National Hellenic Research Foundation (NHRF)
Athens, April 5th -10th 2014

Strategic pipeline planning: from sample preparation to 3D structure determination with bio SAXS and other biophysical technique

PROGRAMME

SATURDAY 05.04.2014

	Structural Biology in Europe 2014 onwards State-of-the-art facilities for cutting-edge research in Europe ○ ESFRI actions Instruct – a success story (more info in →) ○ Large scale facilities in Europe & ○ Opportunities for transnational access
08:45 – 09:30	***Registration***
09:30 – 10:00	Welcome remarks / Introduction NHRF, HeCrA
10:00 – 10:40	**Integrated structural biology. The Instruct vision and some examples** **Prof. DAVID STUART**, FRS, INSTRUCT coordinator Professor of Structural Biology, Director of the Division of Structural Biology, MRC Research Professor *The Nuffield Department of Clinical Medicine, University of Oxford, UK*
10:40 – 11:20	**Cryo-EM structural analysis of macromolecules: The emergence of a new universe of possibilities thanks to automation and new electron detectors.** **Prof. JOSE-MARIA CARAZO**, Director of INSTRUCT image processing centre Head of Biocomputing Unit, CNB and Node Director of Spanish National Bioinformatics Institute *National Centre for Biotechnology (CNB)-CSIC, Madrid, Spain*
11:20 – 12:00	**Integrative use of synchrotron X-ray scattering with other structural techniques to characterize biological macromolecules and complexes.** **Dr DMITRI SVERGUN**, BIOSTRUCT-X coordinator, SAXS Group leader *EMBL-Hamburg Unit, Germany*
12:00 – 12:30	***Coffee break***
12:30 – 13:10	**Structural Biology at Diamond Light Source –An integrated approach** **Dr MARTIN WALSH**, Life Science coordinator *Diamond Light Source, Oxford, UK*
13:10 – 13:50	**Facilities for macromolecular crystallography at HZB-BESSY II in Berlin** **Dr UWE MÜLLER**, Team Leader, Macromolecular Crystallography Group *Institute Soft Matter and Functional Materials* *HZB-Bessy II, Berlin, Germany*

13:50 – 14:15	**Big Data management in Structural Biology** **Prof YANNIS IOANNIDIS**, President & General Director *"Athena"- Research and Innovation Centre in Information Communication and Knowledge technology, Athens, Greece*
14:15 – 15:10	***Lunch break***
	Perspectives in structural biology (part I) An overview of additional main stream methods for structural biology ○ NMR, X-ray imaging, X-ray crystallography
15:10 – 15:50	**Cryo Soft X-ray tomography: an overview** **Dr EVA PEREIRO**, Scientist Responsible of the Soft X-ray microscopy beamline at ALBA Light Source *ALBA Synchrotron facility, Barcelona, Spain*
15:50 – 16:30	**From Single Proteins to Cellular Function: the Contribution of CERM-NMR Infrastructure** **Dr SIMONE CIOFI-BAFFONI**, Faculty member of Magnetic Resonance Center and Department of Chemistry *CERM, Florence, Italy*
16:30 – 17:10	**Synchrotron based fragment screening** **Dr UWE MUELLER**, Team Leader, Macromolecular Crystallography Group Institute Soft Matter and Functional Materials *HZB-Bessy II, Berlin, Germany*
17:10 – 17:30	***Coffee break***
	Career development session: Lessons learnt from mobility of young scientists & prospects in the frame of Horizon 2020
17:30 – 17:45	**Bottlenecks and opportunities of researchers' mobility** **Dr ALEXANDROS SAVVAIDIS,** President of MCFA-Hellas *MCFA-Hellas & Institute of Engineering Seismology and Earthquake Engineering, Thessaloniki, Greece*
	Funding opportunities under Horizon 2020
17:45 – 18:00	**MARIA SAMARA**, Project officer National Contact Point for Horizon-2020 on Marie Sklodowska-Curie Actions
18:00 – 18:15	**GEORGIA TZENOU**, Coordinator of Enterprise Europe Network-Hellas, National Contact Point for Horizon 2020-RIs & Access to Finance Coordinator of EU projects & networks
18:15 – 18:30	**CRISTINA PASCUAL**, National Contact Point for Horizon 2020 on the ERC Programme *National Documentation Center/NHRF, Athens Greece*

