



2nd WG meeting – MuTaLig COST Action

Instituto Universitario de Bio-Organica “Antonio González” (IUBO-AG) - Universidad de La Laguna, Tenerife (Spain), March 15-16 2018



STATUS OF WG ACTIVITIES OF THE MUTALIG COST ACTION

Final program

Thursday March 15th 2018

- 8.30 Registration
- 9.00 **Introduction to the MuTaLig COST Action 2nd WG meeting**
Manuel NORTE (IUBO AG Director) - Universidad de La Laguna, Tenerife (Spain)
Stefano ALCARO (CA15135 Chair) - Università “Magna Græcia” di Catanzaro (Italy)
José M. PADRON (MC substitute for Spain and local organizer) - Universidad de La Laguna, Tenerife (Spain)
- Session I “Reports by WG leaders on the status of WG activities”**
Moderator: Stefano ALCARO (CA15135 Chair) - Università “Magna Græcia” di Catanzaro (Italy)
- 9.15 **WG1 Report**
Danijel KIKELJ (WG1 leader) - University of Ljubljana (Slovenia)
- 9.30 **WG2 Report**
Eugenio GAUDIO (WG2 leader) - Oncology Research Institute, Bellinzona (Switzerland)
- 9:45 **WG3 Report**
Sharon BRYANT (WG3 leader) - Inte:Ligand GmbH, Vienna (Austria)
- 10.00 **WG 4 Report**
Hanoch SENDEROWITZ (WG4 leader) - Bar-Ilan University, Ramat-Gan (Israel)
- 10.15 *Coffee break*
- Session II “Towards new chemical entities within WG1”**
Moderator: Ivo Grabchev (MC member Bulgaria)
- 10.45 **PL1 New molecular entities as inhibitors of HBV and (re)emerging virus replication**
Maria José CAMARASA (invited speaker) - Instituto de Química Médica (IQM, CSIC), Madrid (Spain)

- 11.15 **OC1 Novel indanone derivatives as MAO B/H3R dual targeting ligands for treatment of Parkinson's disease**
Holger STARK (MC member DE) - University Duesseldorf (Germany)
- 11.30 **OC2 Biological activity of novel benzylidene-based (1,3-selenazol-2-yl)hydrazones**
Nenad FILIPOVIĆ - University of Belgrade (Serbia)
- 11.45 **OC3 The utility of the xanthine scaffold for developing MAO-B inhibitors and antioxidants**
David SYNAK - Jagiellonian University Medical College, Kraków (Poland)
- 12.00 **OC4 Chalcogen-based privileged structures in the design of new multitarget drugs**
Óscar LÓPEZ - University of Sevilla (Spain)
- 12.15 **OC5 Development of multi-target agents based on hydroxybenzoic acid scaffold endowed with mitochondriotropic antioxidant and cholinesterase inhibitory activities**
Catarina OLIVEIRA - Universidade do Porto (Portugal)
- 12.30 **OC6 Naphthalimide Molecular Logic Gates as Fluorescence Cellular Imaging and Anticancer Agents**
David MAGRI (MC member ML) - University of Malta (Malta)
- 12.45 **OC7 Multi-target paradigm for innovative ligand identification in anticancer drug discovery process**
Christian MULLER - Université de Strasbourg, Illkirch (France)
- 13.00 **OC8 Symmetry of Ligands: Matriptase-2 Inhibitors as a Case Study in Drug Design**
Michael GÜTSCHOW - University of Bonn (Germany)
- 13.15 *Lunch*
- Session III "Selection of biological targets and assessment of biological data within WG2"**
Moderator: Maria Laura Bolognesi (CA15135 STSM coordinator) "Alma Mater" Università di Bologna (Italy)
- 14.15 **PL2 MicroRNAs in Oncogenesis: Leading or Passenger? It doesn't matter!**
Rami AQEILAN (invited speaker) - The Hebrew University Faculty of Medicine, Jerusalem (Israel)
- 14.45 **OC9 The propargylamine warhead in multi-target compounds for inactivation of MAO**
Rona RAMSAY (MC member UK) - University of St Andrews (UK)
- 15.00 **OC10 Hydrogen sulfide: a candidate multitarget ligand for cardiovascular diseases**
Gunay YETIK ANACAK (MC member TK) - Ege University, Izmir (Turkey)
- 15.15 **OC11 Combinatorial screening of the pan-PI3K inhibitor Copanlisib in T cell lymphomas**
Eugenio GAUDIO (MC member CH, WG2 leader) - Institute of Oncology Research, Bellinzona (Switzerland)
- 15.30 **OC12 Metformin interference with survival signaling in DLBCL**
Mirza SULJAGIC (MC member BA) - International University of Sarajevo (Bosnia and Herzegovina)
- 15.45 **OC13 Mitochondriotropic antioxidants based on cinnamic acid increase cellular stress responses in HepG2 cells**
Ricardo AMORIM - Universidade do Porto (Portugal)
- 16.00 **OC14 Unbiased assessment of direct or indirect targets of any bioactive compound on a proteome-wide scale**
Susana CRISTOBAL (MC member SE) - Linköping University (Sweden)
- 16.15 **OC15 Histamine H₄ receptors a new therapeutic target in postinfectious cardiomyopathy?**
Wiesława Agnieszka FOGEL (MC member PL) - University of Lodz (Poland)
- 16.30 *Coffee break and Poster session*
- Session IV "Development of chemical databases within WG3"**
Moderator: Sharon Bryant (MC member Austria, WG3 leader)
- 17.00 **PL3 Structure of human asparagine synthetase informs the development of new reagents for probing the metabolism of sarcoma cells**
Nigel RICHARDS (invited speaker) - University of Cardiff (UK)
- 17.30 **OC16 Molecular modeling of novel MAO-B/AChE dual inhibitors as potential anti-Parkinson agents**
Donatella BAGETTA - Università "Magna Græcia" di Catanzaro (Italy)
- 17.45 **OC17 Tau-directed polypharmacological approach in Alzheimer's disease: development of a small library of thiazolidinediones**
Annachiara GANDINI - "Alma Mater" Università di Bologna (Italy)
- 18.00 **OC18 Development of a plant genetic toolbox for the production of pharmaceutically-relevant triterpenes**
Christelle ANDRÉ - (MC member LU) Luxembourg Institute of Science and Technology, Belvaux (Luxembourg)
- 18.15 **OC19 New efficient inhibitors of aldose reductase from the family of carboxymethylated indoles**
Magdaléna MÁJEKOVÁ - (MC member SK) Center of Experimental Medicine, Bratislava (Slovakia)
- 18.30 **OC20 Macrocyclic amidinoureas, a valid scaffold for antifungal and chitinase inhibiting compounds**
Francesco OROFINO - Università degli Studi di Siena (Italy)
- 20.30 *Social Dinner at TASCA SIN FRENO, located at Calle Cruz de la Candelaria 35, La Laguna*

