



4th WG meeting – MuTaLig COST Action

Faculty of Pharmacy, Ege University, March 5-6 th 2020

Final status of WG activities within the MuTaLig COST Action



Final program

Thursday March 5th 2020

8.30 Registration

9.00 Introduction to the MuTaLig COST Action 4th WG meeting

Necdet BUDAK (Rector) – Ege University (Turkey)

Ayfer YALÇIN (Dean of Faculty of Pharmacy) – Ege University (Turkey)

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

Günay YETİK-ANACAK (MC member Turkey and local organizer) – Ege University (Turkey)

Body percussion dance show with mortar and pestle "A multi-targeting pharmacist: Galen from Aegean land"

Reports of the WG leaders

Moderator: Fernanda BORGES - (Vice-Chair and MC member Portugal) 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)

10.30 Coffee break

Session I "Multi-targeting agents against cancer and infections"

Moderator: David C. MAGRI – (MC member Malta) University of Malta (Malta)

- 11.00 OC1 Toward Multitarget DNA Gyrase Inhibitors Possessing Antibacterial Activity Danijel KIKELJ (WG1 leader) University of Ljubljana (Slovenia)
- 11.15 OC2 Repositioning of [1,6] Naphthyridines as Antiviral Agents on HSV-1
 Alessandra MONTALBANO University of Palermo (Italy)
- 11.30 OC3 Indolocarbazole maleimides with dual inhibition of kinases and topoisomerase I Florence MCCARTHY (MC member Ireland) University College, Cork (Ireland)

11.45 OC4 Epigenetic Multitargeting in Cancer: Design, Synthesis And Biological Evaluation of Novel Inhibitors

Filipa RAMILO GOMES – University of Lisbon, Lisbon (Portugal)

12.00 OC5 The effect of New Synthesized Resveratrol Derivate H1 on angiogenesis Emine Nur ÖZBEK – Ege University, İzmir (Turkey)

12.15 OC6 A Comparative Study of The Antiangiogenic Activity of Hydroxytyrosyl Alkyl Ethers as Multitargeted Bioactive Compounds

Miguel Ángel MEDINA – University of Málaga, Málaga (Spain)

12.30 OC7 High throughput in-vitro early toxicity and off-target liability assays to rapidly identify limitations of novel thyromimetics

Sheraz GUL – (MC substitute Germany) Fraunhofer Institute, Hamburg (Germany)

12.45 OC8 Cytotoxic Effect of Zn(II)/Au(I), Zn(II)/Ag(I) And Ru(III) Complexes with Schiff Bases in Human Osteosarcoma Cellstitle

Radostina ALEXANDROVA – (MC member Bulgaria) Bulgarian Academy of Sciences (Bulgaria)

13.00 OC9 Multitarget Covalent Inhibitory Property of Klavuzons
Ali ÇAĞIR – Izmir Institute of Technology (IYTE), İzmir (Turkey)

13.15 Lunch and poster session

Session II "Multi-targeting agents against neurodegenerations"

Moderator: Fernanda BORGES – (Vice-Chair and MC member Portugal) University of Porto (Portugal)

14.45 OC10 Expanding the medicinal chemistry Multi-Target Directed Ligands toolbox for neurodegeneration: rationally designed fragment, hybrids and conjugate small molecules Maria Laura BOLOGNESI – (STSM coordinator) University of Bologna (Italy)

15.00 OC11 Natural Product Hybrids are Potent Neuroprotectants in Vitro And in Vivo: Multi-Target Ligands with Unknown Targets?

Michael DECKER – University of Würzburg (Germany)

15.15 OC12 Targeting Alzheimer's Disease with 4-Aminochromane Derivatives
Anthony BURKE – University Evora (Portugal)

15:30 OC13 Combination of Adenosine Antagonism with Additional H3R Antagonism for the Treatment of Parkinson's Disease

Holger STARK – (MC member Germany) Heinrich Heine University of Duesseldorf (Germany)

15.45 OC14 Histamine H3 receptor antagonism as a valuable component for multitarget directed ligands (MTDL)

Wieslawa Agnieszka FOGEL – (MC member Poland) Medical University of Lodz (Poland)