SUNDAY 06.04.2014

	Perspectives in Structural Biology (part II) An overview of additional main stream methods for structural biology
10:00 – 10:45	**High throughput cloning and expression of recombinant proteins for structural biology** **Dr RAY OWENS**, Head of the Oxford Protein Production Facility (OPPF) & Nuffield Department of Medicine Senior Fellow *OPPF- University of Oxford, UK*
10:45 – 11:30	**3D Protein Structure Determination and protein-protein interaction by NMR** **Dr SIMONE CIOFI-BAFFONI**, Faculty member of Magnetic Resonance Center and Department of Chemistry *CERM, Florence, Italy*

11:30 – 12:15	**Macromolecular Crystallography on the low-emittance synchrotron PETRA III** **Dr THOMAS SCHNEIDER**, Coordinator MX@PETRA3, Group Leader *EMBL-Hamburg Unit, Germany*
12:15 – 12:45	***Coffee break***
12:45 – 13:15	**Investigating the effect of structural changes *in vivo* through metabolic flux analysis and metabolomics** **Dr MARIA KLAPA**, Head of Metabolic Engineering & Systems Biology Lab *Institute of Chemical Engineering Sciences (ICE-HT), FORTH-Patras, Greece*
13:15 – 13:45	**Human and Animal Model Tissue Samples as High Quality Protein Sources for Structural and Proteomics Studies** **Dr LASKARINA-MARIA KOROU**, Doctor of Veterinary Medicine *Laboratory for Experimental Surgery and Surgical Research "N.S. Christeas", Medical School University of Athens, Greece*
13:45 – 14:40	***Lunch break***
	Users' perspective
14:40 – 15:00	**Structural Biology by NMR: Knowledge transfer from EU RIs to Greece** **Assoc. Prof. GEORGIOS SPYROULIAS** *Department of Pharmacy, University of Patras, Greece*
15:00 – 17:00	Presentations by the participants on their work and motivation to attend the workshop
17:00 – 17:15	***Coffee break***
17:15 – 19:00	*Case studies – participants will form groups and discuss* *Brain storming and problem solving along with the tutors*
20:30	***Dinner***

MONDAY 07.04.2014

	Sample preparation (part I) What is needed for a "successful" sample preparation ○ Key objectives and how to benchmark the success of a strategy ○ Bottlenecks and trouble shooting ○ Decision making on method selection for 3D structure determination
09:15 – 10:00	**Hybrid Structural Biology: recent examples and future perspectives** **Dr MATTHIAS WILMANNS**, Head of EMBL-Hamburg Unit *EMBL-Hamburg Unit, Germany*
10:00 – 10:45	**Construct design and protein expression** **Dr ROB MEIJERS**, High Throughput Crystallization facility, Team Leader *EMBL-Hamburg Unit, Germany*
10:45 – 11:15	***Coffee break***
11:15 – 12:00	**Quality control and protein optimization** **Dr ROB MEIJERS**, High Throughput Crystallization facility, Team Leader *EMBL-Hamburg Unit, Germany*
12:00 – 12:45	**The power of structural hybridomics** **Prof. Dr SAVVAS SAVVIDES**, Head of Unit for Structural Biology and Biophysics *Lab. for Protein Biochemistry & Biomolecular Engineering (L-ProBE), Ghent University, Belgium*
12:45 – 13:05	**Users' perspective**

12:45 – 13:05	**Integrated molecular and structural biology approaches towards unraveling the unique role of desmin's head domain in intermediate filament structure and function** **Dr MANOLIS MAVROIDIS** Division of Cell Biology, *Biomedical Research Foundation, Academy of Athens*
13:05 – 13:25	**Sensing biomolecular interactions in real time by SPR: principles, examples and caveats".** **Assist. Prof. PAVLOS (BOGOS) AGIANIAN**, *Molecular biology & Genetics Department, Demokritus University of Thrace, Alexandroupolis, Greece*
13:25 – 14:15	***Lunch break***
14:15 – 15:45	Presentations by the participants on their work and motivation to attend the workshop
15:45 – 16:05	***Coffee break***
16:05 – 18:00	*Case studies – participants will form groups and discuss* *Brain storming and problem solving along with the tutors*

