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HELLENIC CRYSTALLOGRAPHIC  
ASSOCIATION

**6th International Conference  
of the  
Hellenic  
Crystallographic Association**

**28-29 September 2012**

**University of Athens**

**ARISTOTELIS Conference Centre, Physics Department, Athens**

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## Programme

<b>Friday 28<sup>th</sup> September</b>	
<b>14.00 – 15.00</b>	<i>Registration -- Poster mounting</i>
<b>15.00 – 15.30</b>	<p><i>Welcome</i></p> <p><b>N. Stefanou</b>, Director of the Department of Solid State Physics, University of Athens, Faculty of Physics, School of Science</p> <p><b>K. Petratos</b>, President of the Hellenic Crystallographic Association</p> <p><b>S. Hamodrakas, M. Calamiotou</b>, Local Organizing Committee</p> <p><b>Απονομή Αναμνηστικών Πλακετών σε αφυπηρητήσαντες Έλληνες συναδέλφους</b></p>
<b>15.30 – 17.30</b>	<i>Chair persons -- S. Hamodrakas, A. Hountas</i>
<b>15.30 – 16.30</b>	<p><b>Manuela Helmer-Citterich</b>, <i>Structural motifs in the annotation of protein binding properties (Invited Lecture)</i></p> <p><b>Presentation Sponsored by EAST-NMR</b></p>
<b>16.30 – 17.30</b>	<b>Carmelo Giacovazzo</b> , <i>New phasing methods for small, medium size molecules and proteins (Invited Lecture)</i>
<b>17.30 – 18.00</b>	<i>Coffe Break – Poster Viewing</i>
<b>18.00 – 20.00</b>	<i>Chair persons -- S.E. Zographos, E. Eliopoulos</i>
<b>18.00 – 19.00</b>	<b>Christos Ouzounis</b> , <i>From reading to writing (and rewriting) the code of life: the future of biology – scientific, ethical, legal, civil and social issues (Invited Lecture)</i>
<b>19.00 – 19.15</b>	D. Sellis, T. Giannakouros, <b>M. Vlassi</b> , <i>Molecular Dynamics Simulations of Arginine/Serine Repeats: Implications for their Role in Molecular Recognition</i>
<b>19.15 – 19.30</b>	G. Patargias, A. W. Bagget, M. S. Han, A. C. Glass, S. Y. Liu, B. J. Nolen, <b>Z. Cournia</b> , <i>Computed-aided optimization of a small molecule inhibitor of Arp2/3 complex, a key regulator of the actin cytoskeleton</i>
<b>19.30 – 19.45</b>	<b>T. Evangelidis</b> , P. Gkeka, Z. Cournia, <i>Elucidating the oncogenic mechanism of the H1047R PI3Kalpha mutant kinase through molecular dynamics simulations</i>
<b>19.45 – 20.00</b>	<b>P. Stavros</b> , C.E. Vorgias, G. Nounesis, <i>Thermodynamic stability of Chitinase60</i>

