

## Agenda for the ISPyB meeting

<b>Tuesday 30<sup>th</sup> January</b>	
<b>14:00 – 14:30</b>	<b>Registration of early participants</b>
14:30 – 16:00	Visit of eBIC cryo-EM facility
16:00 – 17:30	<p style="text-align: center;"><b>Optional session on cryo-EM in ISPyB</b></p> <p><b>Pablo Conesa (CNB-CSIC):</b> Introduction to Scipion</p> <p><b>Olof Svensson (ESRF):</b> Connecting ISPyB and Scipion: current status at ESRF, and future plans</p> <p><b>Free-format discussion</b>, including informal coverage of DLS work</p>
<b>19:30 – 22:00</b>	<b>Dinner (unformatted – individual arrangements)</b>

<b>Wednesday 31<sup>st</sup> January</b>	
<b>08:30 – 09:00</b>	<b>Registration</b>
09:00 – 09:15	Welcome and admin
09:15: – 10:30	<p style="text-align: center;"><b>Updates and Status Reports from Members</b></p> <p><b>Dmitry Molodenskiy (EMBL-HH):</b> BioSAXS in ISPyB, current status</p> <p><b>Solange Delagenière (ESRF):</b> ISPyB status from ESRF</p> <p><b>Alexandra Kastner (HZB):</b> ISPyB status at HZB</p> <p><b>Roeland Boer (ALBA):</b> ISPyB status at ALBA</p> <p><b>Maurizio Polentarutti (ELETTRA):</b> ISPyB status at ELETTRA</p> <p><b>Neil Smith (DLS):</b> ISPyB status at DLS</p> <p><b>Johan Unger (MAX-IV):</b> ISPyB status at MAX-IV</p> <p><b>Gleb Bourenkov (EMBL-HH):</b> ISPyB status at EMBL-HH</p> <p><b>Andrew McCarthy (EMBL-GR):</b> ISPyB status at EMBL-GR</p> <p><b>Edward Daniel (University of Oulu):</b> ISPyB at Oulu University</p> <p><b>Clemens Vonrhein (GPhL):</b> ISPyB-related work at GPhL</p>
<b>10:30 – 11:00</b>	<b>Coffee</b>

<p>11:00 – 12:30</p> <p>15 mn</p> <p>15 mn</p> <p>15 mn</p> <p>15 mn</p> <p>15 mn</p> <p>15 mn</p>	<p style="text-align: center;"><b>Session 1: ISPyB development highlights</b></p> <p><b>Alejandro de Maria Antolinos (ESRF):</b> cryo-EM status, and evolution of EXI</p> <p><b>Timothy Spain (DLS):</b> New column and tables for X-ray PDFs describing sample and capillary geometry</p> <p><b>Aurelien Thureau (SOLEIL):</b> Implementation of membrane proteins in ISPyB-SAXS</p> <p><b>Graeme Winter (DLS):</b> Auto(re)processing at DLS and presentation of results via ISPyB/SynchWeb</p> <p><b>Roeland Boer (ALBA):</b> Data Reprocessing and User Preferences implementation in ISPyB.</p> <p><b>Clemens Vornhein (GPhL):</b> Data processing with autoPROC and STARANISO, and requirements for the full visualisation of results via ISPyB</p>
<p style="text-align: center;"><b>12:30 – 13:30</b></p>	<p style="text-align: center;"><b>Lunch at Diamond House</b></p>
<p>13:30 – 15:30</p> <p>20 mn</p> <p>20 mn</p> <p>20 mn</p> <p>20 mn</p> <p>20 mn</p> <p>15 mn</p>	<p style="text-align: center;"><b>Session 2: Evolving scientific capabilities, logistical requirements and user expectations</b></p> <p><b>Gleb Bourenkov (EMBL-HH):</b> Specific needs of Serial MX in relation to ISPyB.</p> <p><b>Andrea Pica (EMBL-GR):</b> Towards a standardised API for exchange between home labs and ISPyB.</p> <p><b>Juan Sanchez-Weatherby (DLS):</b> the VMX-i beamline and ISPyB</p> <p><b>Alice Douangamath (DLS):</b> Managing high-density pins for the XChem facility with ISPyB</p> <p><b>Rik Wierenga (OU):</b> The Instruct-ULTRA project</p> <p><b>Peter Keller (GPhL):</b> Presenting GPhL Workflow metadata in ISPyB</p>

15:30 – 16:30 15 mn 45 mn	<p align="center"><b>Session 3: The ISPyB collaboration in action</b></p> <p><b>Solange Delagenière (ESRF):</b> How to work together.</p> <p><b>Open discussion:</b> Prospects for enhancing the collaboration towards emerging requirements and expectations</p>
16:30 – 17:00	<b>Coffee</b>
16:30 – 17:00	Scientific Committee meeting // Developers' contact time
17:00 – 17:15	Presentation of Scientific Committee recommendations
17:15 – 18:00	Parallel meetings of Steering and Developers' committees
18:00 – 18:15	Presentation of Steering Committee's meeting outcome
18:15 – 18:30	Presentation of Developers' Committee's meeting outcome
18:30 – 19:00	Formulation of plans for the next 6 months and of resolutions for the medium-term future
<b>19:00 – 20:30</b>	<b>Joint dinner in Diamond House Atrium with MXCuBE participants</b>
20:30 – 21:30	<p><b>Joint discussion session with MXCuBE participants</b></p> <p>Topics to include: "Where ISPyB will (and won't) meet MXCuBE"</p>

