

Macromolecular Crystallography School

MCS2017 5 - 10 May 2017

Instituto de Química-Física "Rocasolano, CSIC, Madrid (Spain), 5-10 May 2017						
	Fri. 5th	Sat. 6th	Sun. 7th	Mon. 8th	Tue. 9th	Wed. 10th
09:30-10:00h	Fundamentals, symmetry and the phase problem Dr. C. Giacovazzo	General overview about <i>SHELX</i> , <i>PHASER</i> and <i>ARCCIMBOLDO</i> Dr. I. Usón	<i>PHENIX</i> : 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	<i>REFMAC</i> and tools for low resolution refinement Dr. R. Nicholls	Data collection on <i>XFEL</i> for serial time-resolved crystallography Dr. J. Martín García
10:00-10:30h						
10:30-11:00h						
11:00-11:30h						
11:30-12:00h	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
12:00-12:30h	Synergic phase refinement Dr. C. Giacovazzo	Data collection. Considerations and compromises. Data quality. Noise, errors, and mistakes Dr. K. Diederichs	<i>PHENIX</i> : Structure solution Dr. P. Adams	<i>PHENIX</i> : Ensemble, ligand and low resolution refinement. Validation and map calculation Dr. P. Afonine	Workshop on <i>REFMAC</i> Dr. E. Krissinel Dr. R. Nicholls	Fundamentals on <i>cryo-EM</i> . Sample preparation, initial screening and optimization Dr. R. Fernández-Leiro
12:30-13:00h						
13:00-13:30h						
13:30-14:00h	Free-time for lunch	Free-time for lunch	Free-time for lunch	Free-time for lunch	Free-time for lunch	Free-time for lunch
14:00-14:30h						
14:30-15:00h						
15:00-15:30h	New phasing approaches from the <i>Bari Factory</i> Dr. C. Giacovazzo	Principles of data processing with <i>XDS</i> Dr. K. Diederichs	Density modification in <i>PHENIX</i> Dr. P. Adams	Workshop on refinement and validation in <i>PHENIX</i> Dr. P. Adams Dr. P. Afonine	Refinement and manual model building using <i>COOT</i> Dr. P. Emsley	From micrographs to atomic model. Data processing overview in <i>cryo-EM</i> Dr. R. Fernández-Leiro
15:30-16:00h						
16:00-16:30h						
16:30-17:00h						
17:00-17:30h	Production of protein samples for crystallization and other biophysical techniques Dr. M. Solá	Workshop on <i>XDS</i> Dr. K. Diederichs	Workshop on <i>MR</i> and phasing in <i>PHENIX</i> Dr. P. Adams Dr. P. Afonine	<i>CCP4</i> : General introduction Dr. E. Krissinel	Workshop on <i>COOT</i> Dr. P. Emsley	Workshop on <i>cryo-EM</i> with <i>Scipion</i> Dr. J.M. Carazo
17:30-18:00h						
18:00-18:30h	Data collection strategies at synchrotron Dr. Roeland Boer	Student's presentations (*)				
18:30-19:00h						
19:00-19:30h					FIESTA !	FAREWELL
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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.