



The International Conference HeCrA-HSCBB-16

The Hellenic Crystallographic Association &
The Hellenic Society for Computational Biology and Bioinformatics

October 7-9, 2016

Agricultural University of Athens

Program

Friday 7th October	
9.00 – 10.00	<i>Registration to the Workshop "Complex Network Analysis for Systems Biology"</i>
10.00 – 13.00	<i>Workshop: "Complex Network Analysis for Systems Biology" (Instructor: Costas Bouyioukos)</i>
13.00 – 15.30	<i>Registration to the HeCrA-HSCBB-16 Conference</i>
15.30 – 16.00	<i>Welcome and opening remarks Prof. Spyridon Kintzios, Dean, School of Food, Biotechnology and Development Prof. Elias Eliopoulos (Agricultural University of Athens, Local Organizing Committee), Dr. Spyros Zographos (President of HeCrA) and Prof. Artemis Hatzigeorgiou (President of HSCBB)</i>
<i>1st Session</i>	<i>Chair persons: Elias Eliopoulos – Spyros Zographos</i>
16.00 – 16.30	<i>Anastassis PERRAKIS "From ARP/WARP to PDB_REDO: a short history and perspectives"</i>
16.30 – 17.00	<i>John VAKONAKIS "Unravelling the centriole architecture, one component at a time"</i>
17.00 – 17.30	<i>Efstratios STRATIKOS "Structural insights on the mechanism of generation of antigenic peptides"</i>
17.30 – 18.00	<i>Demetres D. LEONIDAS et al. "X-ray crystallography screening of plant extracts for the identification of new bioactive agents"</i>
18.00 – 19.00	<i>Poster session / Coffee break</i>
<i>2nd Session</i>	<i>Chair person: Elias Eliopoulos</i>
19.00 – 20.00	Keynote Lecture <i>Simon E.V. PHILLIPS et al. "Mechanism of Hydrogen Activation by [NiFe]-hydrogenases"</i>

Saturday 8th October

<i>1st Session</i>	<i>Chair persons: Irene M. Mavridis - Demetres D. Leonidas</i>
09.30 – 10.00	Savvas SAVVIDES et al. “Structural basis of cytokine sequestration by the viral decoy receptor GIF to achieve immunomodulation”
10.00 – 10.30	Tassos PAPAGEORGIU “Glutathione transferases as molecular tools for green and red biotechnology: Structural insights”
10.30 – 10.45	Christina DRAKOU et al. “A mosquito Odorant Binding Protein that “smells” repellents”
10.45 – 11.00	Anthi METTOU et al. “Aqueous solubility enhancement of small molecule inhibitors and QSPR analysis: a TNF- α study”
11.00 – 11.30	Coffee break
<i>2nd Session</i>	<i>Chair persons: Ioannis Michalopoulos - George Kontopidis</i>
11.30 – 12.00	Konstantinos BEIS “Structural basis for antibacterial peptide transport across membranes”
12.00 – 12.30	Michael KOKKINIDIS et al. “Polysaccharide Deacetylases: Maturation, two Deaths and Resurrection”
12.30 – 13.00	Christina KARATZAFERI et al. “Structure-informed research in skeletal muscle function”
13.00 – 14.00	Poster session / General Assembly of the Hellenic Crystallographic Association
14.00 – 15.00	Lunch break
<i>3rd Session</i>	<i>Chair person: Konstantina Mergia - Kostas Bethanis</i>
15.00 – 15.30	T. CHOLI-PAPADOPOULOU “The Bone Morphogenetic Protein-2 (BMP-2): Bio-immobilization for stem cell recruitment towards their chondrogenic / osteogenic differentiation”
15.30 – 16.00	Pantelis N. TRIKALITIS “Reticular Chemistry and the Development of Novel Metal Organic Frameworks”
16.00 – 16.30	Vassilios. DRACOPOULOS “Structural evolution and stability of Au-Mo-NiO/GDC cermets under reducing/operating conditions: characterization with in-situ (H ₂ or CH ₄)-XRD”
16.30 – 17.00	Coffee break
<i>4th Session</i>	<i>Chair person: Ioannis Michalopoulos - Costas Bouyioukos</i>
17.00 – 17.15	Danai FIMERELI et al. “Detection of gene fusions in breast cancer samples using transcriptome sequencing data”