16.00 OC15 Repurposing Compounds Designed to Treat Mental Diseases as Potential Drugs Against Neurodegenerative Diseases

Agnieszka A. KACZOR – Medical University of Lublin (Poland)

16.15 OC16 Mapping the chromone-3- phenylcarboxamides pharmacophore: structure-activity-toxicity and efflux transport studies

Francesco Mesiti – Università "Magna Græcia" di Catanzaro (Italy)

16:30 Coffee break

Session III "Multi-targeting agents against vascular diseases or oxidative stress"

Moderator: Florence MCCARTHY – (MC member Ireland) University College, Cork (Ireland)

16.45 OC17 Interplay between superoxide dismutase, catalase and peroxidase activities for salenmanganese complexes

Marcelino MANEIRO – University of Santiago de Compostela, Santiago de Compostela (Spain)

17.00 OC18 Mitochondriotropic Cinnamic Acid Antioxidant Improves Cellular Resistance to Stress Ricardo AMORIM – University of Porto, Porto (Portugal)

17.15 OC19 Vascular effects of pioglitazone related to perivascular adipose tissue (PVAT)

Deniz KALELİ DURMAN – Istanbul University, İstanbul (Turkey)

17.30 OC20 The journey from ethnobotanical studies to pharmacological target: The effect of imperatorin and isoimperatorin on penile relaxation

Nazlıcan BELEN – Ege University, Izmir (Turkey)

17.45 OC21 A Potential Repositioning of Trimetazidine for the Treatment of Bladder Dysfunction: Effects on Mouse Detrusor Contractility and Cytoprotection

Yeşim KAYA YAŞAR – Karadeniz Technical University, Trabzon (Turkey)

18.15 Transfer to gala dinner (optional)

Friday March 6th 2020

Session IV: "New methods in Drug Discovery, in silico pharmacology and drug repurpos	ing"
Moderator: Holger STARK - (MC member Germany) Heinrich Heine University of Duesseldorf	(Germany

- 9.00 OC22 A Lab-on-a-Molecule with an Enhanced Fluorescent Readout on Detection of Three Chemical Species
 - David C. MAGRI (MC member Malta) University of Malta (Malta)
- 9.15 OC23 New screening libraries arising from the Prestwick Chemical Drug Library Marie Louise JUNG Prestwick Chemical, Strasbourg (France)
- 9.30 OC24 Lead to Target: A Computational Approach to Identify Possible Protein Targets of Molecules with Known Experimental Biological Activity
 - Sérgio F. SOUSA University of Porto (Portugal)
- 9.45 OC25 Drug design in silico: dream, (next) future or even coming reality?

 Diego LIBERATI National Research Coucil of Italy @ Politecnico di Milano (Italy)
- 10.00 OC26 Computational Approaches in Muti-target Drug Discovery
 Rita GUEDES (MC member Portugal) University of Lisbon (Portugal)
- 10.15 OC27 Multi-Target Ligand Design is Ripe for New Methods
 Alfonso T. GARCÍA-SOSA (MC member EE, communication manager) University of Tartu (Estonia)
- 10.30 OC28 New Inhibitors of the BmrA Pump Identified Through Virtual Screening
 Onur SERÇİNOĞLU Recep Tayyip Erdogan University, Rize (Turkey)
- 10.45 Coffee break
- 11.00 Round table on perspectives of the MuTaLig community

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

Antonio LUPIA – (FAD manager) Net4Science academic spinoff, Catanzaro (Italy)

Fernanda BORGES – (Vice-Chair and MC member Portugal) University of Porto (Portugal)

Danijel KIKELJ – (WG1 leader) University of Liubliana (Slovenia)

Alfonso T. GARCÍA-SOSA – (MC member EE, communication manager) University of Tartu (Estonia) Maria Laura BOLOGNESI – (STSM coordinator) University of Bologna (Italy)

- 12.15 <u>Concluding remarks and best poster awarding ceremony</u>
 Günay YETİK-ANACAK (MC member Turkey and local organizer) Ege University (Turkey)
- 12.45 Snack and farewell

Poster information: Panels for posters have PORTRAIT orientation. The maximum dimensions allowed are **70 cm width x 90 cm** tall.