Session V “Development of Computational methods for multiple ligand design and discovery within WG4”

Moderator: Hanoch Senderowitz (MC member Israel, WG4 leader)

- 9.00 **PL4 MD Derived Feature-based Pharmacophores: A New Way to Enhance Virtual Screening Efficacy in Multitarget Drug Discovery**
Thierry LANGER (MC substitute A) - University of Vienna (Austria)
- 9.30 **OC21 Efficient virtual screening and prediction of binding profiles**
Olli PENTIKÄINEN (new MC member FI) - University of Turku (Finland)
- 9.45 **OC22 Novel techniques for multitarget and multi-antitarget design for blebbistatin analogs**
Alfonso GARCIA-SOSA (MC member EE, communication manager of CA15135) - University of Tartu (Estonia)
- 10.00 **OC23 Self-assembled ligands targeting TLR7: a molecular level investigation**
Andrea DANANI – (MC substitute CH) Università della Svizzera Italiana (USI), Manno (Switzerland)
- 10.15 **OC24 Induced Fit Docking Protocol applied to the *in silico* evaluation of antiviral HIV-1 integrase resistance**
Francesca Alessandra AMBROSIO - Università “Magna Græcia” di Catanzaro (Italy)
- 10.30 **OC25 STD-NMR-in silico Screening: An Effective Combination for Validating ChE and MAO-B Dual Inhibition**
Antony BURKE – Universidade de Évora (Portugal)
- 10.45 **OC26 Multi-level strategy for analysis of bioactive drug conformations**
Sanja ZIVANOVIC – (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona (Spain)
- 11.00 *Coffee break*
- 11.30 **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 GARCIA-SOSA (MC member EE, communication manager of CA15135) - University of Tartu (Estonia)
Maria Laura BOLOGNESI (STSM coordinator of CA15135) - “Alma Mater” Università di Bologna (Italy)
Simona RAPPOSELLI (Associate Editor Frontiers in Chemistry) - Università di Pisa (Italy)
Claire SHOEMAKE (Gender and Inclusiveness coordinator) - University of Malta (Malta)
- 12.30 **Concluding remarks**
- 13.00 **Core meeting (for the MuTaLig Core group only)**

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