<p>17.15 – 17.30</p>	<p>Christoforos NIKOLAOU et al. <i>“Monitoring the development of Rheumatoid Arthritis through focal gene deregulation in four dimensions”</i></p>
<p>17.30 – 18.00</p>	<p>Aris GIOUTLAKIS et al. <i>“PICKLE (Protein InteraCtionKnowLedgebasE) 2.0: Knowledge-driven integration of human protein-protein interaction data via genetic information ontology”</i></p>
<p>18.00 – 19.00</p>	<p style="text-align: center;">Keynote Lecture</p> <p>David GILBERT <i>“Whole genome bacterial metabolic design - principles and challenges for computational synthetic biology”</i></p>

Sunday 9th October

9.30 – end of the day	<i>Voting for the new board of the Hellenic Crystallographic Association</i>
<i>1st Session</i>	<i>Chair persons: Kyriakos Petratos – Irene Mariolaki</i>
9.30 – 10.00	Emmanuel SARIDAKIS et al. “Protein stability, entropy and crystallization”
10.00 – 10.30	Oskar AURELIUS et al. “Making use of longer wavelengths in macromolecular crystallography – the I23 beamline at the Diamond Light Source”
10.30– 11.00	Konstantina MERGIA et al. “Fe⁺ ion irradiation of Fe: structural and magnetic effects”
11.00 – 11.30	<i>Coffee break</i>
<i>2nd Session</i>	<i>Chair persons: Georgia Braliou -Vassiliki Iconomidou</i>
11.30 – 11.45	Metaxia VLASSI et al. “Free Energy Calculations of the Binding of RS-repeat containing Peptides to AKT kinase based on Molecular Dynamics Simulations: a Comparative Study”
11.45 – 12.00	Haralambos TZOUPIS et al. “Conformational Analysis of the Mayaro Virus Non-Structural Protein 3 Macro Domain via Molecular Dynamics (MD) Simulations”
12.00– 12.15	Minos MATSOUKAS et al. “Discovery of novel immunosuppressants targeting Calcineurin through computational methods”
12.15 – 12.30	Christoniki MAGA-NTEVE, et al. “Streamlining GC-MS metabolomic analysis using the M-IOLITE software suite”
12.30 – 13.30	<i>Lunch break</i>
13.30 – 14.30	<i>Poster session /</i> <i>General Assembly of the HSCBB</i>
<i>3rd Session</i>	<i>Chair persons: Christophoros Nikolaou - Margarita Theodoropoulou</i>
14.30 – 14.45	Garyfallia I. MAKRYNITSA et al. “A comparative structure – activity relationship study of alphaviruses’ macro domains via solution NMR spectroscopy”
14.45 – 15.00	Maria SPILIOPOULOU et al. “Structural determination of Coxsackievirus B3 protease 3C via XRPD”
15.30 – 15.45	Catherine VASILOPOULOU et al. “Metabolic Network Analysis of Mammalian Brain; a case study of adult onset hypothyroidism”
15.45 – 16.00	Rafailia BETA et al. “Characterization of the active site of AtHESPERIN”
16.00 – 16.15	Zoe COURNIA et al. “Inhibition studies of the Arp2/3 complex using virtual screening and free energy perturbation calculations”
16.15 – 16.30	Kostas BETHANIS et al. “Structure and anti-proliferative activity of gefitinib-

	<i>cyclodextrin complexes</i>
16.30 – 17.00	HeCrA Ceremony in honor of retired members Award of “ Nikos OIKONOMAKOS ” prize
	Award of " HSCBB Best Student Poster " prize
	Closing remarks