



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 <u>PL1</u> 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-CONTELLES, 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

11:30 <u>SC3</u> Chromone as a promising scaffold for the development of multitarget ligands for neurodegenerative diseases

Joana REIS, University of Porto (Portugal)

11:45 <u>SC4</u> Development of new indole derivatives as multitarget agents for the treatment of neurodegenerative diseases

Maria Rosa BUEMI, University of Messina (Italy)

12:00 <u>SC5</u> 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 <u>SC6</u> Navigation in bile acid chemical space: discovery of novel FXR and GPBAR1 modulators Claudia FINAMORE, University of Naples "Federico II" (Italy)
- 12:30 <u>SC7</u> Synthesis of triclosan derivatives and their biological activity Rudolf VOSÁTKA, Charles University, Hradec Králové (Czech Republic)
- 12:45 <u>SC8</u> 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 <u>SC9</u> 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 <u>SC10</u> 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 <u>PL3</u> Setting up a web-based molecular structure database with open-source software Norbert HAIDER - University of Vienna (Austria)
- 15.15 <u>PL4</u> 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 <u>SC11</u> Let's develop together an exchange virtual compounds computational platform: Updates! Carmine TALARICO, University "Magna Græcia" of Catanzaro (Italy)
- 16:45 <u>SC12</u> Natural Compounds from NuBBE database as Inhibitors of Zika Virus E Protein Črtomir PODLIPNIK, University of Ljubljana (Slovenia)
- 17:00 <u>SC13</u> A computational multitarget screening for the in silico identification of bioactive compounds Roberta ROCCA, University "Magna Græcia" of Catanzaro (Italy) – *PE awarded*
- 17:15 <u>SC14</u> 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)

	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 LER, PZU Moja Klinika-General Hospital Sarajevo (Bosnia and Herzegovina)
10:00	<u>SC19</u> Hydroxycinnamic acid as a valid scaffold for the development of CNS multitarget drugs
	Tiago SILVA, University of Porto, (Portugal) – PE awarded
10:15	<u>SC20</u> 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	<u>SC21</u> Multitargeting prosurvival pathays in human leukemic cells by metformin and thymoquinone
	Mirza SULJAGIC, International University of Sarajevo (Bosnia and Herzegovina)
11:00	<u>SC22</u> 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 activites 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