<b>Saturday 29<sup>th</sup> September</b>	
<b>10.00 – 11.00</b>	<i>Chair persons</i> -- G. Kontopidis, K. Poulas
<b>10.00 – 10.15</b>	M. Vlachou, A. Loutsidou, M. Tsapardoni, M. Birkou, E. Melekis, D. Giannari, F. Karavassili, C.T. Chasapis, D. Bentrop, V. Episkopou, <b>G. A. Spyroulias</b> , <i>NMR-driven structure-function correlation studies of ARKADIA E3 ubiquitin ligase ring finger domain</i>
<b>10.15 – 10.30</b>	<b>S. Floros</b> , S. Papatzelos, G. E. Papadopoulos, <i>Dielectric Behavior of Lysozyme in Water and Urea Solutions studied with MD</i>
<b>10.30 – 10.45</b>	K. Fourtaka, E. Christoforides, D. Mentzafos, C. Pappas, A. E. Nikolopoulou, S. Tsagaropoulou, <b>K. Bethanis</b> , <i>Inclusion compound of IBA in <math>\beta</math>-Cyclodextrin. Preparation, characterization, crystal structure determination and application in plant seeds and vegetative material</i>
<b>10.45 – 11.00</b>	<b>A. Mettou</b> , C. Papanephytou, T. Papakyriakou, E. Eliopoulos, P. Alexiou, E. Couladouros, F. Liepouri, A. Maranti, A. Strongilos, G. Kontopidis, <i>Discovering a lead for Rheumatoid Arthritis by targeting TNF-<math>\alpha</math></i>
<b>11.00 – 11.15</b>	<i>Coffe Break – Poster Viewing</i>
<b>11.15 – 13.45</b>	<i>Chair persons</i> -- K. Vorgias, I. Mavridis
<b>11.15 – 12.15</b>	<b>Alekos Athanasiadis</b> , <i>Z-DNA binding domains and innate immunity (Invited Lecture)</i>
<b>12.15 – 13.15</b>	<b>Emmanuel Mikros</b> , <i>In silico screening in drug discovery (Invited Lecture)</i>
<b>13.15 – 13.35</b>	<b>A. S. Galanis</b> , F. Karavasili, M. Gemmi, I. Margiolaki, S. Nikolopoulos, <i>Combination of 3D diffraction tomography &amp; precession electron diffraction technique as structure analysis tool</i> <b>Presentation Sponsored by Nanomegas</b>
<b>13.35 – 13.45</b>	<b>E. D. Chrygina</b> , <i>Instruct-Ellas: National consortium on structural biology. An update on collaborative efforts, opportunities and challenges</i>
<b>13.45 – 14.45</b>	<i>Lunch break</i> <b>General Assembly of the Hellenic Crystallographic Association</b> <b>Voting for the new board of the Hellenic Crystallographic Association</b>
<b>14.45 – 16.30</b>	<i>Chair persons</i> -- D.D. Leonidas, K. Petratos
<b>14.45 – 15.00</b>	<b>E. Saridakis</b> , J. R. Birtley, E. Stratikos, I. M. Mavridis, <i>Two crystal structures of endoplasmic reticulum aminopeptidase 2 provide atomic level insight on the mechanism of antigen processing</i>
<b>15.00 – 15.15</b>	<b>A.L. Kantsadi</b> , A. Xipnitou, S. Manta, V.T. Skamnaki, J.M. Hayes, C. Kiritsis, A.-M.G. Psarra, Z. Koutsogiannis, A. Dimopoulou, S. Theofanous, N. Nikouleousakos, P. Zoumpoulakis, M. Kontou, S.E. Zographos, D. Komiotis, D.D. Leonidas, <i>The <math>\sigma</math>-hole phenomenon forms the structural basis for the strong inhibitory potency of C-5 halogen substituted glucopyranosyl nucleosides for glycogen phosphorylase</i>

<b>15.15 – 15.30</b>	<b>M.D. Charavgi</b> , M.D. Dimarogona, E. Topakas, P. Christakopoulos, E.D. Chrysina, <i>The crystal structures of a novel glucuronoyl esterase and its S213A mutant from Myceliophthora thermophila in the apo-forms and in complex with a substrate analogue give new insights on its role as a potential biocatalyst</i>
<b>15.30 – 15.45</b>	<b>N. Mitakidis</b> , K. Matsuda, W. Kakegawa, M. Yuzaki, R. Aricescu, Structural studies of C1q-like proteins and their function at the synapse
<b>15.45 – 16.00</b>	<b>P. P. Das</b> , K. W. Krämer, L. Palatinus, H.- B. Bürgi, A. Linden, $\alpha$ -“NaLuF4”: 6 fold twinning with modulation and diffuse scattering
<b>16.00 – 16.30</b>	<b>P. Stewart</b> and S. Kolek, <i>Microseed it! A Theoretical and Practical Exploration of Seed Stability and Seeding Techniques for Successful Protein Crystallization</i> <b>Presentation Sponsored by Anelis &amp; Douglas Instruments</b>
<b>16.30 – 17.00</b>	<i>Coffe Break – Poster Viewing</i>
<b>17.00 – 19.30</b>	<i>Chair persons -- M. Calamiotou, K. Mergia</i>
<b>17.00 – 18.00</b>	<b>Vassilios Psycharis</b> , <i>Crystal Structure study of the twin crystals: Is it a growth or a structure analysis problem? (Invited Lecture)</i>
<b>18.00 – 18.15</b>	<b>M.V. Sofianou</b> , V. Psycharis, N. Boukos, T. Vaimakis, C. Trapalis, <i>Manipulation of the TiO2 anatase crystal habit in order to achieve photocatalytic selectivity in air pollutants</i>
<b>18.15 – 18.30</b>	<b>I.Bakaimi</b> , O. Adamopoulos, C.Stock, M.A Green, A.Lappas, <i>Frustrated manganese oxide systems: The diversity of crystal structures towards novel magnetic behaviors</i>
<b>18.30 – 18.45</b>	<b>K. Papamihail</b> , K. Mergia, Yves Serruys, Th. Speliotis, F. Ott, Effect of iron ion irradiation on the structural and magnetic properties of thin iron films
<b>18.45 – 19.00</b>	<b>P. Kyritsis</b> , D. Maganas, E. Ferentinos, N. Levesanos, C.P. Raptopoulou, A. Terzis, V. Psycharis, <i>Magnetostructural correlations in tetrahedral and octahedral Ni<sup>II</sup> complexes bearing chelating ligands and coordinated solvent molecules</i>
<b>19.00 – 19.30</b>	<i>Closing Remarks</i> “Nikos Oikonomakos award”

