

MedChem2019

*A pan-European network meeting
for Medicinal Chemistry*

Complesso Monumentale San Giovanni - Catanzaro (Italy), June 13th – 15th

Scientific program

Thursday, June 13th

"Sala delle Arti" 1st floor

13:30 Registration and welcome coffee (*cloister*)
15:00 Introduction to the IX Paul Ehrlich Euro-PhD network meeting
Stefano ALCARO (CA15135 Chair and Paul Ehrlich network Coordinator) - UMG di Catanzaro (Italy)

Welcome greetings from the authorities

Giovambattista DE SARRO Rector of Università "Magna Græcia" di Catanzaro (Italy)
Maria PAVIA Director of the Dipartimento di Scienze della Salute - Università "Magna Græcia" di Catanzaro (Italy)

Session PE I

Celebration of the first ten years of the Paul Ehrlich Euro-PhD Network

Moderator: Stefano ALCARO

15:30 PE-PL1/Girolamo CIRRINCIONE - Università degli Studi di Palermo (Italy): Paul Ehrlich Euro-PhD Network: from 2 to 53 members
16:00 PE-PL2/Christa E. MÜLLER - Rheinische Friedrich-Wilhelms-Universität, Bonn, (Germany): Development of chemical tools for nucleotide and lipid receptor-like orphan G protein-coupled receptors

Session PE II

Paul Ehrlich Euro-PhD Network PhD awarding ceremony

Moderator: Serge VAN CALENBERGH

16:30 PE-SC1/Donatella BAGETTA - Università "Magna Græcia" di Catanzaro (Italy): Computational studies on MAO-B and AChE inhibitors as potential anti-Parkinson's and anti-Alzheimer's agents
16:45 PE-SC2/Tommaso FELICETTI - University of Perugia (Italy): Design and chemical optimization of 3-phenylquinolone derivatives as potent nontuberculous mycobacteria efflux inhibitors
17:00 PE-SC3/Carlos FERNANDES - University of Porto (Portugal): PEGylation technology – the second chance for non-bioavailable drug candidates
17:15 PE-SC4/Laura IELO - University of Messina (Italy): Identification of new 4-fluorobenzyl-analogs as tyrosinase inhibitors via computational studies, synthesis and biological evaluation
17:30 PE-SC5/Antonio LUPIA - Università "Magna Græcia" di Catanzaro (Italy): Molecular modeling of epitopes recognized by neoplastic B-cells in Chronic Lymphocytic Leukemia
17:45 PE-SC6/Ester Sofia BENFEITO - University of Porto (Portugal): Design and development of multi-target agents for neurodegenerative diseases
18:00 Introduction and tour to the ROMANO CARRATELLI Codex exposition at San Giovanni Museum
19:00 Free welcome party at the Complesso Monumentale San Giovanni (*cloister*)
22:30 Return to hotels (bus shuttle for registered participants)

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Friday, June 14th

"Sala Gissing" basing floor

Session PE III

Novel chemical entities

Moderator: Athina GERONIKAKI

09:15 PE-SC7/José I. BORRELL - Universitat Ramon Llull, Barcelona (Spain): Pyrido[2,3-d]pyrimidine-7(8H)-ones: synthesis and biomedical applications
09:30 PE-SC8/Vittorio PACE - University of Vienna (Austria): Design and Development of New Chemical Concepts via Controlled Generation of Unstable Carbenoids Species
09:45 PE-SC9/Daniel CHAVARRIA - University of Porto (Portugal): Lessons from black pepper: moving from one to multitarget-directed ligands by diversity-oriented synthesis
10:00 PE-SC10/Amra IBRIC - University of Vienna (Austria): Position-Selective Synthesis and Biological Evaluation of Four Isomeric A-Ring Amino Derivatives of the Alkaloid Luotonin A
10:15 PE-SC11/Ryan D. KRUSCHEL - University College, Cork (Ireland): Synthesis of Cytotoxic Isoquinolinequinone N-oxides as Multitargeted Agents
10:30 PE-SC12/Silvia BALDUCCI - Sapienza University, Rome (Italy): Synergistic inhibition of the Hedgehog pathway by newly designed Smo and Gli antagonists bearing the isoflavone scaffold

10:45 Coffee break (*cloister*)

11:15 Poster session multimedia exposition - small rooms at the basing floor

Session PE IV

Anti-microbial agents

"Sala Gissing" basing floor

Moderator: Danijel KIKELJ

11:45 PE-SC13/Alfonso T. GARCÍA-SOSA - University of Tartu (Estonia): Multi-target design of arginase inhibitors for Leishmania
12:00 PE-SC14/Jakob BOUTON - University of Ghent (Belgium): Synthesis and biological evaluation of 1'-N-homoazanucleosides: discovery of a 5'-methyl-thioadenosine analogue with antitrypanosomal activity
12:15 PE-SC15/Maria Giulia NIZI - University of Perugia (Italy): Halogenated phenothiazines targeting the M. Tuberculosis type II of the NADH dehydrogenase
12:30 PE-SC16/Diego FIORUCCI - University of Siena (Italy): A target for macrocyclic antifungals: the needle in the haystack
12:45 PE-SC17/Yanlin JIAN - University of Ghent (Belgium): Design and synthesis of Mycobacterium tuberculosis thymidylate kinase (MtTMPK) inhibitors

