



PROGRAMME

SUNDAY, JUNE 25

14:00-17:00	Registration	
17:00-17:30	Opening of the Meeting	
A WAY FORWARD TO NEW ANTI-INFECTIVES		
Moderator: Gabriele Constantino (Italy)		
17:30-18:15	PL-1	Nenad Ban (ETH Zürich, CH) <i>Beyond the Prokaryotic Ribosome: Structural and Functional Insights Into Eukaryotic and Mitochondrial Ribosomes</i>
18:15-18:45	KL-1	Pavol Jakubec (Slovak University of Technology, SK; Harvard University, USA) <i>A Platform for the Discovery of New Macrolide Antibiotics</i>
18:45-19:25	PL-2	Martin Krátký (Charles University, CZ) <i>Oligotuftsin-based Carriers for Novel Antimycobacterial Active Agents and Their Conjugates</i>
19:30	Welcome party	

MONDAY, JUNE 26

RATIONAL APPROACH TO THE DESIGN OF NOVEL DRUGS		
Moderator: Margot Ernst (Austria)		
9:00-9:45	PL-3	Gerhard Klebe (University of Marburg, DE) <i>What Thermodynamics Can Help to Understand Protein-Ligand Binding in Medicinal Chemistry</i>
9:45-10:15	KL-2	Nace Zidar (University of Ljubljana, SI) <i>Discovery of N-phenylpyrrolamides as ATPase Inhibitors of DNA Gyrase and Topoisomerase IV</i>
10:15-10:45	Coffee break	
ANTI-INFECTIVE CASE STUDIES		
Moderator: Marko Anderluh (Slovenia)		
10:45-11:25	PL-4	Grigoris Zoidis (National and Kapodistrian University of Athens, GR) <i>Metal Chelating Agents Against Viruses and Parasites</i>
11:25-11:55	KL-3	Marta Kučerová-Chlupáčová (Charles University, CZ) <i>Antimicrobial Potential of 1,2,4-Oxadiazoles and Their Synthesis</i>
11:55-12:25	KL-4	Radim Nencka (Czech Academy of Sciences, CZ) <i>Rational Design of PI4KB Inhibitors as Potential Broad-spectrum Antiviral Agents</i>
12:25-15:00	Lunch – POSTER SESSION I	
FILLING THE GAP IN THE DISCOVERY OF NEW ANTI-CANCER DRUGS		
Moderator: Ivo Piantanida (Croatia)		
15:00-15:40	PL-5	Girolamo Cirrincione (University of Palermo, IT) <i>Marine Environment Inspires Kinases Inhibitors</i>
15:40-16:10	KL-5	Matej Sova (University of Ljubljana, SI) <i>Design and Synthesis of Novel Modulators of Toll-like Receptors and Inhibitors of Indoleamine 2,3-Dioxygenase (IDO1)</i>
16:10-16:30	Coffee break	
16:30-17:10	PL-6	János Wölfling (University of Szeged, HU) <i>Old Scaffolds in New Role: Steroids as Antiproliferative Agents</i>
17:10-17:40	KL-6	Vasiliki Sarli (Aristotle University of Thessaloniki, GR) <i>New Drug Conjugates Based on Azasteroids or Peptides for Targeted Drug Delivery in Cancer Therapy</i>
18:30	Trip to Dubrovnik	

TUESDAY, JUNE 27

LOOKING AT THE EPIGENETIC LEVEL

Moderator: János Wölfling (Hungary)

9:00-9:45	PL-7	Paul Brennan (University of Oxford, UK) <i>Chemical Probes in Target Discovery</i>
9:45-10:15	KL-7	Gianluca Sbardella (University of Salerno, IT) <i>A "Library-on-Library" Screening Approach to Identify Small-Molecule Ligands of Methyl-Lysine Reader Proteins</i>
10:15-10:35	Coffee break	

IN SEARCH FOR NOVEL BIOLOGICALLY ACTIVE MOLECULES

Moderator: Jadwiga Turlo (Poland)

10:35-11:15	PL-8	Margot Ernst (Medical University Vienna, AT) <i>GABA_A Receptor Subtypes: A Structure Guided Path to Selective Compounds</i>
11:15-11:45	KL-8	Maciej Dawidowski (Medical University of Warsaw, PL) <i>Disrupting the PEX14-PEX5 Interaction by Small Molecules Provides a Novel Strategy for Treatment of Trypanosoma Infections</i>
11:45-12:15	KL-9	Krzysztof Kaminski (Jagiellonian University, PL) <i>Hybrid Compounds in the Search for the New Highly Effective Anticonvulsants</i>
12:15-12:45	KL-10	Nektarios Aligiannis (National and Kapodistrian University of Athens, GR) <i>Can Multivariate Statistics Aid to the Reveal of Bioactive Compounds? An NMR and HPTLC Approach</i>
12:45-14:00	Lunch	

TARGETING NEURODEGENERATIVE DISORDERS

Moderator: Vesna Eraković Haber (Croatia)

14:00-14:40	PL-9	Stanislav Gobec (University of Ljubljana, SI) <i>New Hits and Leads for Neurodegenerative Disorders</i>
14:40-15:10	KL-11	Marco Macchia (University of Pisa, IT) <i>Endocannabinoid System Modulation: Therapeutic Implications and Future Perspectives</i>
15:10-15:40	KL-12	Robert Vianello (Ruđer Bošković Institute, HR) <i>Computational Insight into the Catalytic Activity of Monoamine Oxidase Enzyme for Targeting Neurological Diseases</i>
15:40-17:00	Coffee break – POSTER SESSION II	

