

Mu.Ta.Lig. COST Action speeds up the European Drug Discovery process



## 1st Annual Meeting of MuTaLig COST Action CA15135 - Preliminary Program Università della Svizzera Italiana - Lugano (CH) - 21-22 July 2016

[www.mutalig.eu](http://www.mutalig.eu)

Thursday July 21<sup>st</sup> 2016

- 8.30 Registration
- 9.00 **Opening Introduction to the MuTaLig COST Action**  
Stefano **ALCARO** (CA15135 Chair) - Università "Magna Græcia" di Catanzaro (Italy)  
**Session I - moderator Danijel KIKELJ (WG1 leader) - University of Ljubljana (Slovenia)**
- 9.10 **PL1 TBD**  
Michele **PARRINELLO** – ETH-USI, Lugano (Switzerland)
- 9.50 **O1 The first molecule interacting with a host protein for the inhibition of multiple viruses**  
Maurizio **BOTTA** (CA15135 Industrial coordinator) - University of Siena (Italy)
- 10.10 **O2 Development of Ribonuclease H/DNA polymerase HIV-1 RT dual inhibitors**  
Simona **DISTINTO** - University of Cagliari (Italy)
- 10.30 **O3 Multiple Targets Selection for Design of Inhibitors of Ebola Virus Infection**  
Črtomir **PODLIPNIK** - University of Ljubljana (Slovenia)
- 10.50 *Coffee break*  
**Session II – moderator Christa MÜLLER (CA15135 IP coordinator) - University of Bonn (Germany)**
- 11.20 **O4 Standard and advanced simulations in drug design**  
Vittorio **LIMONGELLI** – Università della Svizzera Italiana, Lugano (Switzerland)
- 11.40 **O5 3D-Chemical Feature Based Pharmacophores: Essential Tools for Early Drug Discovery Research**  
Sharon **BRYANT** (WG3 leader) - Inte:Ligand GmbH, Vienna (Austria)
- 12.00 **O6 Let's start from the very beginning: The virtual screening work flow**  
Hanoch **SENDEROWITZ** (WG4 leader) - Bar-Ilan University, Ramat-Gan (Israel)
- 12.20 **O7 Let's develop together an exchange virtual compounds computational platform**  
Francesco **ORTUSO** - Università "Magna Græcia" di Catanzaro (Italy)
- 12.40 **O8 Discovering and designing new drugs considering toxicity and safety from the early stages incorporating multiple targets and anti-targets**  
Alfonso **GARCÍA-SOSA** - University of Tartu (Estonia)
- 13.00 *Lunch*  
**Session III – moderator Maurizio BOTTA (CA15135 Industrial coordinator) - University of Siena (Italy)**
- 14.10 **PL2 Patents: applications in the pharmaceutical field**  
Marco **ZARDI** - Zardi & Co. Attorneys, Lugano (Switzerland)
- 14.50 **O9 Development of dual- and multi-target drugs for the treatment of neurodegenerative diseases**  
Christa **MÜLLER** (CA15135 IP coordinator) - University of Bonn (Germany)
- 15.10 **O10 Multi-Target-Directed-Ligands for Alzheimer's Disease**  
José **MARCO-CONTELLAS** - Consejo Superior de Investigaciones Científicas, Madrid (Spain)
- 15.30 **O11 Development of dual target adenosine A1/A2A receptors antagonists among annelated xanthine derivatives**  
Katarzyna **KIEĆ-KONONOWICZ** - Jagiellonian University, Cracow (Poland)
- 15.50 **O12 Dual targeting of adenosine (A1/A2a) receptors and phosphodiesterase 10A by 2-amino-pyrimidin-3-**

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- Eddy SOTELO** - University of Santiago de Compostela (Spain)
- 16.10 *Coffee break*
- Session IV - moderator Sharon BRYANT (WG3 leader) - Inte:Ligand GmbH, Vienna (Austria)**
- 16.40 **O13 Mitochondrial targets for multi-target ligand design**  
**Rona RAMSAY** - University of St Andrews (UK)
- 17.00 **O14 Hydroxycinnamic acid as a valid scaffold for the development of multitarget ligands for CNS disorders**  
**Tiago SILVA** - University of Porto (Portugal)
- 17.20 **O15 Xanthine derivatives as MAO-B inhibitors and adenosine receptor antagonists**  
**Jakub SCHABIKOWSKI** - Jagiellonian University, Cracow (Poland)
- 17.40 **O16 3D-QSAR and design of dopamine D3 receptor ligands**  
**Slavica FILIPIC** - University of Belgrade (Serbia)
- 20.20 *Social Dinner at Lanchetta Restaurant, Via Castagnola 16, Lugano*

