



1st WG meeting – MuTaLig COST Action Hotel Novotel Budapest Danube - Budapest, November 19-20 2016

POLY-PHARMACOLOGY EXPANDING PAUL EHRLICH'S MAGIC BULLET CONCEPT

www.mutalig.eu

Saturday November 19st 2016

- 8.30 Registration
- 9.00 **Introduction to the MuTaLig COST Action WG meeting**
Stefano ALCARO (CA15135 Chair & LOS) - Università “Magna Græcia” di Catanzaro (Italy)
[Session I “Experts on multi-targeting drug discovery”](#)
moderator Julio Alvarez-Builla (PE Coordinator)
Alcalá University, Madrid (Spain)
- 9.15 **PL1 Cariprazine: A short overview of newest pharmaceutical and medical milestone in the psychiatry**
György NÉMETH - Chemical Works of Gedeon Richter Plc., Hungary
- 10.00 **PL2 Through privileged scaffolds to multi-target drugs: isatin hybrids as anti-viral and anti-tumour agents**
Elias MACCIONI - University of Cagliari (Italy)
- 10.45 *Coffee break*
- [Session II “New chemical entities \(WG1\)”](#)
Moderator Danijel KIKELJ (WG1 leader)
University of Ljubljana (Slovenia)
- 11.00 **SC1 Multi-target-directed-ligands for Alzheimer's disease**
José MARCO-CONTELLAS, CSIC, Madrid (Spain)
- 11:15 **SC2 Inhibition of multiple targets by novel bisindolylmaleimides**
Florence O. MCCARTHY, University College Cork (Ireland)
- 11:30 **SC3 Chromone as a promising scaffold for the development of multitarget ligands for neurodegenerative diseases**
Joana REIS, University of Porto (Portugal)
- 11:45 **SC4 Development of new indole derivatives as multitarget agents for the treatment of neurodegenerative diseases**
Maria Rosa BUEMI, University of Messina (Italy)

- 12:00 SC5 **Design, synthesis and biological evaluation of novel 1-benzylpyrrolidin-3 amine derivatives as potential inhibitors of beta-secretase and cholinesterases**
Wichur TOMASZ, Jagiellonian University Collegium Medicum, Kraków (Poland)
- 12:15 SC6 **Navigation in bile acid chemical space: discovery of novel FXR and GPBAR1 modulators**
Claudia FINAMORE, University of Naples "Federico II" (Italy)
- 12:30 SC7 **Synthesis of triclosan derivatives and their biological activity**
Rudolf VOSÁTKA, Charles University, Hradec Králové (Czech Republic)
- 12:45 SC8 **Isatin-thiazolidinone hybrids as DNA G-quadruplex selective stabilisers: a new potential approach to multitarget anticancer agents**
Claudia MELIS, University of Cagliari (Italy)
- 13:00 SC9 **Interaction of ATP-competitive DNA gyrase inhibitors with the cellular chaperone HSP90 as a potential pathway to inhibit viral replication**
Tihomir TOMAŠIČ, University of Ljubljana (Slovenia)
- 13:15 SC10 **Rational Design and Synthesis of Novel Amidine-Based Scaffolds as BACE1 Inhibitors**
Myriam CIORDIA JIMÉNEZ, Universidad CEU San Pablo, Madrid (Spain) – *PE awarded*
- 13.30 *Lunch*

Session III "Experts on computational methods"

Moderator Stefano ALCARO (CA15135 Chair & LOS)

Università "Magna Græcia" di Catanzaro (Italy)

- 14.30 PL3 **Setting up a web-based molecular structure database with open-source software**

Norbert HAIDER - University of Vienna (Austria)

- 15.15 PL4 **Computational chemogenomics: Is it more than inductive transfer?**

Dragos HORVATH - CNRS Strasbourg, (France)

- 16.00 *Coffee break and poster session*

Session IV "Chemical databases (WG3) and computational methods for multiple ligand design and discovery (WG4)"

Moderator Hanoch SENDEROWITZ (WG4 leader)

Bar-Ilan University, Ramat-Gan (Israel)

- 16:30 SC11 **Let's develop together an exchange virtual compounds computational platform: Updates!**

Carmine TALARICO, University "Magna Græcia" of Catanzaro (Italy)

- 16:45 SC12 **Natural Compounds from NuBBE database as Inhibitors of Zika Virus – E Protein**

Črtomir PODLIPNIK, University of Ljubljana (Slovenia)

- 17:00 SC13 **A computational multitarget screening for the in silico identification of bioactive compounds**

Roberta ROCCA, University "Magna Græcia" of Catanzaro (Italy) – *PE awarded*

- 17:15 SC14 **Validation of Docking and Dynamic protocol for the study of a new class of Oxadiazoles able to inhibit MAO-B and to prevent Neuronal Oxidative damage**

Giulia BIANCO, University of Cagliari (Italy) – *PE awarded*

- 17:30 *Flash communications selected from the poster session*

- 19:00-21:00 **Social Program** (to be announced)

Sunday November 20st 2016

Session V “Biological targets and assessment of biological data (WG2)”

Moderator Eugenio GAUDIO (WG2 leader)

Oncology Research Institute, Bellinzona (Switzerland)

- 9:00 **SC15 Dual enzyme inhibitors: a promising multi-target approach to cancer therapy**
Rita MELEDDU, University of Cagliari (Italy)
- 9:15 **SC16 Surface proteomics, a step to simplify the rapid prototyping of nanodrugs**
Susana CRISTOBAL, Linköping University (Sweden)
- 9:30 **SC17 Screening the central effects of multitarget agent, non-imidazole H3 receptor antagonist/inverse agonists**
W. Agnieszka FOGEL, Medical University of Lodz (Poland)
- 9:45 **SC18 Targeting metastasis-associated in colon cancer-1 (MACC1) via HGF-Met-MAPK pathway as novel predictive marker for breast cancer**
Daria LERA, PZU Moja Klinika-General Hospital Sarajevo (Bosnia and Herzegovina)
- 10:00 **SC19 Hydroxycinnamic acid as a valid scaffold for the development of CNS multitarget drugs**
Tiago SILVA, University of Porto, (Portugal) – *PE awarded*
- 10:15 **SC20 Discovery of a natural feruloyl ester as single inhibitor of HIV-1 RT and synthesis of its dual inhibitors analogues**
Vijay SONAR, University of Cagliari (Italy)
- 10:30 **SC21 Multitargeting prosurvival pathways in human leukemic cells by metformin and thymoquinone**
Mirza SULJAGIC, International University of Sarajevo (Bosnia and Herzegovina)
- 11:00 **SC22 Targeting dietary antioxidants to mitochondria as a therapeutic solution for mitochondrial oxidative stress related diseases**
José TEIXEIRA, University of Porto (Portugal) – *PE awarded*
- 11:15 *Coffee break*

Round table “Status of the WG activities of MuTaLig COST Action”

open to all participants - Moderator Fernanda BORGES (CA15135 Vice-Chair)

University of Porto (Portugal)

11:45

12:45 **Closing remarks**

13:00 **Lunch**