

June 1-3, 2017 • THESSALONIKI



HELLENIC SYMPOSIUM on Medicinal Chemistry

Designing targeted and safer drugs

*Symposium Venue: Aristotle University of Thessaloniki
Amphitheater II Research Dissemination Center (K.E.D.E.A.)*



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SCHOOL OF PHARMACY,
ARISTOTLE UNIVERSITY
OF THESSALONIKI



HELLENIC SOCIETY
OF MEDICINAL
CHEMISTRY

Thursday, June 1, 2017

Satellite: Pharmaceutical Analysis

Session 1

Chairs: TBA

09:00-10:00

Registrations

10:00-10:30

LC-MS/MS based targeted metabolomics. Application in biomarker discovery and the characterization of biological samples.

Georgios Theodoridis, Aristotle University of Thessaloniki, Greece

10:30-10:50

Metabolomics in the discovery of new biomarkers

Evangelos Gikas, National and Kapodistrian University of Athens, Greece

10:50-11:20

Mass Spectrometry-Based Proteomics in Preclinical Drug Discovery, Development and Re-positioning

Michalis Aivaliotis Institute of Molecular Biology and Biotechnology, FORTH, Heraklion, Greece

11:20-11:35

A UHPLC-MS/MS method for the detection of drugs and pharmaceuticals in human bones

Amvrosios Orfanidis¹, Orthodoxia Mastrogianni², Helen Gika¹, Georgios Theodoridis³, Eleni Zaggelidou², Nikolaos Raikos¹

¹Laboratory of Forensic Medicine & Toxicology, Medical School, Aristotle University Thessaloniki

²Laboratory of Forensic Service of Ministry of Justice of Thessaloniki

³School of Chemistry, Laboratory of Analytical Chemistry, Aristotle University Thessaloniki

11:35-12:00

Coffee Break

Session 2

Chairs: TBA

12:00-12:30

2-D and 3-D Printing of solid dosage forms for Personalized Medicine

Dimitrios Fatouros, Aristotle University of Thessaloniki, Greece



12:30-12:50


Dried matrix spots: Applications, challenges and future trends


Yannis Dotsikas, National and Kapodistrian University of Athens, Greece

12:50-13:10	Biomimetic Chromatography as a rapid and efficient tool to investigate ADME properties <i>Fotios Tsopelas, National and Technical University of Athens, Greece</i>
13:10-13:25	An application of ICH guidelines on metronidazole photostability kinetic studies. The sample initial concentration effect. <i>Olga Galanopoulou, ELPEN Pharmaceutical Co. Inc</i>
13:25-13:40	Isolation and Analysis of Fomentariol-An active constituent of mushroom Fomes Fomentarius <i>Jelena Golubović¹, Nevena Maljurić¹, Matjaž Ravnika², Dušan Žigon³, Janko Ignjatović¹, Biljana Otašević¹, Borut Štrukelj²</i> ¹ <i>Department of Drug Analysis, Faculty of Pharmacy, University of Belgrade Serbia</i> ² <i>Chair for Pharmaceutical Biology, University of Ljubljana, Slovenia</i> ³ <i>Jožef Stefan Institute, Ljubljana, Slovenia</i>
15:00-16:30	Registrations
Session 1 Chairs: TBA	
16:30-17:00	Official Opening of the Hellenic Symposium on Medicinal Chemistry
17:00-17:40	Protein Dynamics for Ligand Design <i>Rebecca Wade, Heidelberg University, Germany</i>
17:40-18:20	The challenge of Multi-Targeting Drug Design seen from a computational chemistry point of view <i>Stefano Alcaro, Università "Magna Græcia" di Catanzaro, Italy</i>
18:20-18:50	Metal Chelating Agents against Viruses and Parasites <i>Grigoris Zoidis, National and Kapodistrian University of Athens, Greece</i>
18:50-19:10	Small molecule modulators of utrophin for the treatment of Duchenne Muscular Dystrophy <i>Maria Chatzopoulou, University of Oxford, Oxford, U.K.</i>
19:10-19:30	Quinazoline oxime esters as novel DNA Photo cleavers unser both UVB and UVA Irradiation <i>Konstantina Fylaktakidou, Chemistry of Organic Compounds, Molecular Biology and Genetics Department, Democritus University of Thrace, Alexandroupolis, Greece</i>
19:30	Welcome reception
Friday, June 2, 2017	
Session 2 Chairs: TBA	
09:00-9:30	The crystal structure of glycogen phosphorylase in complex with new potent inhibitors discloses the properties of the catalytic site and sheds light in the design of new antidiabetic agents, converging

