

1st Annual Meeting of MuTaLig COST Action CA15135 - Final Program

Università della Svizzera Italiana - Lugano (CH) – 21-22 July 2016

www.mutalig.eu



Thursday July 21st 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 **O1 The first molecule interacting with a host protein for the inhibition of multiple viruses**

Maurizio BOTTA (CA15135 Industrial coordinator) - University of Siena (Italy)

9.30 **O2 Development of Ribonuclease H/DNA polymerase HIV-1 RT dual inhibitors**

Simona DISTINTO - University of Cagliari (Italy)

9.50 **O3 Multiple Targets Selection for Design of Inhibitors of Ebola Virus Infection**

Črtomir PODLIPNIK - University of Ljubljana (Slovenia)

10.10 **O4 Biofilm targets for the development of novel therapeutics**

Manuel SIMÕES - University of Porto (Portugal)

10.30 **O5 Design, synthesis and biological activity of novel dual ATP-competitive inhibitors of DNA gyrase and topoisomerase IV**

Tihomir TOMAŠIČ - University of Ljubljana (Slovenia)

10.50 *Coffee break*

Session II

moderator Christa MÜLLER (CA15135 IP coordinator)

University of Bonn (Germany)

11.20 **O6 Standard and advanced simulations in drug design**

Vittorio LIMONGELLI - Università della Svizzera Italiana, Lugano (Switzerland)

11.40 **O7 3D-Chemical Feature Based Pharmacophores: Essential Tools for Early Drug Discovery Research**

Sharon BRYANT (WG3 leader) - Inte:Ligand GmbH, Vienna (Austria)

12.00 **O8 Let's start from the very beginning: The virtual screening work flow**

Hanoch SENDEROWITZ (WG4 leader) - Bar-Ilan University, Ramat-Gan (Israel)

12.20 **O9 Let's develop together an exchange virtual compounds computational platform**

Francesco ORTUSO - Università "Magna Græcia" di Catanzaro (Italy)

12.40 **O10 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 (MuTaLig Industrial coordinator)

University of Siena (Italy)

14.10 **PL1 Patents: applications in the pharmaceutical field**

Marco ZARDI - Zardi & Co. Attorneys, Lugano (Switzerland)

14.50 **O11 Development of dual- and multi-target drugs for the treatment of neurodegenerative diseases**

Christa MÜLLER (CA15135 IP coordinator) - University of Bonn (Germany)

15.10 **O12 Development of dual target adenosine A1/A2A receptors antagonists among annelated xanthine derivatives**

Katarzyna KIEĆ-KONONOWICZ - Jagiellonian University, Cracow (Poland)

15.30 **O13 Antimicrobial activity of 1,8-naphthalimide metal complexes**

Ivo GRABCHEV - University of Sofia (Bulgaria)

15.50 **O14 Inhibitors of aldose reductase with multi-target properties**

Magdalena MAJEKOVA Slovak Academy of Sciences, Bratislava (Slovakia)

16.10 *Coffee break*

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Session IV

moderator Sharon BRYANT (WG3 leader)
Inte:Ligand GmbH, Vienna (Austria)

- 16.40 **O15 Mitochondrial targets for multi-target ligand design**
Rona RAMSAY - University of St Andrews (UK)
- 17.00 **O16 Hydroxycinnamic acid as a valid scaffold for the development of multitarget ligands for CNS disorders**
Tiago SILVA - University of Porto (Portugal)
- 17.20 **O17 3D-QSAR and design of dopamine D3 receptor ligands**
Slavica FILIPIC - University of Belgrade (Serbia)
- 17.40 **O18 Multi-Objective Optimization in Drug Design**
Abraham YOSIPOF - Peres Academic Center, Rehovot (Israel)
- 20.20 *Social Dinner at Lanchetta Restaurant,
Via Castagnola 16, Lugano*

Friday July 22nd 2016

Session V

moderator Hanoch SENDEROWITZ (WG4 leader)
Bar-Ilan University, Ramat-Gan (Israel)

- 9.00 **PL2 PI3K inhibition (one Dalton apart)**
Doriano FABBRO (CSO, Piquar Therapeutics), Basel (Switzerland)
- 9.40 **O19 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 **O20 Isoellipticine: targeting cell proliferation by a structured approach**
Florence McCARTHY - University College Cork (Ireland)
- 10.20 **O21 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 **O22 Multi-target paradigm for innovative ligand identification in anticancer drug discovery process**
Christian MULLER University of Strasbourg, (France)
- 11.30 **O23 Synthetic compound binding to anticancer drug target proteins: thermodynamics and structure of interaction**
Asta ZUBRIENÉ - University of Vilnius (Lithuania)
- 11.50 **O24 Molecular hybrids targeting 3D Cancer Stem Cells (CSCs)**
Nenad FILIPOVIĆ - University of Belgrade (Serbia)

- 12.10 **O25 Nur77-induced pro-B cells apoptosis is involving multiple pathways**
Marcel COSTULEANU - University of "Grigore T. Popa", Iași (Romania)
- 12.30 **O26 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 **PL3 Fluctuations and rare events**
Michele PARRINELLO - ETH-USI, Lugano (Switzerland)
- 16.40 **O27 Dual COX-2/5-LOX inhibitors inspired by nature**
Marcela DVORAKOVA - Academy of Sciences of the Czech Republic, Prague (Czech Republic)
- 17.00 *Tea break*

Round table

moderator Fernanda BORGES (CA15135 Vice-Chair)
University of Porto (Portugal)

Discussion on research perspectives and future activities of MuTaLig COST Action

- **Anna ARTESE** (MuTaLig web site manager) - Università "Magna Græcia" di Catanzaro (Italy)
 - **Dora BOGDAN** (MC substitute, organizer of the WG meeting Hungary) - University of Budapest (Hungary)
 - **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)
- 18.30 **Concluding remarks**