

ACAC 2022 SCIENTIFIC PROGRAM

Sunday June 26th 2022

10:30-13:00	Registration Opens
13.30-15.00	Welcome Reception

Monday June 27th 2022

8.30-9.30	Registrations
9.30-9.45	Opening Ceremony Prof. Christiana Mitsopoulou, Head of the Department of Chemistry and Chair of ACAC2022. Prof. I. Emmanouil, Dean of School of Science Assoc. Prof. I. Katsoyiannis, President of Association of Greek Chemists
SESSION 1a. Chairs: A. Danopoulos – P. Falaras	
9.45-10.30	Molecular Nanoparticles. A Molecular Route to Ultra small Nanoparticles of Important Metal Oxides George Christou (<i>University of Florida, USA</i>)
10.30-10.45	“Designed” versus “serendipitous” assembly in the chemistry of 3d/4f-metal coordination complexes. The intermediate case of the “assisted” self-assembly approach Spyros P. Perlepes, Zoi G. Lada, Christina D. Polyzou, Vassilis Psycharis and Catherine P. Raptopoulou (<i>University of Patras, Greece</i>)
10.45-11.00	Actinide cyclo-butadienyl complexes – Synthesis, Reactivity and Evidence of η^4, η^4 Coordination Nikolaos Tsoureas, Richard A. Layfield, Laurent Maronc and Akselli Mansikkamäki (<i>NKUA, Greece</i>)
11.00-11.15	Metal-Organic Frameworks based on hexanuclear secondary (M ₆) ⁿ⁺ (M = Zr ⁴⁺ and trivalent rare earth ions) building units and angular dicarboxylates with sorption and sensing capabilities N. Panagiotou, A. J. Tasiopoulos (<i>University of Cyprus, Cyprus</i>)
11.15-11.45	COFFEE BREAK
SESSION 1b. Chairs: E. Efthimiadou – S. Perlepes	
11.45-12.00	Zero-field splitting and slow relaxation of magnetization in 3d mononuclear metal complexes Panayotis Kyritsis (<i>NKUA, Greece</i>)
12.00-12.15	Orientational Jahn–Teller Isomerism in the Dark-Stable State of Nature's Water Oxidase

	Maria Drosou, Georgia Zahariou, Dimitrios A. Pantazis (<i>Max-Planck-Institut für Kohlenforschung, Germany</i>)
12.15-12.30	Study of the S3 state of nature's water-splitting catalyst by X-ray spectroscopy Maria Chrysina (<i>NCSR "Demokritos", Greece</i>)
12.30-12.45	Possible role of the Tyrosine Z in the S2 to S3 transition of the Oxygen Evolving Complex of Photosystem II Georgia Zahariou (<i>NCSR "Demokritos", Greece</i>)
12.45-13.00	Remarkable blood-brain barrier penetrating diagnostics & therapeutic agents for central nervous system pathologies Barbara Mavroidi, Marina Sagnou, Antonio Shegani, Ioannis Pirmettis, Minas Papadopoulos and Maria Pelecanou (<i>NCSR "Demokritos", Greece</i>)
13.00-13.15	Liposomal Encapsulated Iron Oxide Nanoflowers for the Treatment of Lung Adenocarcinoma via Magnetic Hyperthermia Maria Theodosiou, Elias Sakellis, Nikos Boukos, Vladan Kusigerski, Beata Kalska-Szostko, Eleni Efthimiadou (<i>NKUA, NCSR "Demokritos", Greece</i>)
13.15-13.30	Rhabdomyosarcoma Treatment By Using Polymeric Nanocontainers. Drug Delivery And Therapeutic Outcome Enhancement Sara Seriah, Eleni Efthimiadou, M. Braoudak (<i>University of Hertfordshire, UK; NKUA, NCSR "Demokritos", Greece</i>)
13.30-15.00	LUNCH
SESSION 1c. Chairs: K. Methenitis –V. Psycharis	
15.00-15.45	Establishing photocatalysis as an advanced oxidation-reduction process/technology (AOP-ARP/AOT-ART) Polycarpus Falaras (<i>NCSR "Demokritos", Greece</i>)
15.45-16.00	Exploring the intermolecular interactions in crystals with the Hirshfeld Surface analysis tools Vassilis Psycharis (<i>NCSR "Demokritos", Greece</i>)
16.00-16.15	MOF-74 Analogues and Cu(II) compounds as electrode modifiers for the electrochemical detection of glucose in human perspiration and / or glucose sorption Alexios K. Plessas, Varvara Pagkali, Evangelia Kritikou, Anthi Panara, Anastasios Economou, Nikolaos S. Thomaidis, Christos Kokkinos, Giannis S. Papaefstathiou (<i>NKUA, Greece</i>)
16.15-16.30	A [MnIII2MnII]n Single-Chain Magnet Catherine P. Raptopoulou, Vassilis Psycharis, Michael Pissas, Yiannis Sanakis (<i>NCSR "Demokritos", Greece</i>)
16.30-16.45	Mononuclear trivalent 3d-metal complexes as 'stepping stones' for the synthesis of new polynuclear, heterometallic 3d/3d'-clusters Konstantinos N. Pantelis, Konstantina H. Baka, Catherine P. Raptopoulou, Vassilis Psycharis and Theocharis C. Stamatatos (<i>University of Patras, Greece</i>)
16.45-17.00	DNA/BSA Interaction and in vitro biological evaluation of Ru(II) complex with a