	interdisciplinary data. <i>Evangelia Chrysina, National Research Center, Greece</i>
09:30-10:00	Predicting the acute toxicity of chemicals against female adults of <i>Aedes aegypti</i>. <i>James Devillers, Centre de Traitement de l'Information Scientifique, France</i>
10:00-10:20	Development of Technetium-99m Chelates as Potential Tumor Imaging Agents <i>Dionysia Papagiannopoulou, Aristotle University of Thessaloniki, Greece</i>
10:20-10:35	Contemporary mechanisms on intracellular calcium mobilization <i>Asiye Meriç, Anadolu University, Tepebasi/Eskisehir, Turkey</i>
10:35-10:50	Unpaveling the problems and solutions of Guanidinium Peptide Coupling Reagents for Peptide – Drug Conjugates <i>Nisar Sayyad, Eftychia M. Mavrogiannaki, Vrettos I. Eirinaios, Serafim Papas, Vassiliki Theodorou, Andreas G. Tzakos</i> <i>Department of Chemistry, University of Ioannina, Ioannina, Greece</i>
10:50-11:05	Cu(II)-1D-CPs catalyzed synthesis of N-substituted-1,4-dihydropyridines and polysubstituted pyrroles as potential L-type calcium channel blockers <i>Michael Kallitsakis, D. Andreou, Ioannis N. Lykakis</i> <i>Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece</i>
11:05-11:30	Coffee Break
Session 3 Chairs: TBA	
11:30-12:00	Divergent Synthesis of Natural Sesquiterpene Lactones. En route to the construction of a promising library of anticancer compounds. <i>Alexandros Zografos, Department of Chemistry, Aristotle University of Thessaloniki, Greece</i>
12:00-12:30	Understanding and modulating the function of purine transporters. <i>George Lambrinidis, Faculty of Pharmacy, National and Kapodistrian University of Athens</i>
12:30-12:50	From public domain compound libraries to cell active leads <i>Vassilis Myrianthopoulos, Faculty of Pharmacy, National and Kapodistrian University of Athens</i>
12:50-13:05	Insight into Fyn and SGK1 KIN¹ASES as new targets in Medicinal Chemistry: desing and synthesis of Pyrazolo [3,4-d] Pyrimidine Libraries <i>Francesca Musumeci¹, Silvia Schenone¹, Anna Lucia Fallacara², Iuni Trist², Nicola Perrotti³, Stefano Alcaro³, Francesco Ortuso³, Giovanni Maga⁴</i> ¹ <i>Department of Pharmacy, University of Genoa, Italy</i> ² <i>Department of Biotechnology, Chemistry and Pharmacy,</i>