## Friday July 22<sup>nd</sup> 2016

- Session V - moderator Hanoch SENDEROWITZ (WG4 leader) - Bar-Ilan University, Ramat-Gan (Israel)**
- 9.00 **PL3 PI3K inhibition (one Dalton apart)**  
**Doriano FABBRO** (CSO, Piqu Therapeutics), Basel (Switzerland)
- 9.40 **O17 The BET Bromodomain inhibitor OTX015 affects pathogenetic pathways in preclinical B-cell tumor models and synergizes with targeted drugs**  
**Eugenio GAUDIO** (WG2 leader) Oncology Research Institute, Bellinzona (Switzerland)
- 10.00 **O18 Isoellipticine: targeting cell proliferation by a structured approach**  
**Florence McCARTHY** - University College Cork (Ireland)
- 10.20 **O19 Identification of new multi-targeted molecules, designed as Neuropilin antagonists, with potent anti-angiogenic and anti-tumour activity in vivo**  
**Luc DEMANGE** - CNRS Paris (France)
- 10.40 *Coffee break*
- Session VI - moderator Eugenio GAUDIO (WG2 leader) - Oncology Research Institute, Bellinzona (Switzerland)**
- 11.10 **O20 Multi-target paradigm for innovative ligand identification in anticancer drug discovery process**  
**Christian MULLER** National Cancer Research Center, Belgrade (Serbia)
- 11.30 **O21 Synthetic compound binding to anticancer drug target proteins: thermodynamics and structure of interaction**  
**Asta ZUBRIENĖ** - University of Vilnius (Lithuania)
- 11.50 **O22 Molecular hybrids targeting 3D Cancer Stem Cells (CSCs)**  
**Nenad FILIPOVIĆ** - University of Belgrade (Serbia)
- 12.10 **O23 Nur77-induced pro-B cells apoptosis is involving multiple pathways**  
**Marcel COSTULEANU** - University of "Grigore T. Popa", Iași (Romania)
- 12.30 **O24 Zn(II), Cu(II) and Co(II) complexes with Schiff bases as potential antitumor agents**  
**Radostina ALEXANDROVA** - Bulgarian Academy of Sciences, Sofia (Bulgaria)
- 12.50 *Lunch*
- 14.00 **MC meeting (only for the Management Committee)**
- 14.30 **Poster Session**
- Session VII - moderator Maria Laura BOLOGNESI (STSM coordinator) - "Alma Mater Studiorum" - University of Bologna (Italy)**
- 16.00 **O25 Design, synthesis and biological activity of novel dual ATP-competitive inhibitors of DNA gyrase and topoisomerase IV**  
**Tihomir TOMAŠIČ** - University of Ljubljana (Slovenia)
- 16.20 **O26 Dual COX-2/5-LOX inhibitors inspired by nature**  
**Marcela DVORAKOVA** - Academy of Sciences of the Czech Republic, Prague (Czech Republic)
- 16.40 **O27 Antimicrobial activity of 1,8-naphthalimide metal complexes**  
**Ivo GRABCHEV** - University of Sofia (Bulgaria)
- 17.00 **O28 Biofilm targets for the development of novel therapeutics**  
**Manuel SIMÕES** - University of Porto (Portugal)
- 17.20 **O29 Inhibitors of aldose reductase with multi-target properties**  
**Magdalena MAJEKOVA** Slovak Academy of Sciences, Bratislava (Slovakia)
- 17.40 *Tea break*
- 18.00 **Round table: Discussion on research perspectives and future activities of MuTaLig COST Action - moderator Fernanda BORGES (CA15135 Vice-Chair) - University of Porto (Portugal)**

Anna ARTESE (MuTaLig web site manager) - Università "Magna Græcia" di Catanzaro (Italy)  
Maria Laura BOLOGNESI (STSM coordinator) - "Alma Mater Studiorum" - University of Bologna (Italy)  
Danijel KIKELJ (WG1 leader) - University of Ljubljana (Slovenia)  
Eugenio GAUDIO (WG2 leader) Oncology Research Institute, Bellinzona (Switzerland)  
Sharon BRYANT (WG3 leader) - Inte:Ligand GmbH, Vienna (Austria)  
Hanoch SENDEROWITZ (WG4 leader) - Bar-Ilan University, Ramat-Gan (Israel)  
Maurizio BOTTA (CA15135 Industrial coordinator) - University of Siena (Italy)  
Christa MÜLLER (CA15135 IP coordinator) - University of Bonn (Germany)  
Claire SHOEMAKE (Gender and Inclusiveness coordinator) - University of Malta (Malta)

19.00 **Concluding remarks**