	derivative of 1,10-phenanthroline A. Magiakos, R. Pappa, El. Efthimiadou, B. Mavroidi, M. Pelecanou, M. Paravatou-Petsotas, C. Methenitis (<i>NKUA, Greece; University of Warwick, UK</i>)
17.00-17.15	Dinuclear {Dy ₂ } complexes. a 'playground' for efficient single-molecules magnets Alexandros S. Armenis, Dimitris I. Alexandropoulos, Kim R. Dunbar and Theocharis C. Stamatatos (<i>University of Patras, Greece</i>)
17.15-18:30	POSTER SESSION (odd numbers)

Tuesday June 28th 2022

SESSION 2a. Chairs: C. Proestos – A. Sakellari	
9.30-10.15	The chemistry of carotenoids and their key actions in agro-food and health Antonio J. Meléndez Martínez (<i>Universidad de Sevilla, Spain</i>)
10.15-10.30	Greek honey authenticity and characterization– studying the gold of nature Marilena Dasenaki, Georgios Koulis, Panagiotis-Loukas Gialouris, Charalampos Proestos, Nikolaos Thomaidis (<i>NKUA, Greece</i>)
10.30-10.45	Chemometric analysis of the mineral content of honey originating from different botanical and geographical origins Carolina S. Silva, Ioannis Gkikopoulos, Sotirios Karavoltsos, Aikaterini Sakellari, Charalampos Proestos, Owen Falzona, Vasilis Valdramidis (<i>University of Malta, Malta</i>)
10.45-11.00	Experimental brewing and measurement of ochratoxin, gluten and vitamins B9, B12 in beer samples by ELISA Antonios Liapis, Konstantina Pasvanka, Eleni Kollia, Charalampos Proestos (<i>NKUA, Greece</i>)
11.00-11.30	COFFEE BREAK
SESSION 2b. Chairs: E. Emmanouilidou - E. Dasenaki	
11.30-11.45	The role of polymorphic variation in intracellular antigen processing Efstratios Stratikos (<i>NKUA, Greece</i>)
11.45-12.00	Poly[oligo(ethylene glycol) methacrylate]-b-poly[(vinyl benzyl trimethylammonium chloride)]-based ternary hybrid complexes encapsulating magnetic nanoparticles and DNA Angeliki Chroni, Aleksander Forys, Barbara Trzebicka, Adam Alemayehu, Václav Tyrpekl and Stergios Pispas (<i>N.H.R.F., Greece</i>)
12.00-12.15	Lipid-Functionalized Dendrimers as Corneocyte Lipid Envelope Mimics Panagiota Velissari, Kateřina Vávrová (<i>Charles University, Czech Republic</i>)
12.15-12.30	Characterization of organic matter and metal complexation in the marine surface microlayer of coastal areas Sotirios Karavoltsos, Aikaterini Sakellari, Marta Plavšić, Georgios Bekiaris, Dimitra Tagkouli, Anastasios Triantafyllidis, Antonia Giannakourou, Sultana

