

H2020 - INFRADEV-03-2018-2019

Ensuring long-term sustainability of excellence in chemical biology within Europe and beyond

“CoriolanDragulescu” Institute of Chemistry, Timisoara, 24 Mihai  
Viteazu Ave., 300223, Timis, Romania

## EU-OPENSREEN DRIVE Workshop 2022

Wednesday 19 October 2022

“Medicinal chemistry in drug discovery, new therapeutical approaches”

**11:00 - 11:15** Welcome - Liliana Pacureanu, Costin-IoanPopescu

**11:15 - 11:25** EU-OPENSREEN – BahneStechmann EU-OPENSREEN DRIVE WP-1 leader

**11:25 - 11:35** Tumor Cell Death Induced by Magnetic Hyperthermia Using Functionalized Magnetic Nanoclusters - IoanaBaldea, AncaPetran, Adriana Filip, Adrian Florea, Maria Letitia Macavei, Mihai Cenariu, Maria TeodoraRadu, Cristian Iacovita, Faculty of Medicine, “Iuliu Hatieganu” University of Medicine and Pharmacy Cluj-Napoca

**11:35 - 11:45** Ketoconazole: from Fundamentals to New Antifungal Formulations Based on PAMAM Dendrimers with Improved Biodisponibility - Flavia Martin, Irina Kacso, IoanaGrosu, Maria Miclaus, Xenia Filip, OcsanaOpris, IoanaBâldea, SorinaDănescu, Dan Vodnar, Mihaela Pop, Faculty of Medicine, “Iuliu Hatieganu” University of Medicine and Pharmacy Cluj-Napoca

**11:45 - 11:55** Antimicrobial Agents: Design, Synthesis, Molecular Docking and Antibacterial Evaluation - Lucia Pintilie, Adela Staras, AnamariaHanganu, Maria Maganu, Miron T. Caproiu, National Institute for Chemical-Pharmaceutical Research - Development Bucharest

**11:55 - 12:20** Coffee break

**12:20 - 12:30** Fluorescence-Based Assays for the Discovery of RAGE Inhibitors – Carmen Tanase, IoanaPopa - Institute of Biochemistry of the Romanian Academy, Bucharest

**12:30 - 12:40** Natural Secretagogues of Hormons Involved in Glucose Metabolism Discovered with Novel Luciferase-Based Assays - SorinaAndreeaAnghel, RodicaBadea, Gabi Chiritoiu, David Patriche, Florentina Pena - Institute of Biochemistry of the Romanian Academy, Bucharest

**12:40 - 12:50** High Throughput Virtual and Experimental Screening of New Free Fatty Acid Receptor 1 Modulators - Cosmin Trif, SorinaAndreeaAnghel, TeodorAsvadurSulea, Maria Alexandra Banica, LaurentiuSpiridon, SorinTunaru - Institute of Biochemistry of the Romanian Academy, Bucharest

**12:50 - 13:50** Lunch

**13:50 - 14:00** Improving the Selection of Protein Crystal Structures for Drug Discovery Docking - SorinAvram, “CoriolanDragulescu” Institute of Chemistry Timișoara

**14:00 - 14:10** Generation of a Receptor Cell Line Suitable for High Throughput Screening of Molecules with Anti-Inflammatory Capacity - Gabriela Chiritoiu<sup>1</sup>, Simona Ghenea<sup>1</sup>, Cristian V.A. Munteanu<sup>1</sup>, Cosmin Trif<sup>1</sup>, CostinIoan Popescu<sup>1</sup>, Laurentiu Spiridon<sup>1</sup>, Mihaela Uta<sup>1</sup>, Livia Sima<sup>1</sup>, Sorin Tunaru<sup>1</sup>, Stefana M. Petrescu<sup>1</sup>, Gina

Simion<sup>2</sup>, Gheorghita Isvoranu<sup>2</sup>, Marioara Chiritoiu-Butnaru<sup>1,2</sup> Institute of Biochemistry of the Romanian Academy, Bucharest, Romania, <sup>2</sup> "Victor Babeş" National Institute of Pathology, Bucharest, Romania

**14:10 - 14:20** Chemically Modified Peptides as Immunomodulatory Agents - Gabi Chiritoiu, Cristian Munteanu, Stefana Petrescu, Institute of Biochemistry of the Romanian Academy, Bucharest

**14:20 - 14:30** Mass-Spectrometry Based Proteomics Approaches Unravel Protein Interactions Networks - Cristian Munteanu, Gabriela Chiritoiu, Cristian Butnaru, Marioara Chiritoiu, Andrei Petrescu, Stefana Petrescu, Institute of Biochemistry of the Romanian Academy, Bucharest

**14:30 - 14:40** Next Generation of Drug Targets for Schizophrenia - Sorin Tunaru, Institute of Biochemistry of the Romanian Academy, Bucharest

**14:40 - 14:50** Spectrophotometric Determinations of Metronidazol - Review - Georgiana Atodiresei-Pavalache, Verginica Schroder, Faculty of Pharmacy, "Ovidius" University Constanța

**14:50 - 15:00** Design and Synthesis of Organic and Inorganic Compounds, Coordination Complexes and Hybrid Materials with Targeted Properties for Applications in Biological and Catalytic Fields - Elisabeta I. Szerb, "Coriolan Dragulescu" Institute of Chemistry Timișoara

**15:00 - 15:30** Coffee break

**15:30 - 15:40** Multifunctional Organic, Hybrid, and Polymeric Compounds with Controlled Properties and Applications - Aurelia Visa, "Coriolan Dragulescu" Institute of Chemistry Timișoara

**15:40 - 15:50** DrugCentral: an Open-Access Drug Compendium Supporting Drug Discovery and Repositioning - Ramona Curpan "Coriolan Dragulescu" Institute of Chemistry Timișoara

**15:50 - 16:00** Deposition of Chemical Compounds in European Academic Compound Library - opportunities and bottlenecks, Liliana Pacureanu, "Coriolan Dragulescu" Institute of Chemistry Timișoara

**16:00 - 16:10** RoChemBioNet Actual Situation and Future Steps Costin-Ioan Popescu, Liliana Pacureanu, "Coriolan Dragulescu" Institute of Chemistry Timișoara

**16:10 - 16:20** Open discussions – participants questions, comments, etc.

**16:20** Event closure – Liliana Pacureanu, Costin-Ioan Popescu, all participants

Thursday 20 October 2022

**13:00 – 15:00** Round table

Participants: Liliana Pacureanu, Costin-Ioan Popescu, Sorin Tunaru, Ioana Popa, Liliana Cseh, Narcisa Marangoci, Cosmin Trif, Laurentiu Spiridon, Ramona Curpan, Elisabeta Szerb, Florentina Pena

Introducing of participants. (2 min)

1. Presentation of the main topics: compound submission to EACL, collaboration inside RoChemBioNet, database management. (8 min)
2. Discussions, ideas and suggestions or experience that relates to the topic. (90 min)
3. Conclusions (20 min)

