



MuTaLig COST ACTION CA15135
3rd WG meeting 2019
Paris (France), February 23-24 2019



3rd WG meeting – MuTaLig COST Action

Faculté de Pharmacie de Paris, Université Paris DESCARTES, February 23-24 2019

Activities of young investigators within the WG MuTaLig COST Action



Final program

Friday February 22nd 2019

MuTaLig Session at the Young Research Fellows Meeting, French Medicinal Chemistry Society
Moderator: Luc DEMANGE (MC member FR – LOS) - Université Paris DESCARTES (France)

15:00 - 17.30 Information at the web site www.sct-asso.fr/yrfm.html

Saturday February 23rd 2019

8.30 Registration

9.00 **Introduction to the MuTaLig COST Action 3rd WG meeting**

Stefano ALCARO (CA15135 Chair) - Università “Magna Græcia” di Catanzaro (Italy)

Luc DEMANGE (MC member for France and local organizer) - Université Paris DESCARTES (France)

Session I “Drug repositioning and kinase opportunities”

Moderator: David MAGRI (MC member MT) - University of Malta (Malta)

9.30 **PL1 Repositioning approach to fish new multitarget bioactive molecules: Application to the development of analogues to bisacodyl.**

Maité SYLLA - Conservatoire national des arts et métiers, Paris (France)

10.00 **PL2 Towards selective Kinase Inhibitors. Elucidation of their Molecular Mechanism of Action**

Hervé GALONS (Editor in Chief of Eur J Med Chem) - Université Paris DESCARTES (France)

10.30 *Coffee break and Poster session*

Session II “Selected WG1 and WG2 young investigators in anticancer field”

Moderator: Gilles HANQUET (MC member FR) - Université de Strasbourg (France)

11:00 **OC1 Synthesis and Antagonist Study of CXCR1 and CXCR2 Receptors for Oncology Applications**

Lou MATEO - Université côte d’Azur, Nice (France)

11.20 **OC2 A branching inhibitor in plants as a new antiangiogenic and antitumoral drug candidate**

Paloma CARRILLO - University of Malaga (Spain)



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Session II “Selected WG1 young investigators in CNS field”

Moderator: Hoger STARK (MC member DE) - Heinrich-Heine University, Düsseldorf (Germany)

- 11.40 **OC3 Development of novel MTDL combining 5-HT4R agonism and antioxidant properties in Alzheimer’s disease**
Caroline LANTHIER - (CERMN), Normandie Univ, UNICAEN, Caen (France)
- 12.00 **OC4 Development of Dual-Target Agents Based on Piperine Scaffold**
Daniel CHAVARRIA - University of Porto (Portugal)
- 12.20 **OC5 Studies on novel tacrine-donepezil hybrids with potent MTDL profile**
Gülşah BAYRAKTAR - Ege University, Izmir (Turkey)
- 12.40 **OC6 Design and development of new chemical entities for the treatment of Parkinson disease**
Francesco MESITI - Università “Magna Græcia” di Catanzaro (Italy)
- 13.00 **OC7 Highly Selective and Antioxidant BChE Inhibitors with Controllable Duration of Action Showing Neuroprotective Properties *in vivo***
Matthias HOFFMANN - Julius-Maximilians University, Würzburg (Germany)
- 13.20 *Lunch and Poster session*

Session III “Selected WG2, WG3 and WG4 young investigators”

Moderator: Emmanuel MIKROS (MC member EL) - University of Athens (Greece)

- 15.00 **OC8 Novel Fubinaca/Rimonabant Hybrids as Endocannabinoid System Modulators**
Azzurra STEFANUCCI - “G. d’Annunzio” University, Chieti (Italy)
- 15.20 **OC9 Tracking the Oxypeucedanin: from ethnobotanical studies to pharmacological target**
Elif ALANÇAY - Ege University, Izmir (Turkey)
- 15.40 **OC10 Targeting metabolism and apoptosis signaling in cancer cells: a structure-based virtual screening approach toward Hexokinase 2 inhibitors**
Sara N. GARCIA - Universidade de Lisboa (Portugal)
- 16.00 **OC11 The Mu.Ta.Lig. Chemotheca: Chemoinformatic tool for Multi-Target Drugs Identification and Compounds Repurposing**
Raffaella CATALANO - Università “Magna Græcia” di Catanzaro (Italy)
- 16.20 **OC12 Funnel-Metadynamics Automated Protocol (FMAP): three steps to disclose drug pharmacodynamics**
Stefano RANIOLO - Università della Svizzera italiana (USI), Lugano (Switzerland)
- 16.40 **OC13 The *in silico/in vitro* metabolism identification of the series promising xanthine- and tert-amylphenoxyalkyl piperidine derivatives with confirmed multi target directed activity**
Gniewomir LATACZ - Jagiellonian University Medical College, Kraków (Poland)
- 17.00 *Jazz free event (organized by the student’s associations of the Faculty of Pharmacy)*
- 18.30 **Core meeting (for the MuTaLig Core group only)**
- 19.30 *Optional social activity (cruise & dinner)*



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Sunday February 24th 2019

Session IV: "New ideas and updates from Working Groups"

Moderator: Stefano ALCARO (CA15135 Chair) - Università "Magna Græcia" di Catanzaro (Italy)

9:00 **OC14 Zn(II) complexes with pyridine-based thiazolyl-hydrazones as potent multi-targeting anticancer agents**

Nenad FILIPOVIĆ (MC substitute SR) - University of Belgrade (Serbia)

9.20 **OC15 Pyridoindole compounds with multi-target effects**

Magdaléna MÁJEKOVÁ (MC member SK) - Institute of Exp Pharm and Tox, Bratislava (Slovakia)

9.40 **OC16 Recent Progress on Naphthalimide Molecular Logic Gate Anticancer Agents**

David MAGRI (MC member MT) – University of Malta (Malta)

10.00 **OC17 Multi-Target Qualities and Ligand Pharmacology for Neurodegenerative, Cancer, and Other Inhibitors in the Chemotheca**

Alfonso T. GARCÍA-SOSA (MC member EE, communication manager) - University of Tartu (Estonia)

10.20 **OC18 Isatin-Triazole Hybrids: Lymphoma Anti-Proliferation and BuChE Inhibition**

Antony BURKE - University of Évora (Portugal)

10.40 *Coffee break*

11.15 **Round table and best poster awarding ceremony**

Moderator: 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)

Alfonso T. GARCÍA-SOSA (MC member EE, communication manager) - University of Tartu (Estonia)

Maria Laura BOLOGNESI (STSM coordinator) - "Alma Mater" Università di Bologna (Italy)

12.30 **Concluding remarks**

Poster information: Panels for posters have PORTRAIT orientation. The maximum dimensions allowed are 95 cm width x 150 cm tall.