	Zervoudaki, Ioannis Gkikopoulos, Nick Kalogeropoulos (<i>NKUA, Greece</i>)
12.30-12.45	Established measures for MSFD Descriptors 8 & 9 in the Greek Programme of Measures; Are they fit for purpose? Theodora Paramana, Manos Dassenakis (<i>NKUA, Greece</i>)
12.45-13.00	Unmanned Surface Vehicles as a complement tool for water quality monitoring of EYDAP's Reservoirs Georgios Katsouras, Nikolaos Defteraios, Phani Miskaki, Anastasia Kagiara, Eugenia Gialia, Marina Despotidou, Nikos Tsalas, Alekos Dosis, Stylianos Samios, Efthymios Lytras and Giorgos Sachinis (<i>E.Y.D.A.P., Greece</i>)
13.00-14.30	LUNCH
SESSION 2c. Chairs: N. Thomaidis - A. Markou	
14.30-16.30	Flash Presentations
14.30-14.35	Bis(picolinoylhydrazone)pyridine as a ligand for the synthesis of Dy-based single-molecule magnets Georgia P. Bakali, Athina Dimitriadi, Christianna Brantley, George Christou and Theocharis C. Stamatatos (<i>University of Patras, Greece</i>)
14.35-14.40	Metal - involving reactions of the oxime group. The case of 2-pyridyl chloroxime Chrysi Chaikali, Sokratis T. Tsantis, Demetrios I. Tzimopoulos, Catherine P. Raptopoulou, Vassilis Psycharis and Spyros P. Perlepes (<i>University of Patras, Greece</i>)
14.40-14.45	IR spectral shifts of amorphous trichloroacetonitrile films during crystallization N. Efthymiadis, G. Kanellopoulos, L. Tsagri, K. Meris, M. Giota, A. Tsekouras (<i>NKUA, Greece</i>)
14.45-14.50	Production & purification of monoclonal antibodies. a first step towards the characterisation of the MHC I immunopeptidome in the A375 melanoma cell line Martha- Spyridoula Nikopaschou and Efstratios Stratikos (<i>NCSR "Demokritos", Greece; NKUA, Greece</i>)
14.50-14.55	Structure assignment, conformational analysis and discovery of potential targets of the thiosemicarbazone and thiocarbonylhydrazide derivatives N. Georgiou, A. Katsogiannou, D. Tzeli, S. Vassiliou, Uroš Javornik, Janez Plavec, T. Mavromoustakos (<i>NKUA, Greece</i>)
14.55-15.00	Comparison of the properties of polyurea-crosslinked alginate aerogels prepared from different types of isocyanates under various reaction conditions Argirios Gomatos, Grigorios Raptopoulos, Patrina Paraskevopoulou (<i>NKUA, Greece</i>)
15.00-15.05	Modelling the $\{UO_2\}^{2+}$ extraction from seawater using amidoxime extractants and its competition with VIV and VV Maria Iliopoulou, Sokratis T. Tsantis, Demetrios I. Tzimopoulos, Vassilis Psycharis, Catherine P. Raptopoulou and Spyros P. Perlepes (<i>University of Patras, Greece</i>)