	<p>University of Siena, Italy ³Department of "Scienze della Salute", University "Magna Graecia" of Catanzaro, Italy ⁴Institute of Molecular Genetics, IGM-CNR, Pavia, Italy</p>
13:05-14:15	Lunch
14:15-15:30	Poster session and coffee
Session 4 Chairs: TBA	
15:30-16:00	<p>Binding Site Description Analysis of Some New Benzothiazole Derivatives as hGST P1-1 Enzyme Inhibitors <i>Ismail Yaltsin, Ankara University, Turkey</i></p>
16:00-16:30	<p>Design and Synthesis of Topoisomerase II inhibitors. <i>Ioannis Kostakis, Faculty of Pharmacy, National and Kapodistrian University of Athens, Greece</i></p>
16:30-16:45	<p>Research in Antibacterial and Antioxidant activity of essential oils deriving from herbs of Mediterranean flora <i>Eleftheria Chorti-Tripsa</i>¹, Christos Kontogiorgis¹, Diamanto Lazari², Dimitra Hadjipavlou-Litina³, Athanasios Tselemonis¹, Theodoros Constantinidis¹ ¹Medical Department, Democritus University of Thrace, Alexandroupolis, Greece ²Laboratory of Pharmacognosy, Faculty of Pharmacy, Aristotle University of Thessaloniki, Thessaloniki, Greece ³Laboratory of Pharmaceutical Chemistry, Faculty of Pharmacy, Aristotle University of Thessaloniki, Thessaloniki, Greece</p>
16:45-17:00	<p>Synthesis of new pyrazoline analogues and their evaluation in terms of their anti-oxidant and soubean lipoxynesane inhibitory activity <i>Ioanna Kostopoulou¹, Antonia Diassakou¹, Eleni Kavetsou¹, Andromachi Tzani¹, Marina Roussaki¹, Dimitra Hadjipavlou-Litina², Eleni Pontiki², Anastasia Detsi¹</i> ¹School of Chemical Engineers, National Technical University of Athens, Greece ²Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Aristotle University of Thessaloniki, Thessaloniki, Greece</p>
17:00-17:30	Coffee  
17:30- 18:10	<p>Autophagic pathways in health and disease: Mitophagy and neurodegeneration <i>Nektarios Tavernarakis, Foundation for Research and Technology, Greece</i></p>
18:10-18:25	<p>Design and pharmacochemical study of novel compounds containing antioxidant acids and CNS-Acting moieties <i>Georgios Papagiouvannis, Evangelia Papapostolou, Ourania Stogianopoulou, Panos Kourounakis, Eleni Rekka</i></p>

	<i>Department of Medicinal Chemistry, School of Pharmacy, Aristotle University of Thessaloniki</i>
18:30-18:45	In honor of Emeritus Professor Panos Kouroumakis <i>Eleni Rekka, Aristotle University of Thessaloniki Department of Medicinal Chemistry, School of Pharmacy, Aristotle University of Thessaloniki</i>
18:45-19:15	Thoughts on teaching and research in Medicinal Chemistry <i>Panos Kourounakis, Aristotle University of Thessaloniki Department of Medicinal Chemistry, School of Pharmacy, Aristotle University of Thessaloniki</i>
Saturday, June 3, 2017	
Session  Chairs: TBA	
09:15-9:45	Development of phosphinic pseudopeptide inhibitors of Zn-metalloproteases associated with the modulation of immune response <i>Dimitris Georgiadis, Department of Chemistry, National and Kapodistrian University of Athens, Greece</i>
09:45:10:05	Dynamic origins of MHC-I function in antigenic peptide selection <i>Athanassios Papakyriakou, University of Southampton, U.K.</i>
10:05-10:20	New artemisin hybrid molecules: synthesis and In Vitro antileukemic activity <i>Antonios S. Letis¹, Ean-Jeong Seo², Sotiris S. Nikolaropoulos¹, Thomas Efferth², Athanassios Giannis³, Manolis A. Fousteris¹</i> ¹ Laboratory of Medicinal Chemistry, Department of Pharmacy, University of Patras, Greece ² Department of Pharmaceutical Biology, Institute of Pharmacy and Biochemistry, University of Mainz, Germany ³ Institute of Organic Chemistry, Faculty of Chemistry and Mineralogy, University of Leipzig, Germany
10:20-10:35	New C-nor-D-homo spiro-steroids with potential activity in Hedgehog signaling pathway <i>Aggeliki Roumana¹, Dimanthi Pliatsika², Marina Bantzi², Sotiris S. Nikolaropoulos¹, Athanassios Giannis², Manolis A. Fousteris¹</i> ¹ Laboratory of Medicinal Chemistry, Department of Pharmacy, University of Patras, Greece ² Institute of Organic Chemistry, Faculty of Chemistry and Mineralogy, University of Leipzig, Germany
10:35-10:50	Synthesis and pharmacological activity of structurally diverse chemical analogues of compound PQ-10 <i>Agnieszka Zagórska¹, Anna Partyka², Adam Bucki¹, Grażyna Chłoń-Rzepa¹, Magdalena Jastrzębska-Więsek², Agata Siwek³, Monika Głuch-Lutwin⁴, Maciej Pawłowski¹</i> Department of ¹ Medicinal Chemistry, ² Clinical Pharmacy, ³ Pharmacobiology, ⁴ Pharmacodynamic, Jagiellonian University Medical College, Kraków, Poland
10:50-11:05	NMR conformational dynamics of LAM, RRM1 and RRM2

