



3rd Annual meeting - MuTaLig COST Action October 18-19 2018

“MuTaLig & Companies: the multi-targeting drug discovery with implications at industrial level”

University of Malta - Campus Historical building - Saint Paul street, Valletta (Malta)



3rd Annual meeting – MuTaLig COST Action

Final program

Thursday October 18th 2018

- 8.30 Registration
- 9.00 **Introduction to the MuTaLig COST Action 3rd Annual meeting**
Stefano ALCARO (CA15135 Chair) - Università “Magna Græcia” di Catanzaro (Italy)
Lilian M. AZZOPARDI Head of Department of Pharmacy, University of Malta and President of the European Association of Faculties of Pharmacy
- Session I: patents and anticancer agents**
Moderator Nigel Richards (MC member for UK) - University of Cardiff, UK
- 9.15 **PL1 From Bench to Spin-off: How to reach results able to be patented**
Bruno BOTTA (MC substitute for Italy) - MoLiRom Srl spinoff, Roma (Italy)
- 9.45 **OR1 Discovery of a new small molecule with strong and selective *in vitro* and *in vivo* therapeutic activity in human lymphomas**
Eugenio GAUDIO (WG2 leader) - Oncology Research Institute, Bellinzona (Switzerland)

- 10.00 **OR2 Angiogenesis inhibitors: better if multi-targeted**
Ana QUESADA University of Malaga (Spain)
- 10.15 **OR3 *In vitro* evaluation of anticancer activity and *in silico* estimation of mechanisms of action of newly synthesized 9-aminoacridine derivatives**
Vladimir DOBRIČIĆ (MC member for Serbia) - University of Belgrade (Serbia)
- 10.30 **OR4 Inhibition of Glutamine Metabolism as a Multitarget Therapy against Pancreatic Ductal Carcinoma**
José M. PADRON (MC substitute for Spain) - Universidad de La Laguna, Tenerife (Spain)
- 10.45 *Coffee break*
- Session II: proprietary products and neurodegeneration**
Moderator Maria Laura BOLOGNESI (MC member for Italy) - "Alma Mater" Università di Bologna (Italy)
- 11.15 **PL2 Lead Discovery Siena: Development of Proprietary Products for Infective diseases and Oncology**
Annalaura BRAI Lead Discovery Siena Srl spinoff, Siena (Italy)
- 11.45 **OR5 Coumarin – One Core to Rule Them All**
Olli PENTIKÄINEN (MC member for Finland) - University of Turku (Finland)
- 12.00 **OR6 Structure-based Discovery of Dual Inhibitors of Disparate Drug Targets for Parkinson's Disease**
Jens CARLSSON (MC member for Sweden) Uppsala University, Sweden
- 12.15 **OR7 Discovery and Characterisation of Tacrine/Huprine-Tryptophan Heterodimers as Novel Multipotent Compounds Against Alzheimer's Disease**
Jan KORABECNY (MC member for Czech Republic) - University Hospital, Hradec Kralove (Czech Republic)
- 12.30 **OR8 In the search for selective cholinesterase inhibitors against Alzheimer's disease**
Óscar LÓPEZ University of Sevilla (Spain)
- 12.45 **OR9 History in the Making: development of multi-target-directed ligands for Alzheimer's disease that modulate oxidative stress/mitochondria quality and the cholinergic system**
Sofia BENFEITO University of Porto (Portugal)
- 13.00 **OR10 ABAD (17β-HSD10) inhibitors with implications to neurodegenerative diseases and cancer treatment (from molecular design to in vivo data)**
Kamil MUSILEK (MC member for Czech Republic) - University of Hradec Kralove (Czech Republic)
- 13.15 *Lunch*
- Session III: against different (multi)targets**
Moderator Maurizio BOTTA (Industrial coordinator of CA15135) - Università di Siena (Italy)
- 14.30 **PL3 Towards the discovery of new correctors of Cystic Fibrosis Transmembrane conductance Regulator (CFTR) based on a repositioning study of photosensitizers**
Paola BARRAJA (Associate Editor of European Journal of Medicinal Chemistry) - Università di Palermo (Italy)
- 15.00 **OR11 Toward Dual Gyrase A/Gyrase B Inhibitors as Antibacterial Agents**
Danijel KIKELJ (WG1 leader) - University of Ljubljana (Slovenia)
- 15.15 **OR12 Increasing Functional Cellular Uptake of Small Molecules Using Deoxycholic Acid Conjugation**
Pavel STARKOV Tallinn University of Technology, Tallinn (Estonia)
- 15.30 **OR13 Rutin fatty acid esters as multi-target compounds**
Magdalena MAJEKOVA Slovak Academy of Sciences, Bratislava (Slovakia)
- 15.45 **OR14 Discovery of Novel Methyl Jasmonate Derivatives and Evaluation of Their Mechanisms in Cancer**
Mustafa GUZEL (MC substitute for Turkey) - Medipol University International, Istanbul (Turkey)
- 16.00 **OR15 Trans-National Fraunhofer small molecule drug discovery projects**
Sheraz GUL (MC substitute for Germany) Fraunhofer Institute, Hamburg (Germany)
- 16.15 **OR16 Physicochemical clustering of pharmaceuticals in the WHO Anatomical Therapeutic Chemical Classification**
Claude FARRUGIA University of Malta, Msida (Malta)
- 16.30 *Coffee break and Poster session*
- 17.00 MC meeting (for MC members/substitutes only)
- 18.00 *Social activity (optional)* www.um.edu.mt/events/mutaliq2018/socialevent

