



National Hellenic Research Foundation (NHRF)
Athens, February 14th -17th 2016

Dilemmas in structural biology: selection & integration of methods

PROGRAMME

SUNDAY 14.02.2016

<i>Seminar room</i>	Session title
08:45 – 09:15	Registration
09:15 – 09:20	Welcome remarks / Introduction
09:20 – 10:00	Crystallographic Fragment Screening at the HZB-MX Beamlines MANFRED WEISS <i>Helmholtz-Zentrum Berlin für Materialien und Energie Macromolecular Crystallography (HZB-MX), Bessy II, Berlin, Germany</i>
10:00 – 10:40	I. Microseed matrix-screening (rMMS): introduction, theory, practice and a new technique for membrane protein crystallization in LCP
10:40 – 11:20	II. Setting up rMMS experiments by hand or with a robot – practical session PATRICK SHAW STEWART <i>Douglas Instruments Ltd, UK</i>
11:20 – 11:40	Coffee break
11:40 – 12:20	Protein structures for drug discovery: homologous proteins as seeds in crystallization Areej AbuHammad <i>Faculty of Pharmacy, University of Jordan, Jordan</i>
12:20 – 12:40	Structure-based drug design: Hits discovery through crystallography screening of extracts from natural resources Demetres D. Leonidas <i>Dept. of Biochemistry and Biotechnology, University of Thessaly, Greece</i>
12:40 – 13:10	The Power of Powder: Protein-based drug screening & Environmental Response of Protein Crystals using XRPD IRENE MARGIOLAKI <i>Department of Biology, University of Patras, Greece</i>
13:10 – 13:40	Introduction to SAS Model Determination DANIEL FRANKE <i>European Molecular Biology Laboratory (EMBL)-Hamburg Unit, Germany</i>
13:40 – 14:30	Lunch break
14:30 – 16:00	SAXS practical
16:00 – 16:30	Coffee break
16:30 – 18:30	Presentations by the participants on their work and motivation to attend the workshop (12 x 10min)

MONDAY 15.02.2016

Amphitheatre
L. Zervas

Challenges in Structural Biology throughout the years

- 09:00 – 09:30 **X-ray Crystallography: 100 years after**
IRENE MAVRIDIS
Institute of Nanoscience and Nanotechnology, National Center for Scientific Research "Demokritos", Athens, Greece
- 09:30 – 10:10 **Cryo-EM of macromolecules: From sample to atomic structure**
CHRISTOS SAVVA
Electron Microscopy Facility, MRC Laboratory of Molecular Biology, Cambridge Biomedical Council, UK
- 10:10 – 10:50 **Neutron crystallography – prospects at the European Spallation Source**
ESKO OKSANEN
European Spallation Source, Lund, Sweden

10:50 – 11:20 **Coffee break**

Amphitheatre
L. Zervas

Structural Biology Data Management Omics – Metabolic Engineering & Systems Biology

- 11:20 – 12:00 **The Small Angle Scattering Biological Data Bank, SASBDB**
CY M. JEFFRIES
European Molecular Biology Laboratory (EMBL)-Hamburg Unit, Germany
- 12:00 – 12:30 **Title**
Christos OUZOUNIS
Chemical Process & Energy Resources Institute (CPERI), Centre for Research & Technology Hellas (CERTH), Thessaloniki, Greece
- 12:30 – 13:00 **Metabolomics vs metabolic flux analysis as a cell culture monitoring tool in pharmaceutical industry**
MARIA KLAPA
Metabolic Engineering & Systems Biology Lab, Institute of Chemical Engineering Sciences (ICE-HT), FORTH-Patras, Greece
- 13:00 – 13:30 **Emerging information technologies and infrastructures relevant to Structural Biology: Experiences from the Biological Magnetic Resonance Data Bank (BMRB)**
YANNIS IOANNIDIS
"Athena"- Research and Innovation Centre in Information Communication and Knowledge technology, Athens, Greece

13:30 – 14:15 **Lunch break**

Seminar room

High throughput Protein Crystallization

- 14:15 – 15:30 **Sample optimization and quality control on challenging samples**
- 15:30 – 16:30 **The axon guidance cue Netrin-1 switches receptors to change cell fate**
ROB MEIJERS
Sample Preparation & Characterization (SPC) facility, European Molecular Biology Laboratory (EMBL)-Hamburg Unit, Germany

16:30 – 16:45 **Coffee break**

Amphitheatre
L. Zervas

16:45 – 18:05 Presentations by the participants (8 x 10min)

