



MuTaLig COST ACTION CA15135
WG meeting 2016, Budapest (HU),
November 19-20 2016



List of accepted posters

Poster #	WG	Presenting author	Title
1.	1	Christelle ANDRE, Luxembourg Institute of Science and Technology, Esch/Alzette (Luxembourg)	Unravelling triterpene-hydroxycinnamate biosynthesis in apple
2.	1	Michaela BARANČOKOVÁ, University of Ljubljana (Slovenia)	Discovery of novel gyrase B and gyrase B/topoisomerase IV (ParE) dual inhibitors with in vitro antibacterial activity
3.	1	Sofia BENFEITO, University of Porto (Portugal)	Development of bifunctional agents for ameliorating the oxidative stress associated with aging related diseases
4.	1	Elvira BRUNO, University of Messina (Italy)	Development of a new class of benzensulfonamides as selective CA inhibitors
5.	1	Nuria CABEDO, Health Research Institute INCLIVA, Valencia (Spain)	1-Substituted tetrahydroisoquinolines and 7-phenyl-hexahydrocyclopenta[ij] isoquinolines as D2-like dopaminergic receptor ligands
6.	1	Fernando CAGIDE, University of Porto (Portugal)	Design and development of novel and selective A3 adenosine receptor ligands based on chromone-2-carboxamide
7.	1	Alessia CASO, University "Federico II" of Napoli (Italy)	Total synthesis of ent-smenamide A and c-16-epi-smenamide A
8.	1	Daniel CHAVARRIA, University of Porto (Portugal)	Insights on the development of novel neuroprotective agents: a comparative study between ferulic acid and related sulfanyl derivatives
9.	1	Luc DEMANGE, Université Paris-Descartes, Sorbonne Paris (France)	A chemical toolbox applied to original syntheses of druggable C-nucleosides analogues
10.	1	Jenny DESANTIS, University of Perugia (Italy)	Design and synthesis of potent anti-influenza small molecules that disrupt the RNA polymerase PA-PB1 subunits interaction
11.	1	Christoph ENZENSBERGER, Friedrich Schiller University, Jena (Germany)	Homobivalent carbolines as potential designed multiple ligands for the therapy of neurodegenerative disorders



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12.	1	Carlos FERNANDES, University of Porto (Portugal)	Nanomedicine as a tool to surpass physicochemical and bioavailability constrains: delivering of a coumarin-based MAO-B inhibitor using functionalized PLGA nanoparticles
13.	1	Andrè FONSECA, University of Porto (Portugal)	Coumarin <i>versus</i> chromone monoamino oxidase B inhibitors: Quo vadis?
14.	1	Justyna GODYŃ, Jagiellonian University, Kraków (Poland)	Lipophilic properties of multiple ligands targeting cholinesterases and amyloid beta determined by micellar electrokinetic chromatography and reversed-phase thin-layer chromatography
15.	1	Laura IELO, Università di Messina (Italy)	Tyrosinase inhibitors: synthesis, biological assays and docking studies of a new class of compounds
16.	1	Martin KRÁTKÝ, Charles University, Hradec Kralove (Czech Republic)	Salicylanilide carbamates active against Mycobacterium tuberculosis and other bacteria including drug-resistant strains
17.	1	Andraž LAMUT, University of Ljubljana (Slovenia)	Design, synthesis and biological evaluation of novel DNA gyrase B inhibitor-siderophore conjugates
18.	1	Daniel MARTINS, University of Porto (Portugal)	Optimizing Nature: development of novel antioxidants based on ferulic acid
19.	1	Giulia NESI, University of Pisa (Italy)	Symbiotic approach applied to the synthesis of new agents for the treatment of Alzheimer's disease
20.	1	David NOVAK, Palacky University (Czech Republic)	Cyclopentenediones as a relatively new group of bioactive substances
21.	1	Catarina OLIVEIRA, University of Porto (Portugal)	Benzoic based amide nitrones: a new class of cholinesterase inhibitors endowed with neuroprotective activity
22.	1	Jose M. ORDUÑA, University San Pablo CEU, Madrid (Spain)	Synthesis of a disaccharide rigid lanthanide binding tag to aid NMR studies of a coat protein of human norovirus
23.	1	Miryam PASTOR-FERNÁNDEZ, University San Pablo CEU, Madrid (Spain)	Multi Target Drug Discovery "MTDD" a new approach for the treatment of cancer
24.	1	Thanigaimalai PILLAIYAR, University of Bonn (Germany)	Diindolylmethanes (DIMs): from nutrients to multitarget anti-cancer drugs