ORAL PRESENTATIONS – section I

Moderator: Magdaléna Májeková (Slovak Republic)

17:00-17:15	OP-1	Manabu Kawada (Institute of Microbial Chemistry - BIKAKEN, JP) <i>Anti-Helicobacter Pylori Activity of a Novel Derivative of Intervonin</i>
17:15-17:30	OP-2	Nela Malatesti (University of Rijeka, HR) <i>In vitro Photodynamic Activity of a New Tri-Cationic Amphiphilic Porphyrin Against Herpes Simplex Virus 1, Bacteria And Cancer Cells</i>
17:30-17:45	OP-3	Giannamaria Annunziato (University of Parma, IT) <i>Discovery of New, Potential Anti-Infective Compounds Based on Carbonic Anhydrase Inhibitors by Rational Target-Focus Repurposing Approach</i>
17:45-18:00	OP-4	Michaela Barančoková (University of Ljubljana, SI) <i>Discovery of Novel Gyrase B Inhibitors and Gyrase B/Topoisomerase IV (ParE) Dual Inhibitors with In Vitro Antibacterial Activity</i>
18:00-18:15	OP-5	Tommaso Felicetti (University of Perugia, IT) <i>Fighting Antimicrobial Resistance by Breaking Resistance Mechanisms</i>
18:15-18:30	OP-6	Dmitry Tselikhovsky (The Hebrew University of Jerusalem, IL) <i>α-Enaminones: New Building Blocks for Direct Synthesis of Biologically Active Alkaloids</i>
18:30-18:45	OP-7	Marcin J. Cieślak (Polish Academy of Sciences, PL) <i>Novel Benzo[b]furan Derivatives – Biological Activity and Protein Target Identification in Leukemic Cells</i>
18:45-19:00	OP-8	Moran Shubely (Bar-Ilan University, IL) <i>Development of Novel Drug Candidate Against Prostate Cancer</i>

ORAL PRESENTATIONS – section II		
Moderator: Jarmila Vinšová (Czech Republic)		
17:00-17:15	OP-9	Rafał Kurczab (Polish Academy of Sciences, PL) <i>Evaluation of Halogen Bonding Hot Spots by Virtual Screening of Commercial Databases – a Case Study of 5-HT_{2R}</i>
17:15-17:30	OP-10	Jaroslav Polanski (University of Silesia, PL) <i>Big Data: Avogadro Stoichiometry Explains Hyperbolic Ligand Efficiency Trend</i>
17:30-17:45	OP-11	Vassilios Myrianthopoulos (University of Athens, GR) <i>From Public Domain Compound Collections to Cell-Active Epigenetic Modulators. The Case of the NCI Repository</i>
17:45-18:00	OP-12	Thavendran Govender (University of KwaZulu Natal, ZA) <i>Mass Spectrometric Imaging as a Preclinical Tool for Medicinal Chemists</i>
18:00-18:15	OP-13	David Chan Bodin Siebert (Technical University Vienna, AT) <i>Pyrazoloquinolinones, Revisited GABA_A Receptor Tool Compounds</i>
18:15-18:30	OP-14	Svetlana Maklakova (Lomonosov Moscow State University, RU) <i>Synthesis of Tissue-Specific Conjugates for Targeted Drug Delivery Into Hepatic Cells</i>
18:30-18:45	OP-15	Rosana Leiva (Universitat de Barcelona, ES) <i>Novel Polycyclic N-acylpyrrolidines as 11β-HSD1 Inhibitors</i>
18:45-19:00	OP-16	Maria Majellaro (University of Santiago de Compostela, ES) <i>Enantiospecific Modulation Of A_{2B} Adenosine Receptor</i>
20:00	Gala Dinner	
WEDNESDAY, JUNE 28		
LIGAND-BASED APPROACH		
Moderator: Gianluca Sbardella (Italy)		
9:00-9:40	PL-10	Jadwiga Turlo (Medical University of Warsaw, PL) <i>Polysaccharides as Biological Response Modifiers: Structure-Activity Relationship</i>
9:40-10:10	KL-13	Magdaléna Májeková (Slovak Academy of Sciences, SK) <i>Ligand-based Drug Design of Novel Aldose Reductase Inhibitors from Databases of Indole-1-Acetic Acids</i>
10:10-10:40	KL-14	Hannes Mikula (Technical University Vienna, AT) <i>Pretargeted Prodrug Activation Through Bioorthogonal Elimination</i>
10:40-11:00	Coffee break	
FROM MOLECULAR PROBES TO CLINICS		
Moderator: Hannes Mikula (Austria)		
11:00-11:40	PL-11	Ivo Piantanida (Ruđer Bošković Institute, HR) <i>Design of Small Molecular Probes for Proteins and DNA / RNA</i>
11:40-12:10	KL-15	Vesna Eraković Haber (Fidelta Ltd., HR) <i>Patient Derived Testing Systems – Reaching Beyond Targeted Based Drug Discovery</i>
12:15-12:45	WINNING POSTERS FLASH PRESENTATIONS	
12:45-13:00	CLOSING	