TUESDAY 08.04.2014

	Bio Small Angle X-ray Scattering (SAXS) (part I) ○ Bio SAXS at the forefront of structural biology ○ Basic principles of small angle X-ray scattering ○ Supporting biophysical techniques (e.g. Dynamic Light Scattering) ○ SAXS data analysis software *In vitro* and *in silico* SAXS challenges
09:00 – 09:45	**Basics of SAXS by macromolecular solutions** **Dr DMITRI SVERGUN**, BIOSTRUCT-X coordinator, SAXS Group leader *EMBL-Hamburg Unit, Germany*
09:45 – 10:30	**It is worth the investment!** **Strategies to significantly improve SAXS data quality with a few additional biochemical/ biophysical steps.** **Dr MELISSA (Ann) GRAEWERT** *EMBL-Hamburg Unit, Germany*
10:30 – 11:00	***Coffee break***
11:00 – 11:45	***Ab initio* shape determination** **Dr DMITRI SVERGUN**, BIOSTRUCT-X coordinator, SAXS Group leader *EMBL-Hamburg Unit, Germany*
	Users' perspective
11:45 – 12:05	**Protein aggregation** **Dr CONSTANTINOS VORGIAS, Professor of Biochemistry** *Department of Biochemistry & Molecular Biology, Faculty of Biology, School of Science, National & Kapodistrian University of Athens, Greece*
12:05 – 12:25	**Multiangle dynamic light scattering: the method and some applications to protein solutions** **Dr STERGIOS PISPAS** *Institute of Theoretical and Physical Chemistry, NHRF, Athens, Greece*
12:25 – 13:25	BioSAXS - Practical session
13:25 – 14:15	***Lunch break***
14:15 – 16:00	BioSAXS - Practical session
16:00 – 16:20	***Coffee break***
16:20 – 18:00	BioSAXS - Practical session

WEDNESDAY 09.04.2014

	Bio Small Angle X-ray Scattering (SAXS) (part II)
09:00 – 10:30	**The use of high-resolution structures for SAXS-based modelling.** **Dr MAXIM PETOUKHOV** *EMBL-Hamburg Unit, Germany*
10:30 – 11:00	***Coffee break***
11:00 – 11:45	**Characterization of mixtures & intermolecular interactions by SAXS** **Dr PETR KONAREV** *EMBL-Hamburg Unit, Germany*
11:45 – 13:45	BioSAXS - Practical session
13:45 – 14:30	***Lunch break***
14:30 – 16:30	BioSAXS - Practical session
17:00 – 17:20	***Coffee break***
16:00 – 17:00	Questions and answers session
17:20 – 18:00	Presentations by the participants on their work and motivation to attend the workshop

THURSDAY 10.04.2014

	Sample preparation (part II) What is needed for a "successful" sample preparation ○ Key objectives and how to benchmark the success of a strategy ○ Bottlenecks and troubleshooting ○ Decision making on method selection for 3D structure determination
09:00 – 09:45	**Highways, biways and detours in crystallization** **Prof. TERESE BERGFORS,** *Department of Cell and Molecular Biology, Biomedical Centre, Uppsala University, Sweden*
09:45 – 10:30	**Seeding Strategies for "Random" Crystal Screening and Crystal Optimization** **Dr PATRICK SHAW STEWART** *Douglas Instruments Ltd, UK*
10:30 – 12:00	Protein crystallization practical session
12:00 – 12:30	***Coffee break***
12:30 – 13:00	**New approaches to the search for crystallisation conditions and to crystal optimisation** **Dr EMMANUEL SARIDAKIS** *Institute of Physical Chemistry NCSR- "Demokritos", Athens, Greece*
	Users' perspective
13:00 – 13:30	**From molten globules to bio-inspired materials** **Prof. MIKE KOKKINIDIS** *University of Crete/Institute of Molecular Biology & Biotechnology, FORTH-Heraklion, Greece*
13:30 – 14:00	**The Thermodynamic Stability of Proteins: Structure-based Issues and Interactions** **Dr GEORGE NOUNESIS**, Deputy Director *Institute of Radioisotopes & Radiodiagnostic Products, NCSR- "Demokritos", Athens, Greece*

14:00 – 14:30	**Assessing protein integrity, stability and interactions by spectroscopy-based methods** **Dr Prof. ANASTASIA S. POLITOU**, Assist. Prof. of Biological Chemistry *Medical School, University of Ioannina/Biomedical Research Division-FORTH-Ioannina, Greece*
14:30 – 15:15	***Lunch break***
14:00 – 15:45	Case studies – participants will form groups and discuss Brain storming and problem solving along with the tutors
15:15 – 15:45	***Coffee break***
15:45 – 18:00	Questions and answers session
18:00 – 18:15	**Closing remarks**