Friday October 19th 2018

- Session IV : computational methods and multi-target drug design**
Moderator Sharon BRYANT (WG3 leader) - Inte:Ligand GmbH, Vienna (Austria)
- 9.00 **PL4 Methods for protein ligand unbinding kinetics estimation**
Sergio DECHERCHI BIKI Technologies Srl spinoff, Genova (Italy)
- 9.30 **OR17 Machine-learning and ligand pharmacology for multi-target ligand design**
Alfonso GARCIA-SOSA (MC member EE, communication manager CA15135) - University of Tartu (Estonia)

- 9.45 **OR18 Binding Estimation After Refinement (BEAR): a post-docking tool for drug design**
Giulio RASTELLI Università di Modena e Reggio Emilia (Italy)
- 10.00 **PL5 A Multi-level strategy for the generation of bioactive conformational ensembles**
Robert SOLIVA NOSTRUM Biodiscovery, Barcellona (Spain)
- 10.30 *Coffee break and Poster session*
- Session V: GPCR ligands**
Moderator Bart ROMAN (MC member for Belgium) – Ghent University (Belgium)
- 11.00 **PL6 Navigating Structural GPCR-Ligand Interaction Space for Computer-Aided Drug Design**
Chris DE GRAAF - HEPTARES therapeutics, Cambridge (UK)
- 11.30 **OR19 Case studies for succesful combination of cholinesterase inhibitors and GPCR ligands with procognitive *in vivo* activity**
Michael DECKER - Julius Maximilian University of Würzburg (Germany)
- 11.45 **OR20 In vitro, in silico and in vivo studies of D2AAK4 as a potential multi-target anti-psychotic**
Agnieszka Anna KACZOR Medical School of Lublin (Poland)
- 12.00 **Round table and best poster awarding ceremony**
Moderator Thierry LANGER (MC substitute for Austria) - University of Vienna (Austria)
Fernanda BORGES (CA15135 Vice-Chair) - University of Porto (Portugal)
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 (Industrial coordinator of CA15135) - Università di Siena (Italy)
Maria Laura BOLOGNESI (STSM coordinator of CA15135) - “Alma Mater” Università di Bologna, Bologna (Italy)
Alfonso GARCIA-SOSA (Communication manager of CA15135) - University of Tartu (Estonia)
- 13.00 **Announcements for the next MuTalig meetings and concluding remarks**
Stefano ALCARO (CA15135 Chair) - Università “Magna Græcia” di Catanzaro (Italy)
Sheraz GUL (MC substitute for Germany) Fraunhofer Institute, Hamburg (Germany)
Luc DEMANGE (MC member for France) Université Paris-Descartes, Paris (France)
Claire SHOEMAKE and David MAGRI (local organizers and Malta MC members) - University of Malta (Malta)

Poster information: Panels for posters have PORTRAIT orientation. The maximum dimensions allowed are 90 cm width x 100 cm tall.