



**National Hellenic Research Foundation,
Institute of Organic & Pharmaceutical Chemistry**

**Structure– & Computer– Aided Design Workshop:
Bioactive Molecules & Materials**

7 – 11 November, 2011

MONDAY, 7 November 2011		
9.00 – 10.15	Registration	
10.15 – 10.30	Welcome & opening remarks	
10.30 – 11.15	Lucia Banci Structural-based design of new vaccines: towards Structural Vaccinology	
11.15 – 12.00	Matthias Wilmanns How bioactive nitrogen incorporation in metabolites is regulated in glutamine amidotransferases	
12.00 – 12.30	Coffee break	
12.30 – 13.15	Jose Maria Carazo Challenges in Three-dimensional Electron Microscopy	
13.15 – 14.00	Sarah Butcher Discovery of new drug targets by cryo-electron tomography and image reconstruction	
14.00 – 15.00	Lunch break & Poster session	
15.00 – 15.45	Georgios Spyroulias NMR Structural Biology at University of Patras & The SEE-DRUG project	
15.45 – 16:45	Practical session virtual screening Manos Mikros (Group A)	Instruct-ELLAS meeting of current and potential users
16.45 – 17.15	Coffee break	
17.15 - 18.15	Practical session virtual screening Manos Mikros (Group B)	Instruct-ELLAS meeting of current and potential users

TUESDAY, 8 November			
09.30 – 10.15	Darren Hart ESPRIT: Library-based construct screening for difficult-to-express proteins		
10.15 – 11.00	Patrick Shaw Stewart (Douglas Instruments) Random micro-seeding: a theoretical and practical exploration of seed stability and seeding techniques for successful protein crystallization		
11.00 – 11.30	Coffee break		
11.30 – 12.15	Elsbeth Garman From hot to cool and more for less.		
12.15 – 13.00	George Kontopidis Optimise outcome from ligand soaking: consideration and results		
13.00 – 14.00	Lunch break & Poster session		
14.00 – 15.30	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 50%; padding: 5px;">Practical session Robotic Crystallization Patrick Shaw Stewart (Group A)</td> <td style="width: 50%; padding: 5px;">Practical session X-ray data collection Elsbeth Garman (Group B)</td> </tr> </table>	Practical session Robotic Crystallization Patrick Shaw Stewart (Group A)	Practical session X-ray data collection Elsbeth Garman (Group B)
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15.30 – 16.00	Coffee Break		
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19.00	Reception Dinner		

WEDNESDAY, 9 November	
9.30 – 10.15	Thomas Steinbrecher Free Energy Calculations in Ligand Protein-Binding Studies
10.15 – 11.00	Rod Hubbard Structure and Fragment-Based Ligand Discovery Methods and Applications
11.00 – 11.30	Coffee break
11.30 – 12.15	Michael Szardenings Exploring Proteins with Peptide Phage Display
12.15 – 13.00	Masha Niv Computational Design of Protein Kinase-Inhibiting Peptides and Peptidomimetics
13.00 – 14.00	Lunch break & Poster session
14.00 – 14.45	Elias Eliopoulos Designing inhibitors for Rheumatoid arthritis. A "hit to lead" approach
14.45 – 15.15	Joe Hayes Molecular modeling targeting glycogenolysis control

THURSDAY, 10 November	
09.30 – 10.15	Josep Maria Luis Exploring the exohedral reactivity and selective encapsulation of fullerene compounds
10.15 – 11.00	Giannis Papaefstathiou Assembling Polynuclear Metal Complexes into Supramolecular Architectures
11.00 – 11.30	Coffee break
11.30 – 12.15	Zoe Cournia Nanoparticle-lipid bilayer interactions: Insights from Molecular Dynamics and free energy calculations
12.15 – 12.45	Haralambos Tzoupis Binding of Novel Fullerene Inhibitors to HIV-1 Protease: Insight through Molecular Dynamics and Molecular Mechanics Poisson–Boltzmann Surface Area Calculations
12.45 – 13.45	Lunch break & Poster session
13.45 – 14.30	Thomas Mavromoustakos Rational Drug Design
14.30 – 15.15	Georgios Leonis Molecular Dynamics and Binding Free Energy Calculations in Protein Systems: Advancements on Hypertension Treatment
15.15 – 16.00	Christiana Mitsopoulou Dithiolene Complexes: Properties and applications in material science and bioinorganic/biological chemistry.
16.00 – 16.30	Coffee Break
16.30– 18.30	Practical session: Desmond software <i>Interactive Session</i> Istvan Kolossvary (Group A)

FRIDAY, 11 November	
09.30 – 11.30	Practical session: Desmond software <i>Interactive Session</i> Istvan Kolossvary (Group B)
11.30 – 12.00	Coffee break
12.00 – 12.45	Kostas Iatrou Odorant binding protein-based screens for discovery of natural compounds effecting mosquito olfactory responses
12.45 – 13.30	Pavlos Agianian Direct insecticide binding to malaria mosquito GSTs
13.30 – 14.30	Lunch break & Poster session
14.30 – 15.15	Joanna Andreadou Novel targets as pharmacological tools for the development of new therapeutic strategies for the coronary heart disease
15.15 – 16.00	Andreas Papapetropoulos Hydrogen sulfide a novel signalling molecule in mammalian cells
16.30 – 17.15	Ioannis Emiris Geometric algorithms for modeling molecular structure
17.15 – 17.30	Closing remarks

Supported by:



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