20:30 **Dinner**

TUESDAY 16.02.2016

Seminar room

Sample preparation, Integrated approaches, iNEXT

- 09:00 – 09:30 **Engineering *E. coli* for high-level production of eukaryotic integral membrane proteins**
GEORGIOS SKRETAS
Institute of Biology, Medicinal Chemistry & Biotechnology, National Hellenic Research Foundation (NHRF) Athens, Greece
- 09:30 – 10:00 **Eukaryotic recombinant protein expression systems and their applications to structural immunology**
STRATOS STRATIKOS
Institute for Nuclear & Radiological Sciences & Technology, Energy & Safety, National Centre for Scientific Res. "Demokritos" Athens, Greece
- 10:00 – 11:00 **iNEXT, NMR and gene regulation**
ROLF BOELENS
Bijvoet Center for Biomolecular Research, Utrecht University, The Netherlands
- 11:00 – 11:30 **Coffee break**
- 11:30 – 12:00 **Novel synthetic neurosteroidal agonists of Nerve Growth Factor (NGF) receptors: biomolecular NMR studies and *in silico* considerations**
MARIA ZERVOU
Institute of Biology, Medicinal Chemistry & Biotechnology, National Hellenic Research Foundation (NHRF), Athens, Greece
- 12:00 – 12:30 ***In situ* diffraction as complementary technique in structure solution**
ANASTASSIOS C. PAPAGEORGIOU
Turku Centre for Biotechnology, University of Turku and Åbo Akademi University, Finland.
- 12:30 – 13:00 **Strategies and dilemmas in protein purification**
DIMITRIS HATZINIKOLAOU
Department of Biology, University of Athens, Greece
- 13:00 – 14:00 **Lunch break**
- 14:00 – 14:40 **Crystal structure of natural and synthetic peptides containing α -aminoisobutyric acid**
KYRIAKOS PETRATOS
Institute of Molecular Biology & Biotechnology, Foundation for Research and Technology (IMBB-FORTH) Crete, Greece
- 14:40 – 15:10 **Practical suggestions to overcome common problems in macromolecular crystallography**
PETROS GIASTAS
Hellenic Pasteur Institute, Athens, Greece
- 15:10 – 16:30 **Practical on 3D structure determination from MX data**
MAGDA CHEGKAZI
European Molecular Biology (EMBL)-Hamburg Unit, Germany
MARIA DIMAROGONA
School of Chem. Eng. National Technical Univ. of Athens (NTUA) Greece
- 16:30 – 17:00 **Coffee break**
- 17:00 – 17:50 Presentations by the participants (5 x 10min)

WEDNESDAY 17.02.2015

Seminar room **Biophysical & Computational approaches in Structural Biology**

09:00 – 09:30 **Interaction of lysozyme with polymeric nanostructures: Strategies for immobilization of enzymes?**

STERGIOS PISPAS

Institute of Theoretical & Physical Chemistry, National Hellenic Research Foundation (NHRF) Athens, Greece

09:30 – 10:00 **Design and structure of bimodal carriers for binding of drugs and cell internalization**

KONSTANTINA YANNAKOPOULOU

Institute of Nanoscience and Nanotechnology, National Center for Scientific Research "Demokritos", Athens, Greece

10:00 – 10:30 **Identifying key molecules using animal models and -omics methodologies**

IOANNIS VLACHOS

*Laboratory for Experimental Surgery and Surgical Research «N.S. Christeas», Medical School of Athens, University of Athens
DIANA-Lab, Department of Computer & Communication Engineering, University of Thessaly / Hellenic Pasteur Institute, Greece*

10:30 – 11:00 **Introduction to drug discovery**

EMMANUEL MIKROS

Faculty of Pharmacy, University of Athens, Greece

11:00 – 11:30 **Coffee break**

11:30 – 12:00 **Towards the design of novel inhibitors using evolutionary, structure-based virtual screening and protein-ligand co-complex X-ray crystallography. The PG N-deacetylase paradigm**

ELIAS ELIOPOULOS

Genetics Laboratory, Agricultural University of Athens, Greece

12:00 – 12:30 **Computational methods in the study of enzyme function: The case of β -lactamases**

STATHIS D. KOTSAKIS

Laboratory of Bacteriology, Hellenic Pasteur Institute, Athens, Greece

12:30 – 13:00 **Practical Considerations in Structure-Based Virtual Screening**

ATHANASIOS PAPAKYRIAKOU

Institute of Nanoscience and Nanotechnology, National Center for Scientific Research "Demokritos" Athens, Greece

13:00 – 14:00 **Lunch break**

Seminar room **Career development session: prospects for the young scientists in the frame of Horizon 2020**

14:00 – 14:30 **Funding opportunities under the calls of the Marie Skłodowska Curie Actions**

MARIA SAMARA

National Documentation Centre, National Hellenic Research Foundation (NHRF) Athens, Greece

14:30 – 15:00 **ERC the Programme of Excellence**

CRISTINA PASCUAL

National Documentation Centre, National Hellenic Research Foundation (NHRF) Athens, Greece

15:00 – 15:10 *Closing remarks*