15.05-15.10	<p>A new, domino O-H/C-H activation reaction towards the synthesis of oxygen-doped polyaromatic molecules with potential technological and biological applications</p> <p><u>Entzy Kaplanai</u>, Eftathios Tonis, Maria Drymona, Yulian Zagranyski, and Georgios C. Vougioukalakis (NKUA, Greece)</p>
15.10-15.15	<p>Synthesis of Co^{II} and Fe^{II} Complexes Coordinated with Pincer Ligands bearing NHC Donors and Their Use in Ketone Hydrogenation Reactions</p> <p><u>Irene Ligielli</u>, Konstantinos P. Zois, Georgios Vougioukalakis and Andreas Danopoulos (NKUA, Greece)</p>
15:15-15:20	<p>A combinatorial approach for the discovery of selective inhibitors of Zn aminopeptidases ERAPs/IRAP Sandra</p> <p><u>Sandra Llamas-Rizo</u>, Evgenia-Galateia Georgaki, Efstratios Stratikos, Dimitris Georgiadis (NKUA, Greece)</p>
15:20-15:25	<p>Production of recombinant ERAP enzymes and their use in evaluating inhibitor libraries that probe substrate specificity pockets</p> <p><u>Evgenia-Galateia Georgaki</u>, Sandra Llamas Rizo, Anastasia Mpakali, Dimitris Georgiadis and Efstratios Stratikos (NCSR "Demokritos", Greece)</p>
15:25-15:30	<p>Magnetoliposomes encapsulated DNR against cervical cancer. characterization and biological evaluation</p> <p><u>Dimosthenis Pourdalas</u>, Danai Prokopiou, Maria Theodosiou, Eleni Efthimiadou (NCSR "Demokritos", Greece; NKUA, Greece)</p>
15:30-15:35	<p>Evaluation of polyurea-crosslinked alginate aerogels for water decontamination from heavy metals</p> <p><u>Sigala Evangelia</u>, Zoi Artemisia, Raptopoulos Grigorios, Sakellari Aikaterini, Karavoltzos Sotirios, Paraskevopoulou Patrina</p>
15:35-15:40	<p>Controlling crystallization of Sb₂S₃ films for efficient solar cells</p> <p><u>L. Theofylaktos</u>, L. Gkivalou, K. Gkini, C. Kouzios, S. Orfanoudakis, M. Konstantakou, T. Stergiopoulos (AUTH, Greece; NKUA, Greece)</p>
15:40:15:45	<p>Spent coffee grounds as an unconventional source of polysaccharides with application as carriers for pulmonary insulin delivery</p> <p><u>Sara A. Valente</u>, Margarida Pais, Paulo Gomes, Guido R. Lopes, Margarida Almeida, Paula Ferreira, Manuel A. Coimbra and Cláudia P. Passos (University of Aveiro, Portugal)</p>
15:45-15:50	<p>One pot synthesis of thiazolidin-2-ylideneamines</p> <p><u>Leandros P. Zorba</u> and Georgios C. Vougioukalakis (NKUA, Greece)</p>
15:50-15:55	<p>NMR structural characterization of mannan (polymannose) conjugate with the myelin oligodendrocyte glycoprotein 35-55 epitope (MOG₃₅₋₅₅)</p> <p><u>Nikoletta Zoupanou</u>, Areti Gkika, Maria-Eleni Androutsou, Theodore Tselios, Thomas Mavromoustakos (NKUA, Greece)</p>
15:55-16:00	<p>Development of a novel, step-growth polymerization strategy, based on a multi-component coupling reaction</p> <p><u>Dimitrios Giannopoulos</u>, Leandros Zorba, Christos Zisis, Marinos Pitsikalas, and Georgios C. Vougioukalakis (NKUA, Greece)</p>
16.00-16.30	<p>Discussion / Questions</p>

