i>XDS</i> . Serial Crystallography at Synchrotron  <b>Dr. K. Diederichs</b>	<i>AUTO-RICKSHAW</i> : New automated procedures for Multidata sets processing/phasing  <b>Dr. S. Panjikar</b> Break	Density modification in <i>PHENIX</i>  <b>Dr. P. Adams</b>	Workshop on refinement and validation in <i>PHENIX</i>  <b>Dr. P. Adams</b> <b>Dr. P. Afonine</b>	Refinement and manual model building using <i>COOT</i>  <b>Dr. P. Emsley</b>	Free-time for lunch
14:00-14:30h						
14:30-15:00h						
15:00-15:30h						
15:30-16:00h	Break		Break	Break	Break	From micrographs to atomic model: Data processing overview in <i>cryo-EM</i> <b>Dr. R. Fernández-Leiro</b>
16:00-16:30h	Workshop on <i>XDS</i>  <b>Dr. K. Diederichs</b>	Break	Workshop on <i>MR</i> and phasing in <i>PHENIX</i>  <b>Dr. P. Adams</b> <b>Dr. P. Afonine</b>	<i>CCP4</i> : General introduction  <b>Dr. E. Krissinel</b>	Workshop on <i>COOT</i>  <b>Dr. P. Emsley</b>	Break
16:30-17:00h						
17:00-17:30h						
17:30-18:00h						
18:00-18:30h	Student's presentations (*)	Student's presentations (*)	Discussions, questions and time for student's projects (*)			<b>Dr. A.J. McCoy</b>
18:30-19:30h		Discussions, questions and time for student's projects (*)				
...				<b>FIESTA !</b>		<b>FAREWELL</b>

At the end of each day, discussion sections will be moderated by Drs. J.A. Hermoso, A. Albert, I. Usón, M. Solá and X. Gomis-Rüth, 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.