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25.	1	Antonio QUOTADAMO, University of Modena and Reggio Emilia (Italy)	Pteridine derivatives as potent PTR1 inhibitors for the treatment of trypanosomiasis and leishmaniasis
26.	1	Lucia SEMELKOVÁ, Charles University, Hradec Králové (Czech Republic)	Microwave assisted synthesis and antibacterial evaluation of 3-aminopyrazine-2- carboxamide derivatives
27.	1	Peter ŠRAMEL, University of Bratislava (Slovakia)	Design and Synthesis of TKIs Specifically Interacting with SBCP (VEGFR2 TK)
28.	1	Pavel STARKOV, Tallinn University of Technology (Estonia)	Target and sub-target identification and modulation using the bimolecular approach
29.	1	Davide Benedetto TIZ, University of Ljubljana,(Slovenia)	Novel N-Phenyl-4,5-dibromopyrrolamides and N-Phenyl-3,4-dichloro-5-methylpyrrolamides Targeting DNA Gyrase B and Topoisomerase IV
30.	2	Hafidh AKKARI, Université de la Manouba (Tunisia)	First report of the <i>in vitro</i> nematicidal effects of camel milk
31.	2	Adina ARVINTE, Institute of Macromolecular Chemistry, Iasi (Romania)	Studies on Inclusion complexes of cyclodextrins
32.	2	Camilla CRISTOFARI, University of Padova (Italy)	Structural characterization of C-rich sequence in EGFR promoter region
33.	2	Richard A. ENGH, The Arctic University of Norway, Tromsø, (Norway)	Dealing with dynamics and disorder of protein kinase inhibitors and their targets as revealed by crystallography and complementary techniques
34.	2	Christiana A. MITSOPOULOU, National and Kapodistrian University of Athens (Greece)	DNA binding and biological activity of two novel Cu(ii) – quinoxaline complexes
35.	2	Gunay YETIK-ANACAK, Ege University, Izmir (Turkey)	New drug candidates targeting hydrogen sulfide
36.	3	José M. PADRÓN, Universidad de La Laguna, Tenerife (Spain)	SAR-DB: A Structure-Activity Database for Virtual Screening
37.	3	Ugo PERRICONE, Università di Palermo (Italy)	Conf-VLKA: A structure-based revisit of the Virtual Lock-and-Key Approach
38.	4	Bruno DI GERONIMO, Universidad CEU San Pablo, Madrid (Spain)	Novel drug discovery strategy against alcoholism, in silico approach to the protein tyrosine phosphatase receptor Z1 (PTPRZ1).



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39.	4	Simona DISTINTO, University of Cagliari (Italy)	Combination of pharmacophore and docking methods: a success story on the repositioning approach for the discovery of EBOV VP35 inhibitors
40.	4	Vladimir DOBRIČIĆ, University of Belgrade (Serbia)	Molecular docking studies of novel 9-aminoacridine derivatives with potential multi-target - based antiproliferative activity
41.	4	Rita GUEDES, University of Lisbon, Lisbon (Portugal)	Computational Approaches for the Discovery of Human Proteasome Inhibitors
42.	4	Jakub JOŃCZYK, Jagiellonian University, Kraków (Poland)	Multi-Approach Virtual Screening. Complex solution in the design of multitarget directed ligands.
43.	4	Isabella ROMEO, Università Magna Græcia di Catanzaro (Italy)	Identification of anti-obesity side effects of FDA-approved drugs through computer-aided repurposing techniques
44.	4	Jelica VUCICEVIC, University of Belgrade (Serbia)	Application of 3D-QSAR and virtual screening methods for design of novel antidepressants affecting serotonin transporters and histamine H3 receptors
45.	4	Abraham YOSIPOF, Bar-Ilan University, Ramat-Gan (Israel)	The Big Data Challenge in Drug Design: Data Visualization