Wednesday June 29th 2022

SESSION 3a. Chairs: D. Georgiadis – S. Stratikos	
9.30-10.15	Bruker BioSpin Progress in NMR technology from benchtop to Ultra High Field Angelo Ripamonti (<i>Bruker BioSpin / Regional Manager South&Western Europe</i>)
10.15-10.30	Comprehensive screening of migrating substances from container closure systems and filters into pharmaceutical formulations Chrysoula Kanakaki, Sofia Eleni Tsorotioti, Panagiotis Kaloudis and Magda Xenou (<i>DEMO S.A. Pharmaceutical Industry</i>)
10.30-10.45	All-3D printed enzymatic microchip for the simultaneous determination of cholesterol and choline in blood Eleni Koukouvitzi, Christos Kokkinos (<i>NKUA, Greece</i>)
10.45-11.00	Inhibition of ER aminopeptidases leads to shifts in the immunopeptidome of cancer cells and the presentation of novel and potentially antigenic peptides Ioannis Temponeras, George Stamatakis, Martina Samiotaki, George Panayotou and Efstratios Stratikos (<i>NCSR "Demokritos", Greece</i>)
11.00-11.30	COFFEE BREAK
SESSION 3b. Chairs: V. Magrioti – S. Vassiliou	
11.30-11.45	Mechanisms for allosteric inhibition of Insulin-Regulated Aminopeptidase Anastasia Mpakali, Petros Giastas and Efstratios Stratikos (<i>NCSR "Demokritos", Greece</i>)
11.45-12.00	Galactomannan microparticles as vehicles for pulmonary insulin delivery Miguel F. Galrinho, Bernardo Ferreira, Sara Valente, Lisete M. Silva, Paulo Gomes, Margarida Almeida, Manuel A. Coimbra and Cláudia P. Passos (<i>University of Aveiro, Aveiro, Portugal</i>)
12.00-12.15	Comparative interaction studies of quercetin with 2-hydroxyl-propyl-cyclodextrin and 2,6-methylated-cyclodextrin. Vasiliki Vakali, Michael Papadourakis, Uros Javornik, Georgia Valsami, Zoe Cournia, Thomas Mauromoustakos (<i>NKUA, Greece</i>)
12.15-12.30	Advanced Migration Studies of Food Contact Materials – Facing Current and Future Challenges Chrysoula Kanakaki, Theodora Traka, Eleni Tratari, Erasmia Bizani and Nikolaos Thomaidis (<i>NKUA, Greece</i>)
12.30-12.45	Iron-Catalyzed C–H Activation by Weak O-Carbonyl Chelation. Development and Mechanistic Investigation Antonis M. Messinis, Lars H. Finger, João C. A. Oliveira, Lianrui Hu, Claudia A. Stückl and Lutz Ackermann (<i>Georg-August-Universität Göttingen, Germany</i>)
12.45-13.00	Upcycling bread waste into Ag-doped carbon functional material for fabricating screen-printed electrodes applied to the analysis of halogenated compounds Wenchao Duan, Martí Gich, César Fernández-Sánchez (<i>ICMAB (CSIC), Spain</i>)

13.00-14.30	LUNCH
SESSION 3c. Chairs: T. Mavromoustakos - G. Vougioukalakis	
14.30-15.15	Development and effective use of new virtual ligand screening algorithms for rapid transition to clinical phase stages Serdar Durdagi (<i>Bahçeşehir University, Turkey</i>)
15.15-15.30	Progress in the synthetic and medicinal chemistry of bioactive organophosphorus peptidomimetics. Dimitris Georgiadis (<i>NKUA, Greece</i>)
15.30-15.45	Organic Synthetic Photochemistry. The Awakening of a Sleeping Giant Christoforos G. Kokotos (<i>NKUA, Greece</i>)
15.45-16.00	Rational development of bacterial ureases inhibitors V. Ntatsopoulos, A. Pagoni, A. Mucha, S.Vassiliou, L. Berlicki (<i>NKUA, Greece</i>)
16.00-16.15	Design, Synthesis and Antimycobacterial Activity of Long and Medium Chain β -Lactones Victoria Magrioti, Christina Dedaki, Alexandros Athanasoulis, Kanellos Albanis, Filippos Foteinakis, Pierre Santucci, Stephane Canaan, Jean-Francois Cavalier (<i>NKUA, Greece</i>)
16.15-16.30	Development of an inquiry-based laboratory experiment on enzymes for secondary education Aliki Zentefia and Katerina Paschalidou (<i>NKUA, Greece</i>)
16.30-18.00	POSTER SESSION (even numbers)
20.30	CONFERENCE DINNER

Thursday June 30th 2022

SESSION 4a. Chairs: D. Tzeli – S. Karavoltsos	
9.30-10.15	The Use of Cellulose Nanocrystals as Molecular Scaffolds; Supramolecular Chemistry Using Nature's Most Abundant Template Dimitris S. Argyropoulos (<i>North Carolina State University, USA</i>)
10.15-10.30	Electrospun nanofibrous scaffolds based on marinebiopolymers for biomedical applications Stefanos Kikionis, Efstathia Ioannou and Vassilios Roussis (<i>NKUA, Greece</i>)
10.30-10.45	The role of feature selection in untargeted metabolomics schemes I. Barla, E. Papagiannopoulou, K. Antoniadis, S. Polychronopoulou, N. Thomaidis, E. Gikas (<i>NKUA, Greece</i>)
10.45-11.00	Poly(vinyl pyridine) and its Quaternized Derivatives. Understanding their Solvation and Solid State Properties Katerina Mavronasou, Alexandra Zamboulis, Panagiotis Klonos, Apostolos Kyritsis, Dimitrios N. Bikiaris, Raffaello Papadakis and Ioanna Deligkiozi (<i>Creative Nano PC</i>)

