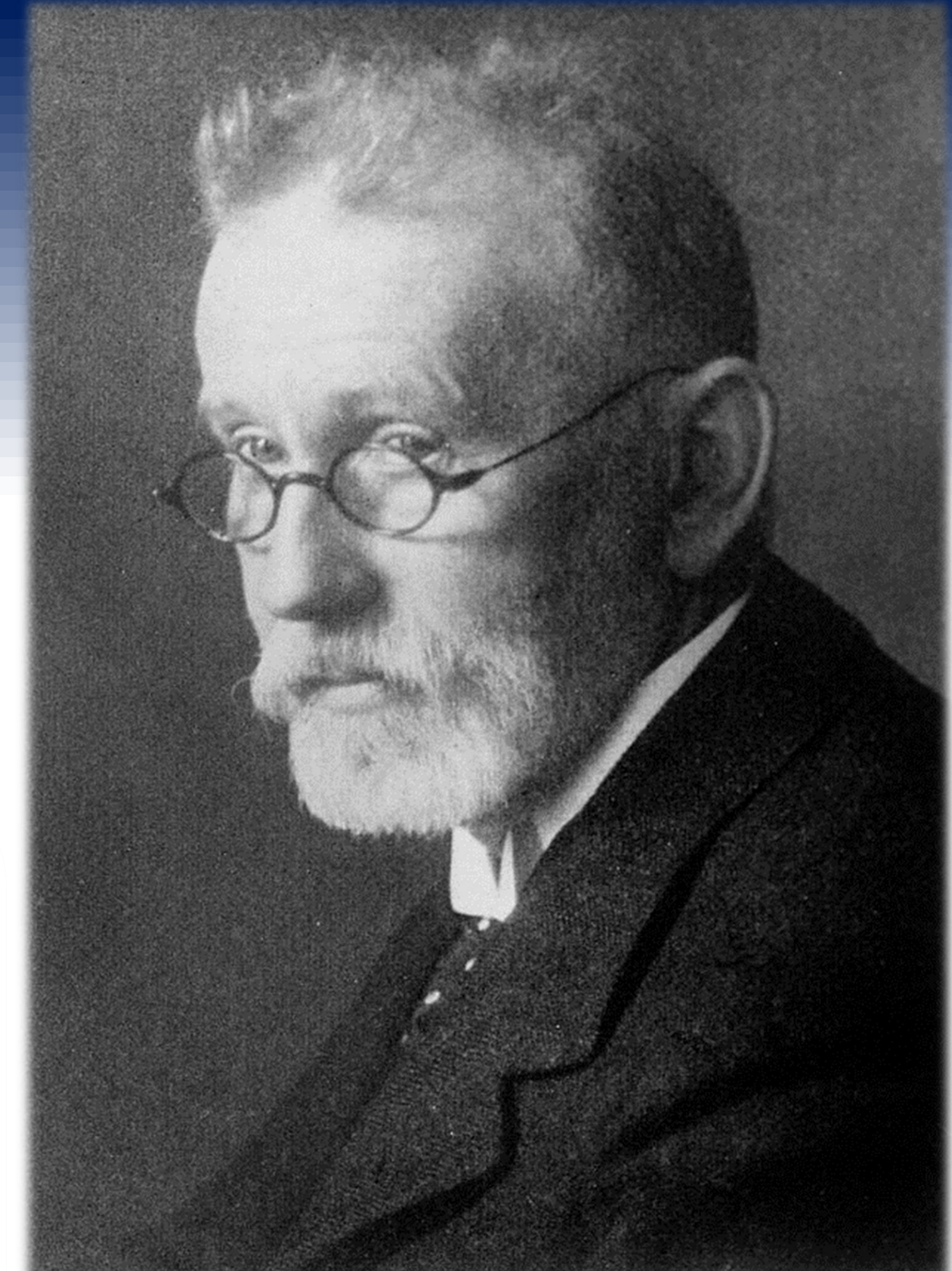


1st WG meeting – MuTaLig COST Action

Hotel Novotel Budapest Danube

Budapest, November 19-20 2016

POLY-PHARMACOLOGY EXPANDING PAUL EHRLICH'S MAGIC BULLET CONCEPT



Prof. Ehrlich

Supported by



Life Science PhD programme
Università Magna Graecia
Catanzaro (Italy)

Program of the 1st WG meeting

Saturday November 19th 2016

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)

- 8.30 Registration
- 9.00 Introduction to the MuTaLig COST Action WG meeting
Stefano **ALCARO** (CA Chair & LOS) - Università "Magna Graecia" 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., Budapest (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-CONTELLI**, 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** (CA Chair & LOS) - Università "Magna Graecia" 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

- 16:30 **SC11** Let's develop together an exchange virtual compounds computational platform: Updates!
Carmine **TALARICO**, University "Magna Graecia" 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 Graecia" 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
Social Program

