

# Macromolecular Crystallography School

## MCS2020 13 - 18 April 2020

Instituto de Química-Física "Rocasolano, CSIC, Madrid (Spain), 13-18 April 2020

|             | Mon. 13th   | Tue. 14th   | Wed. 15th   | Thu. 16th  | Fri. 17th  | Sat. 18th   |  |
|-------------|---|---|---|--|--|---|--|
| 08:30-09:00 | Production of protein samples for crystallization and other biophysical techniques<br><br><b>Dr M. Solá</b> | Data collection. Considerations and compromises. Data quality. Noise, errors, and mistakes<br><br><b>Dr K. Diederichs</b> | New phasing approaches from the <i>Bari Factory</i><br><br><b>Dr C. Giacovazzo</b>                                  | <i>PHENIX</i> . General introduction to structure refinement and <i>phenix.refine</i><br><br><b>Dr P. Afonine</b>          | <i>REFMAC</i> and tools for low resolution refinement<br><br><b>Dr R. Nicholls</b> | Micro ED  |  |
| 09:00-09:30 |   |   |   |  |  | <b>Dr C. Millán</b>   |  |
| 09:30-10:00 |   |   |   |  |  | Fundamentals on cryo-EM   |  |
| 10:00-10:30 |   |   |   |  |  | <b>Dr C. San Martín</b>   |  |
| 10:30-11:00 | Coffee break  | Coffee break  | Coffee break  | Coffee break   | Coffee break   | Coffee break  |  |
| 11:00-11:30 | Automated pipelines for protein crystallography and fragment screening<br><br><b>Dr J. Márquez</b>          | Principles of data processing with XDS. Serial Crystallography at Synchrotron<br><br><b>Dr K. Diederichs</b>              | <i>PHENIX</i> : General introduction and general overview of automated structure solution<br><br><b>Dr P. Adams</b> | <i>PHENIX</i> : Ensemble, ligand and low-resolution refinement. Validation and map calculation<br><br><b>Dr P. Afonine</b> | Workshop on <i>REFMAC</i><br><br><b>Dr R. Nicholls</b>                             | Sample preparation, initial screening and optimization for cryo-EM    |  |
| 11:30-12:00 |   |   |   |  |  | <b>Dr R. Fernández-Leiro</b>  |  |
| 12:00-12:30 |   |   |   |  |  | <b>Dr R. Fernández-Leiro</b>  |  |
| 12:30-13:00 | Free-time for lunch   | Free-time for lunch   | Free-time for lunch   | Free-time for lunch  | Free-time for lunch  | Free-time for lunch   |  |
| 13:00-13:30 | <i>AUTO-RICKSHAW</i> : New automated procedures for processing / phasing<br><br><b>Dr. S. Panjikar</b>      | Workshop on XDS<br><br><b>Dr K. Diederichs</b>  | Density modification in <i>PHENIX</i><br><br><b>Dr P. Adams</b>   | Workshop on refinement and validation in <i>PHENIX</i><br><br><b>Dr P. Adams</b><br><b>Dr P. Afonine</b>                   | Refinement and manual model building using COOT<br><br><b>Dr P. Emsley</b>         | From micrographs to atomic model: Data processing overview in cryo-EM |  |
| 13:30-14:00 |   |   |   |  |  | <b>Dr R. Fernández-Leiro</b>  |  |
| 14:00-14:30 |   |   |   |  |  |   |  |
| 14:30-15:00 |   |   |   |  |  |   |  |
| 15:00-15:30 |   |   |   |  |  |   |  |
| 15:30-16:00 | Break   | Break   | Break   | Break  | Break  | FAREWELL  |  |
| 16:00-16:30 | Multidata sets<br><br><b>Dr S. Panjikar</b>   | General overview about <i>SHELX</i> , <i>PHASER</i> and <i>ARCIMBOLDO</i><br><br><b>Dr I. Usón</b>                        | Workshop on MR and phasing in <i>PHENIX</i><br><br><b>Dr P. Adams</b><br><b>Dr P. Afonine</b>                       | CCP4: General introduction<br><br><b>Dr E. Krissinel</b>   | Workshop on COOT<br><br><b>Dr P. Emsley</b>  |   |  |
| 16:30-17:00 |   |   |   |  |  |   |  |
| 17:00-17:30 |   |   |   |  |  |   |  |
| 17:30-18:00 | Biophysical methods in solution<br><br><b>Dr. B. Monterroso</b>   | Student's presentations (*)   | Student's presentations (*)   | FIESTA !   |  |   |  |
| 18:00-18:30 |   | Discussions, questions and time for student's projects (*)  | Discussions, questions and time for student's projects (*)  |  |  |   |  |
| 18.30-19:00 |   |   |   |  |  |   |  |
| ...         |   |   |   |  |  |   |  |
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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.