

COSMX2012

Training course in Complementary Optical Spectroscopies in Macromolecular Crystallography

Programme

08:30 - 08:45 Registration in the ESRF entrance hall

Wednesday, Sep. 19th - Lectures

Venue: room MD-1-21

Session: General introduction to complementary spectroscopies

Chair: D. de Sanctis

09:00 - 09:10 Welcome by Bauke Dijkstra (Director of Research of the ESRF)

09:10 - 09:50 Why using complementary spectroscopies? (Antoine Royant, IBS/ESRF)

09:50 - 10:30 Raman-assisted crystallography (RaX): principles and applications
(Philippe Carpentier, ESRF)

10:30 - 10:50 Coffee break in room MD-1-21

Session: Instrumentation & sampling strategies

Chair: A. Royant

10:50 - 11:30 Various instrumentation setups for complementary optical spectroscopies at the
ESRF (David von Stetten, ESRF)

11:30 - 12:10 Making the most of multiple methods (at Diamond and beyond) (Robin Owen, DLS)

12:10 - 12:50 SLS SpectroLab multi-mode spectroscopy - on-axis integration and sampling
geometries (Martin Fuchs, SLS)

12:50 - 14:00 Lunch at the ESRF/ILL restaurant

Session: Radiation damage

Chair: R. Owen

14:00 - 14:40 Radiation damage modeling and data collection strategy (Sasha Popov, ESRF)

14:40 - 15:20 Radiation damage - online UV/vis absorption applications (Martin Weik, IBS/ESRF)

15:20 - 15:40 Coffee break in room MD-1-21

Session: Specific technical aspects

Chair: M. Fuchs

15:40 - 16:20 UV and X-ray damage for experimental phasing (Max Nanao, EMBL)

16:20 - 17:00 UV-RIP and complementary spectroscopy on ID29 (Daniele de Sanctis, ESRF)

17:00 - 17:40 Spectroscopic data analysis (Florian Dworkowski, SLS)

19:00 - 20:30 Dinner at the ESRF/ILL restaurant

Thursday, Sep. 20th - Practicals

Venues: ID14-eh1, ID29, ID29S, ID23

Practicals - Participants will be divided in 4 groups

P1: On-line UV-vis absorption / fluorescence microspectrophotometry (beamline ID14-eh1, Philippe Carpentier & Martin Weik)

P2: On-line Raman spectroscopy (beamline ID29, Daniele de Sanctis & David von Stetten)

P3: Off-line UV-vis absorption / fluorescence microspectrophotometry (ID29S-Cryobench, Antoine Royant & Florian Dworkowski)

P4: UV-RIP phasing (beamline ID23, Max Nanao)

<u>Locations</u>	<u>ID14-eh1</u>	<u>ID29</u>	<u>ID29S</u>	<u>ID23</u>
08:30 - 10:15	Group 1	Group 2	Group 3	Group 4
<i>10:15 - 10:45</i>	<i>Coffee break in room 18-1-11</i>			
10:45 - 12:30	Group 2	Group 3	Group 4	Group 1
<i>12:30 - 14:00</i>	<i>Lunch at the ESRF/ILL restaurant</i>			
14:00 - 15:45	Group 3	Group 4	Group 1	Group 2
<i>15:45 - 16:15</i>	<i>Coffee break in room 18-1-11</i>			
16:15 - 18:00	Group 4	Group 1	Group 2	Group 3
<i>18:30 - 21:00</i>	<i>Poster Session and Cocktail Dinatoire on the ESRF mezzanine</i>			

Friday, Sep. 21st - Lectures: examples

Venue: room MD-1-21

Session: Examples I

Chair: M. Nanao

09:00 - 09:40 Resonance Raman and UV-vis absorption to fingerprint ligand and redox states in heme proteins (Mike Hough, U. of Essex)

09:40 - 10:20 Dynamic crystallography: combining single crystal spectroscopy and X-ray crystallography to study time-resolved changes (Arwen Pearson, U. of Leeds)

10:20 - 10:40 *Coffee break in room MD-1-21*

Session: Examples II

Chair: P. Carpentier

10:40 - 11:20 Mechanisms underlying dioxygen reduction in laccases (Isabel Bento, ITQB)

11:20 - 12:00 Concluding remarks

12:00 - 13:00 *Farewell buffet lunch in room MD-1-21*

End of course