13:00 Lunch (*cloister*)

14:15 Poster session multimedia exposition - small rooms at the basing floor

15:00 Paul Ehrlich Euro-PhD network coordinator meeting

Session MuTaLig III

Advanced computational methods

14:45 CA-SC12/Hanoch SENDEROWITZ - University of Bar Ilan, Ramat-Gan (Israel): Computational tools for multi-target drug discovery
15:00 CA-SC13/Agnieszka A. KACZOR - University of Lublin (Poland): In silico methods for multi-target drug development
15:15 CA-SC14/Federica MORACA - University "Federico II", Napoli (Italy): Combined FAAH and COX inhibition by Flurbiprofen amide derivatives for the treatment of pain and inflammation
15:30 CA-SC15/Mario PREJANO - Università della Calabria, Rende (Italy): On the inhibition mechanism of glutathione transferase p1 by piperlongumine. Insight from theory
15:45 CA-SC16/Annachiara TINIVELLA - University of Modena e Reggio Emilia (Italy): In silico repurposing of the hexahydrocyclopenta[c]quinoline scaffold as potent Carbonic Anhydrase inhibitors
16:00 Coffee break (*cloister*)
16:15 Poster session multimedia exposition - small rooms at the basing floor
17:00 Social activity for booked participants only (optional)

Saturday, June 15th

"Sala Gissing" basing floor

09:00 Welcome coffee (*cloister*)
09:30 Best poster voting deadline & MuTaLig MC meeting (MC members only)

Session MuTaLig IV

Opportunities for cooperation research projects

10:30 CA-SC17/Frank MARX - Deputy Head of Unit, Research Executive Agency, Bruxelles (Belgium): Marie Skłodowska-Curie Actions – mobility and training for researchers
10:45 CA-SC18/Gianluca SBARDELLA - (MC substitute for Italy) University of Salerno (Italy): The Innovative Medicines Initiative: Europe's partnership for health
11:00 CA-SC19/Menotti LUCCHETTA - Regione Calabria, Catanzaro (Italy): Calabria regional policies for research and innovation
11:15 CA-SC20/Antonio MAZZEI - CalabriaInnova-Fincalabra, Settingiano, Catanzaro (Italy): Exploitation of Research Results: European fund and network
11:30 Joint Paul Ehrlich and MuTaLig round table and best poster(s) awarding ceremony / Best poster award released by **Sharon BRYANT**, CEO of Inte:Ligand GmbH, Vienna (Austria) / Best poster award released by **Rita PODZUNA**, Director of Schrödinger GmbH, Mannheim (Germany) / Announcements about next Paul Ehrlich and MuTaLig meetings
12:30 Joint Paul Ehrlich and MuTaLig meeting concluding remarks
12:45 Social activity with lunch for booked participants only (optional)

"Sala delle Arti" 1st floor

Session MuTaLig I

Anti-neurodegenerative agents

Moderator: Fernanda BORGES

09:00 Introduction to **IV MuTaLig annual meeting**
09:15 CA-SC1/Rona R. RAMSAY - University of St Andrews, (United Kingdom): Maintaining the neuro-transmitter pool in degenerating brain: parameters for propargylamine inhibition of monoamine oxidase
09:30 CA-SC2/Leonardo PISANI - University "Aldo Moro", Bari (Italy): Expanding the coumarin toolbox directed at CNS multitargeting agents
09:45 CA-SC3/Giulia ROTONDI - Sapienza University, Rome (Italy): 4-(3-Nitrophenyl)thiazol-2-ylhydrazone derivatives as selective hMAO-B inhibitors: synthesis, biological activity and computational analysis
10:00 CA-SC4/Mariagrazia RULLO - University "Aldo Moro", Bari (Italy): Probing fluorine-effects in multitarget anti-Alzheimer agents
10:15 CA-SC5/Anthony BURKE - University of Évora (Portugal): Novel Chromane Derivatives for Alzheimer's Disease
10:30 CA-SC6/Francesco MESITI - Università "Magna Græcia" di Catanzaro (Italy): Looking for the Pharmacophore of Benzopyran MAO-B Inhibitors

Session MuTaLig II

Anti-cancer agents

"Sala delle Arti" 1st floor

Moderator: Eugenio GAUDIO

11:45 CA-SC7/Maria Paola COSTI - University of Modena e Reggio Emilia (Italy): Protein-protein interaction studies on thymidylate synthase leads to the identification and characterization of interface inhibitors as anticancer agents
12:00 CA-SC8/Francesco TRAPASSO - Università "Magna Græcia" di Catanzaro (Italy): A candidate multi-targeting approach to block the CD98hc oncoprotein
12:15 CA-SC9/Camilla CRISTOFARI - University of Padova (Italy): The untranslated region of the BCL2 gene and its noncanonical secondary structures
12:30 CA-SC10/Serenella DEPLANO - University of Cagliari (Italy): Multi-enzyme inhibitors for the treatment of cancer
12:45 CA-SC11/Maria DICHIAIA - University of Catania (Italy): Development of NO-releasing sigma receptor hybrids as anticancer agents

"Sala Gissing" basing floor

"Sala delle Arti" 1st floor

Moderator: Vittorio LIMONGELLI

"Sala delle Arti" 1st floor

Moderator: Maria Laura BOLOGNESI