Sunday November 20th 2016

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

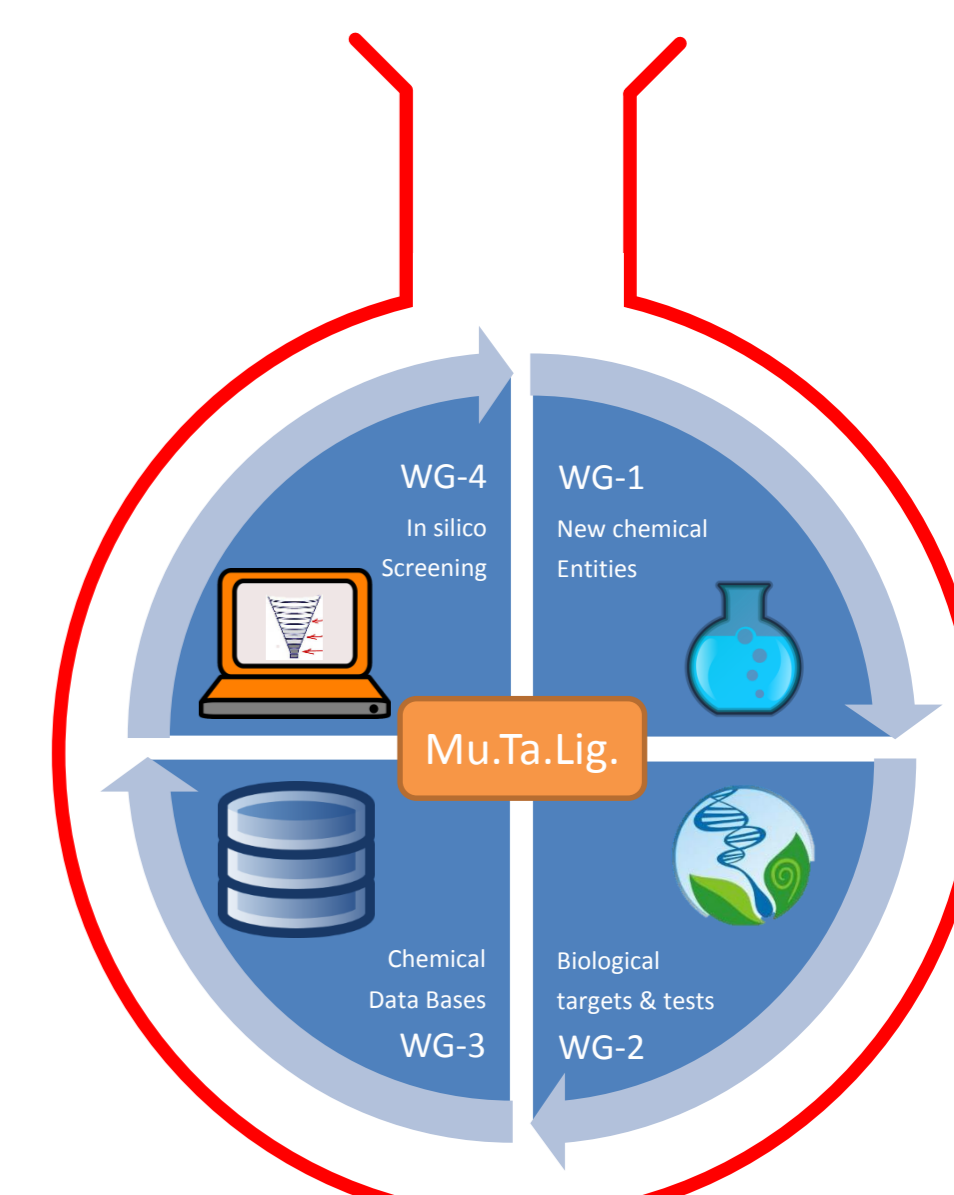
Moderator Eugenio **GAUDIO** (WG2 leader) - Oncology Research Institute, Bellinzona (CH)

- 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 **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 **SULJAGIĆ**, 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
- 15:00 Core group meeting



Info about MuTaLig COST Action
www.cost.eu/COST_Actions/ca/CA15135
www.mutalig.eu

COST ACTION CA15135 Core group

Stefano Alcaro (Italy) - Chair
Fernanda Borges (Portugal) - Vice Chair
Danijel Kikelj (Slovenia) - WG1 leader
Eugenio Gaudio (Switzerland) - WG2 leader
Sharon Bryant (Austria) - WG3 leader
Hanoch Senderowitz (Israel) - WG4 leader
Maria Laura Bolognesi (Italy) - STSM coordinator
Maurizio Botta (Italy) - Industrial coordinator

COST Association officers - Bruxelles

Lucia Forzi - Science officer
Svetlana Voinova - Administrative officer

Grant Holder

Joana Abrantes (Portugal) - GH manager

Local Organizer

Peter Matyus (Hungary) - MC member

Horizon 2020
European Union Funding
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