## Agenda for the MXCuBE meeting

<b>Wednesday 31<sup>st</sup> January</b>	
<b>16:30 – 17:00</b>	<b>Coffee / Registration of early participants Sign-up for visit of Diamond MX beamlines on Friday afternoon</b>
<b>19:00 – 20:30</b>	<b>Joint dinner in Diamond House Atrium with ISPyB participants</b>
<b>20:30 – 21:30</b>	<b>Joint discussion session with ISPyB participants</b> Topics to include: "Where ISPyB will (and won't) meet MXCuBE"

<b>Thursday 1<sup>st</sup> February</b>	
<b>08:30 – 09:00</b>	<b>Registration Sign-up for visit of Diamond MX beamlines on Friday afternoon</b>
<b>09:00 – 09:15</b>	Welcome and admin
<b>09:15: – 10:30</b>	<p style="text-align: center;"><b>Updates and Status Reports from Members</b></p> <p><b>Marizio Polentarutti (Elettra):</b> MXCuBE status at Elettra</p> <p><b>Michael Hellmig (HZB):</b> MXCuBE status at HZB</p> <p><b>Johan Unge (MAX IV):</b> MXCuBE status at MAX IV)</p> <p><b>Antonia Beteva (ESRF):</b> MXCuBE status at ESRF</p> <p><b>Jan Meyer (DESY):</b> MXCuBE status at DESY</p> <p><b>Roeland Boer (ALBA):</b> MXCuBE status at ALBA</p> <p><b>Martin Savko (SOLEIL):</b> MXCuBE status at SOLEIL</p> <p><b>Gleb Bourenkov (EMBL-HH):</b> MXCuBE status at EMBL-HH</p> <p><b>Gerard Bricogne (GPhL):</b> MXCuBE-related developments at GPhL</p>
<b>10:30 – 11:00</b>	<b>Coffee</b>

11:00 – 12:30	<p style="text-align: center;"><b>Session 1: MXCuBE development highlights</b></p> <p><b>Frederik Bolmsten (MAX IV):</b> Scientific data management and integration in MXCuBE</p> <p><b>Marcus Oskarsson (ESRF):</b> MXCuBE3 release and deployment at ESRF</p> <p><b>Ivars Karpics (EMBL-HH):</b> New interactive graphical features in Qt4 MXCuBE</p> <p><b>Andrew Thompson (SOLEIL):</b> Taming the SmarGon multi-axis goniometer</p> <p><b>Rasmus Fogh (GPhL):</b> Connection and execution of GPhL workflows through MXCuBE: status report and demonstration</p>
12:30 – 13:30	Lunch at Diamond House
13:30 – 15:00	<p style="text-align: center;"><b>Session 2: Evolving scientific capabilities at beamlines and in MXCuBE</b></p> <p><b>Roeland Boer (ALBA):</b> Implementation of a dual gripper sample changer in MXCuBE</p> <p><b>Martin Savko (SOLEIL):</b> Integration of new/non-traditional data collection methods in MXCuBE</p> <p><b>Olof Svensson (ESRF):</b> Multi-crystal data collection capabilities at ESRF</p> <p><b>Gleb Bourenkov (EMBL-HH):</b> Performance issues arising in Mesh&amp;Collect-like experiments</p>
15:00 – 16:30 20 mn 20 mn 20 mn 30 mn	<p style="text-align: center;"><b>Session 3: The MXCuBE collaboration in action</b></p> <p><b>Rasmus Fogh (GPhL):</b> A hitch-hiker's guide to MXCuBE development – a discussion starter</p> <p><b>Matias Guijaro (ESRF):</b> "Less is more": a proposal for enhancing collaboration</p> <p><b>Peter Keller (GPhL):</b> Licensing MXCuBE under the LGPL</p> <p><b>Open discussion</b>, including: how to improve the integration, or the clean separation, of the main components in MX experiments: ISPyB, MXCuBE, workflows and autoprocessing.</p>
16:30 – 17:00	Coffee
17:00 – 18:30	<b>Chaired general discussion</b> , including: how to improve the integration, or the clean separation, of the main components in MX experiments: ISPyB, MXCuBE, workflows and autoprocessing.
18:30 – 20:00	Dinner in Diamond House Atrium
20:00 – 21:30	Scientific Committee meeting // Developers' contact time

<b>Friday 2<sup>nd</sup> February</b>	
09:00 – 09:30	Presentation of Scientific Committee recommendations
09:30: – 10:30	Parallel meetings of Steering and Developers' committees
<b>10:30 – 11:00</b>	<b>Coffee</b>
11:00 – 11:15	Presentation of Steering Committee's meeting outcome
11:15 – 11:30	Presentation of Developers' Committee's meeting outcome
11:30 – 12:30	Formulation of plans for the next 6 months and of resolutions for the medium-term future
<b>12:30 – 14:00</b>	<b>Lunch at the Diamond canteen</b>
14:00 – 15:30	Guided visit of Diamond MX beamlines (for those who signed up)
14:00 – 17:00	Free-format contact and activity time.