

- 12:00 SC5 **Design, synthesis and biological evaluation of novel 1-benzylpyrrolidin-3 amine derivatives as potential inhibitors of beta-secretase and cholinesterases**
Wichur TOMASZ, Jagiellonian University Collegium Medicum, Kraków (Poland)
- 12:15 SC6 **Navigation in bile acid chemical space: discovery of novel FXR and GPBAR1 modulators**
Claudia FINAMORE, University of Naples "Federico II" (Italy)
- 12:30 SC7 **Synthesis of triclosan derivatives and their biological activity**
Rudolf VOSÁTKA, Charles University, Hradec Králové (Czech Republic)
- 12:45 SC8 **Isatin-thiazolidinone hybrids as DNA G-quadruplex selective stabilisers: a new potential approach to multitarget anticancer agents**
Claudia MELIS, University of Cagliari (Italy)
- 13:00 SC9 **Interaction of ATP-competitive DNA gyrase inhibitors with the cellular chaperone HSP90 as a potential pathway to inhibit viral replication**
Tihomir TOMAŠIČ, University of Ljubljana (Slovenia)
- 13:15 SC10 **Rational Design and Synthesis of Novel Amidine-Based Scaffolds as BACE1 Inhibitors**
Myriam CIORDIA JIMÉNEZ, Universidad CEU San Pablo, Madrid (Spain) – *PE awarded*
- 13.30 *Lunch*

[Session III "Experts on computational methods"](#)

Moderator Stefano ALCARO (CA15135 Chair & LOS)

Università "Magna Græcia" di Catanzaro (Italy)

- 14.30 PL3 **Setting up a web-based molecular structure database with open-source software**
Norbert HAIDER - University of Vienna (Austria)
- 15.15 PL4 **Computational chemogenomics: Is it more than inductive transfer?**
Dragos HORVATH - CNRS Strasbourg, (France)

16.00 *Coffee break and poster session*

[Session IV "Chemical databases \(WG3\) and computational methods for multiple ligand design and discovery \(WG4\)"](#)

Moderator Hanoch SENDEROWITZ (WG4 leader)

Bar-Ilan University, Ramat-Gan (Israel)

- 16:30 SC11 **Let's develop together an exchange virtual compounds computational platform: Updates!**
Carmine TALARICO, University "Magna Græcia" of Catanzaro (Italy)
- 16:45 SC12 **Natural Compounds from NuBBE database as Inhibitors of Zika Virus – E Protein**
Črtomir PODLIPNIK, University of Ljubljana (Slovenia)
- 17:00 SC13 **A computational multitarget screening for the in silico identification of bioactive compounds**
Roberta ROCCA, University "Magna Græcia" of Catanzaro (Italy) – *PE awarded*
- 17:15 SC14 **Validation of Docking and Dynamic protocol for the study of a new class of Oxadiazoles able to inhibit MAO-B and to prevent Neuronal Oxidative damage**
Giulia BIANCO, University of Cagliari (Italy) – *PE awarded*
- 17:30 Flash communications selected from the poster session
- 19:00-21:00 **Social Program** (to be announced)

Session V “Biological targets and assessment of biological data (WG2)”

Moderator Eugenio GAUDIO (WG2 leader)

Oncology Research Institute, Bellinzona (Switzerland)

- 9:00 SC15 **Dual enzyme inhibitors: a promising multi-target approach to cancer therapy**
Rita MELEDDU, University of Cagliari (Italy)
- 9:15 SC16 **Surface proteomics, a step to simplify the rapid prototyping of nanodrugs**
Susana CRISTOBAL, Linköping University (Sweden)
- 9:30 SC17 **Screening the central effects of multitarget agent, non-imidazole H3 receptor antagonist/inverse agonists**
W. Agnieszka FOGEL, Medical University of Lodz (Poland)
- 9:45 SC18 **Targeting metastasis-associated in colon cancer-1 (MACC1) via HGF-Met-MAPK pathway as novel predictive marker for breast cancer**
Daria LER, PZU Moja Klinika-General Hospital Sarajevo (Bosnia and Herzegovina)
- 10:00 SC19 **Hydroxycinnamic acid as a valid scaffold for the development of CNS multitarget drugs**
Tiago SILVA, University of Porto, (Portugal) – PE awarded
- 10:15 SC20 **Discovery of a natural feruloyl ester as single inhibitor of HIV-1 RT and synthesis of its dual inhibitors analogues**
Vijay SONAR, University of Cagliari (Italy)
- 10:30 SC21 **Multitargeting prosurvival pathays in human leukemic cells by metformin and thymoquinone**
Mirza SULJAGIC, International University of Sarajevo (Bosnia and Herzegovina)
- 11:00 SC22 **Targeting dietary antioxidants to mitochondria as a therapeutic solution for mitochondrial oxidative stress related diseases**
José TEIXEIRA, University of Porto (Portugal) – PE awarded
- 11:15 *Coffee break*

Round table “Status of the WG activites of MuTaLig COST Action”

open to all participants - Moderator Fernanda BORGES (CA15135 Vice-Chair)

University of Porto (Portugal)

11:45

12:45 **Closing remarks**

13:00 **Lunch**