11.00-11.30	COFFEE BREAK
SESSION 4b. Chairs: A. Tsekouras – G. Souliotis	
11.30-11.45	Electronic structure and bonding properties of iron-sulfur model complexes. $[\text{Fe}(\text{SMe})_4]_q$, $[\text{Fe}_2\text{S}_2(\text{SMe})_4]_q$, $[\text{Fe}_3\text{S}_4(\text{SMe})_3]_q$, & $[\text{Fe}_4\text{S}_4(\text{SMe})_4]_q$ Demeter Tzeli (NKUA, Greece)
11.45-12.00	The Nuclear Equation of State. From Nuclei to Neutron Stars T. Depastas, G.A. Souliotis, A. Bonasera (NKUA, Greece)
12.00-12.15	Micellar Aggregation of Surfactants and Encapsulation of Organic Molecules through Molecular Dynamics Simulations Emmanouil Kainourgiakis and Jannis Samios (NKUA, Greece)
12.15-12.30	Theoretical Investigation of the reactivity of α -Lithiated aryl benzyl ethers Sofia Kiriakidi, Carlos Sedano, Samuel Suárez-Pantigna, Roberto Sanz and Carlos Silva López (Universidad de Vigo, Campus Lagoas-Marcosende, Spain)
12.30-12.45	An AI tool-kit for the design of zeolitic-imidazolate frameworks with separation performance on demand Panagiotis Krokidas, Stelios Karozis, Salvador Moncho, Edward N. Brothers, Ioannis G. Economou, Michael E. Kainourgiakis, George Giannakopoulos and Theodore A. Steriotis (NCSR "Demokritos", Greece)
12.45-13.00	Molecular studies on lipoxxygenase enzyme and its potent inhibitors Eleni Chontzopoulou, Christina Papaemmanouil, Maria V. Chatziathanasiadou, Dimitrios Kolokouris, Sofia Kiriakidi, Athina Konstantinidi, Ioannis K. Kostakis, Evangelia D. Chrysinia, Dimitra Hadjipavlou-Litina, Demeter Tzelia, Andreas G. Tzakos, Juan Jose Nogueira Perez, Thomas Mavromoustakos (NKUA, Greece)
13.00-14.30	LUNCH
SESSION 4c. Chairs: A. Economou - M. Chatzichristidi (co-organized with Micro-Nano Scientific Society)	
14.30-14.45	Bio-functional surfaces of fluoropolymers via lithography Christina Gkioka, Anastasia Nika, Fotini Macharioti, Panagiota Petrou, Margarita Chatzichristidi (NKUA, Greece)
14.45-15.00	Lab on Chip on PCB for Bio and Chemical Analysis M.K. Filippidou, G. Kaprou, C. Moritz Loukas, Panagiota Petrou, A. Tserepia, S. Chatzandroulis (NCSR "Demokritos", Greece)
15.00-15.15	Legionella spp. diagnosis in 2 hours. A lab-on-a-chip for rapid, colorimetric detection in water Katerina Tsougeni, Kosmas Ellinas, Evangelos Gogolides, and Angeliki Tserepi (Nanoplasmas Private Company, TEPA Lefkippos, NCSR "Demokritos")
15.15-15.30	Detection of ewe's milk adulteration with cow's milk using immersible optical immunosensors D. Kourti, M. Angelopoulou, K. Misiakos, E. Makarona, A. Salapatas, A. Economou, P. Petrou and S. Kakabakos (NCSR "Demokritos", Greece)
15.30-15.45	PDMS surface functionalization for enhanced mesenchymal stem cell growth in bone marrow-on-a-chip platforms

	Dionysia Kefallinou, Maria Grigoriou, Dimitrios T. Boumpas, Evangelos Gogolides, and Angeliki Tserepi (<i>NCSR "Demokritos", Greece</i>)
15.45-16.30	Round Table of Young Researchers Chairs: S. Kiriakidi, K. Moldovan, A. Plessas
16.30-16.45	Flash & Poster Awards To be sponsored by Association of Greek Chemists

Friday July 1st 2022

10.30-12.30	Round table of O.C. and M.C.
12.30-13.00	CLOSING CEREMONY