	<p>domains of LA protein <u>Aikaterini Argyriou</u>¹, <u>Maria Apostolidi</u>, <u>Christos T.Chasapis</u>¹, <u>Dionysios Vourtsis</u>¹, <u>Parthena Konstantinidou</u>², <u>Denis Drainas</u>², <u>Detlef Bentrop</u>³, <u>Constantinos Stathopoulos</u>², <u>Georgios A. Spyroulias</u>¹ ¹Department of Pharmacy, University of Patras, Greece. ²Department of Biochemistry, School of Medicine, University of Patras, Greece. ³Institute of Physiology II, University of Freiburg, Germany</p>
11:05-11:30	Coffee Break
<p>Session  Chairs: TBA</p>	
11:30-11:50	<p>An in silico multi-pharmacophore virtual screening methodology for the discovery of novel compounds against pharmacological targets <u>Minos Matsoukas</u>, University of Patras, Greece</p>
11:50-12:05	<p>Breakthrough in rational design of hMAO B inhibitors: SB and LB 3-D QSAR driven generation of novel anti-Parkinson's drug-like structures <u>Milan Mladenovic</u>¹, <u>Alexandros Patsilnakos</u>^{2,3}, <u>Adele Pirolli</u>^{2,4}, <u>Manuela Sabatino</u>^{2,3}, <u>Rino Ragno</u>^{2,3} ¹Kragujevac Center for Computational Biochemistry, University of Kragujevac, Serbia ²Faculty of Pharmacy and Medicine, Rome Sapienza University, Italy ³Alchemical Dynamics srl, Rome, Italy ⁴Department of Information Technology, IRBM Science Park, Rome, Italy</p>
12:05-12:20	<p>In Silico tool for probing the multiple antibacterial profiles of nanoparticles by a QSAR perturbation model <u>M. Natália D.S. Cordeiro</u>, <u>A. Speck-Planche</u> LAQV@REQUIMTE, Faculty of Sciences, University of Porto, Portugal</p>
12:20-12:35	<p>Computer – Aided drug design for binding pose and affinity predictions in the D3R Grand Challenge 2 <u>Christina Athanasiou</u>¹, <u>Sofia Vasilakaki</u>¹, <u>Dimitris Dellis</u>², <u>Woody Sherman</u>, <u>Zoe Cournia</u>¹ ¹ Biomedical Research Foundation Academy of Athens, Greece ² Greek Research and Technology Network, Athens, Greece ³ Silicon Therapeutics, Boston, United States</p>
12:35-12:50	<p>Consensus docking: development, evaluation and experimental application in hit identification <u>Poli Giulio</u>¹, <u>Tuccinardi Tiziano</u>² ¹Department of Biotechnology, Chemistry and Pharmacy, University of Siena, Italy. ²Department of Pharmacy, University of Pisa, Italy</p>
12:50-13:30	<p>The First Molecule Interacting with a Host Protein for the Inhibition of Multiple Viruses Maurizio Botta, Università degli Studi di Siena, Italy</p>
13:30-13:45	Closing of the Symposium