### Posters

M. Calamiotou, G. Golfinopoulos, D. Lampakis, J. Karpinski, N.D. Zhigadlo, E. Liarokapis	THE T-O STRUCTURAL PHASE TRANSITION OF THE SLIGHTLY DOPED NdFeAsO <sub>1-x</sub> Fx SUPERCONDUCTING SYSTEM
C. T. Chasapis, A. Argyriou, P.-J. Corringer, D. Bentrop, G.A. Spyroulias	SOLUTION NMR STUDY OF THE MONOMERIC EXTRACELLULAR DOMAIN OF A nAChR PROKARYOTIC HOMOLOGUE
D. Chatzileontiadou, C. Hamakou, P. Maragozidis, S. Bougiatioti, V.T. Skamnaki, V. Parmenopoulou, S. Manta, J. Delbe, J. Courty, D. Komiotis, N.A.A. Balatsos, D.D. Leonidas	NOVEL SYNTHETIC NUCLEOSIDE ANALOGS AS RIBONUCLEASE A/ ANGIOGENIN INHIBITORS
M. Chegkazi, A. Pantzou, D. Sovantzis, E.D. Chrysina, T. Gimisis	GLYCOGEN PHOSPHORYLASE: A STRUCTURE-BASED DRUG DESIGN TARGET FOR TREATMENT OF TYPE 2 DIABETES
M. Dimarogona, M. Moukouli, E. Topakas, P. Christakopoulos, E.D. Chrysina	STRUCTURAL STUDIES OF A TYPE C FERULOYL ESTERASE FROM FUSARIUM OXYSPORUM
C.E. Drakou, K.E. Tsitsanou, S.E. Zographos	CRYSTAL STRUCTURE OF ODORANT BINDING PROTEIN 4 FROM ANOPHELES GAMBIAE
R. Gessmann, D. Axford, G. Evans, H. Brückner, K. Petratos	THE CRYSTAL STRUCTURES OF SAMAROSPORIN I AT ATOMIC RESOLUTION
A.E. Giannopoulou, F. Karavassili, E. Kotsiliti, M. Norrman, G. Schluckebier, Y. Watier, J. Wright, A. Fitch, I. Margiolaki	INVESTIGATION OF INSULIN POLYMORPHISM VIA SYNCHROTRON X-RAY POWDER DIFFRACTION
P. Giastas, A. Andreou, S. Balomenou, D. Koutsoulis, K.Poulas, S. Tzartos, E. Eliopoulos and V. Bouriotis	EXPRESSION AND STRUCTURAL ANALYSIS OF BC1974, A PEPTIDOGLYCAN DEACETYLASE FROM BACILLUS CEREUS
P. Gkeka, P. Angelikopoulos, Z. Cournia	NANOPARTICLE-MEMBRANE INTERACTIONS: INSIGHTS INTO EFFICIENT DELIVERY OF NANOMEDICINE USING MD SIMULATIONS
A.L. Kantsadi, V. Peppas, V.T. Skamnaki, S.E.Zographos, S.R. Inamdar, B.M. Swamy, D.D. Leonidas	THE CRYSTAL STRUCTURE OF SCLEROTIUM ROLFSII LECTIN VARIANTS WITH FINE CARBOHYDRATE SPECIFICITY
M. Karamolegkou, V. Iconomidou, V. Gionis, G. Chryssikos, S. Hamdrakas	STUDIES OF AMYLOID FIBRIL FORMATION OF THE CA (CENTRAL CONSERVATIVE DOMAIN OF THE A-CLASS) SILKMOTH CHORION PROTEIN PEPTIDE-ANALOGUE UTILIZING MICRO-RAMAN AND ATR FT-IR SPECTROSCOPY
F. Karavassili, A. E. Giannopoulou, E. Kotsiliti, M. Norrman, G. Schluckebier, J. Wright, A. Fitch, I. Margiolaki	PHASE MAPPING OF INSULIN USING SYNCHROTRON X-RAY POWDER DIFFRACTION METHODS
V. Kargas, N. Papandreou, P. Bagos, S. Hamdrakas	STRUCTURAL STUDIES ON THE EFFECT OF NON-SYNONYMOUS POLYMORPHISMS IN HUMAN MELANOCORTIN-1 RECEPTOR INVOLVED IN HEALTH AND DISEASE
E. Kotsiliti, A. Valmas, Y. Watier, L. Saunders, B. Coutard, V. Lantéz, E. A. Gould, A. N. Fitch, J. P.Wright, B. Canard, N. Papageorgiou, I. Margiolaki	CRYSTALLISATION AND STRUCTURAL STUDIES OF THE nsP3 MACRO DOMAIN OF THE MAYARO VIRUS

