



## 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

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

## Saturday 8<sup>th</sup> October

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

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

## Sunday 9<sup>th</sup> October

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

<b>16.15 – 16.30</b>	<b>Zoe CURNIA</b> <i>et al.</i> “ <i>Inhibition studies of the Arp2/3 complex using virtual screening and free energy perturbation calculations</i> ”
<b>16.30 – 17.00</b>	<b>HeCrA Ceremony</b> in honor of retired members Award of “ <b>Nikos OIKONOMAKOS</b> ” prize
	Award of “ <b>HSCBB Best Student Poster</b> ” prize
	<b>Closing remarks</b>