<u>T. Koutsourj</u> , N. Louros, P. Tsiolaki, G. Baltatzis, E. Patsouris, V. Iconomidou, S. Hamodrakas	AN 'AGGREGATION-PRONE' PEPTIDE OF APOLIPOPROTEIN A-I (ApoA-I) AND ITS RELATION TO ApoA-I AMYLOIDOSES
<u>E. Lappa</u> , N. Louros, P. Tsiolaki, E. D. Chrysina, V. Iconomidou, S. Hamodrakas	'HACKING' THE CODE OF A NATURAL PROTECTIVE AMYLOID: STRUCTURAL STUDIES OF A HEXAPEPTIDE-ANALOGUE FROM THE CENTRAL DOMAIN OF SILKMOTH CHORION PROTEINS OF THE A FAMILY
<u>A. Michaelides</u> , S. Skoulika, M.G. Siskos	HIGH-DIMENSIONAL PHOTOREACTIVE LANTHANIDE MOFS OF TRANS,TRANS-MUCONIC ACID
<u>Th. Mouschountj</u> , G. Tsaousis, S.J. Hamodrakas	RELATIONS OF 'AGGREGATION-PRONE' PEPTIDES AND 'INTRINSICALLY DISORDERED REGIONS' IN TWELVE (12) AMYLOIDOGENIC PROTEINS
D. Papadopoulou, E.D. Chrysina, I.Z. Emiris, <u>A. Tartas</u>	MAPPING OF THE SOLVENT STRUCTURE REVEALS POTENTIAL PROTEIN BINDING SITES
M. Papadovasilaki, D. Oberthür, C. Betzel, E. Scoulica, <u>K. Petratos</u>	HETEROLOGOUS EXPRESSION, PURIFICATION AND CHARACTERIZATION OF AMINOGLYCOSIDE ADENYLYL-TRANSFERASE (AadA6) FROM PSEUDOMONAS AERUGINOSA
<u>G. Stravodimos</u> , A.L. Kantsadi, S. Theofanous, A.-M.G. Psarra, E. Adamou, K. Kotsona, D. Kouretas, S.A. Haroutounian, D.D. Leonidas	EXTRACTS FROM GREEK GRAPE VARIETIES INHIBIT GLYCOGEN PHOSPHORYLASE b. BIOCHEMICAL AND BIOLOGICAL ASSESSMENT.
<u>D. Vourtsis</u> , P.V. Gkazonis, C.T. Chasapis, D. Bentrop, G.A. Spyroulias	EXPRESSION AND NMR STUDY OF THE N- & C-TERMINAL POLYPEPTIDES OF ANTHRAX LETHAL FACTOR METALLOPROTEASE
<u>E. Zarkadas</u> , M. Zouridakis, P. Giastas, E. Eliopoulos, S. Tzartos	DESIGN AND EXPRESSION OF EXTRACELLULAR DOMAINS OR TRUNCATED FORMS OF THE NEURONAL $\alpha 7$ AND $\alpha 9$ HUMAN NICOTINIC ACETYLCHOLINE RECEPTORS, SUITABLE FOR BOTH FUNCTIONAL AND STRUCTURAL STUDIES

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