

PEVM2021 Scientific Programme

Monday, July 26th

Tuesday, July 27th

Wednesday, July 28th

14:45 Welcome to #PEVM2021
Stefano ALCARO
Università "Magna Græcia" di Catanzaro (Italy)

12:00 Paul Ehrlich Euro-PhD network coordinator meeting
(Reserved only for PE Local Coordinators)

14:45 Opening
Rita PODZUNA
Senior Director at Schrödinger - München (Germany)

14:45 Opening
Michelangelo SIMONELLI
Senior Government Affairs Director at Gilead Sciences (Italy)

Paul Ehrlich Network Projects (PENP)

PENP Session I - Topic: "Cancer diseases"

Chairs **Beatriz de PASCUAL-TERESA**
Universidad CEU San Pablo (Spain)
Luc DEMANGE
Université Paris Descartes (France)
Rita GUEDES
Universidade de Lisboa (Portugal)

15:00 **PENP-1/Marilia BARRECA**
Università di Palermo (Italy)
Pyrrolo[2',3':3,4]cyclohepta[1,2-d][1,2]oxazoles, a new class of anti-mitotic agents active against multiple malignant cell types
Supervisor Paola Barraja

15:20 **PENP-2/Adriana CORICELLO**
Università "Magna Græcia" di Catanzaro (Italy)
Model optimization and site-mapping of hASNS, a novel target in the treatment of ALL
Supervisor Stefano Alcaro

15:40 **PENP-3/Lisa SEQUEIRA**
Università di Cagliari (Italy)
Development of Tumour-Associated Carbonic Anhydrases Inhibitors based on Benzopyrone Scaffold
Supervisor Elias Maccioni

16:00 **Coffee break and Sponsor Slideshow**

Paul Ehrlich Euro-PhD Awards (PEEPA)

Moderator **Serge VAN CALENBERGH**
Ghent University (Belgium)

16:10 **PEEPA-1/Francesca Alessandra AMBROSIO**
Università "Magna Græcia" di Catanzaro (Italy)
Molecular modeling studies on antiviral targets: drug resistance mechanisms and rational drug design

16:25 **PEEPA-2/Ghada BOUZ**
Charles University (Czech Republic)
Derivatives of Pyrazinecarboxylic Acid as Potential Antimycobacterial Active Drugs

16:40 **PEEPA-3/Jessica CERAMELLA**
Università della Calabria (Italy)
Au and Ag NHC-metal complexes as effective multi-target agents in breast cancer treatment

16:55 **PEEPA-4/Daniel CHAVARRIA**
Universidade do Porto (Portugal)
Development of new chemical entities based on natural scaffolds with therapeutic potential towards age-related disorders

17:10 **PEEPA-5/Bruno DI GERONIMO**
Universidad San Pablo-CEU (Spain)
Behind the allosteric inhibition of PTPRZ1, a current druggable phosphatase.

Flash PENP Communications (5 min)

Moderator **Claudia SISSI**
Università di Padova (Italy)

17:25 - 18:00
FC-1/Marianna BUFANO - Università di Roma "La Sapienza" (Italy)
Modeling Epac1 interactions with the allosteric inhibitor AM-001 by co-solvent molecular dynamics

FC-2/Valentina DEL GENIO - Università di Napoli "Federico II" (Italy)
Delivery for infectious diseases

FC-3/Maria Giulia NIZI - Università di Perugia (Italy)
Discovering selective Poly (ADP-ribose) Polymerase (PARP) Inhibitors to expand the precision medicine approach

FC-4/Michela PUXEDDU - Università di Roma "La Sapienza" (Italy)
Inhibition of ZIKA virus replication by novel inhibitors of NS2B/NS3 complex

FC-5/Jessica SEBASTIANI - Università di Roma "La Sapienza" (Italy)
The interaction between gab2 with sh3-domain of gbr2 as a new potential target in cancer therapy

FC-6/Kedmany SISOUKLATH - Université de Paris (France)
Development of innovative analytical tools to improve the safety of plant-based health products, application to the case of plants of the genus Tinospora used in Laos and in Europe

FC-7/Lorenzo TAGLIAZUCCHI - Università di Modena e Reggio Emilia (Italy)
Proteomic contribution to the omic path for the identification of novel drugs overcoming resistance in Leishmaniasis

18:15 **Closing**

PENP Session II - Topic: "Neurodegenerative diseases"

Chairs **Fernanda BORGES**
Universidade do Porto (Portugal)
Jose Ignacio BORRELL
Ramon Llull University (Spain)
Elias MACCIONI
Università di Cagliari (Italy)

15:00 **PENP-4/Bianca FIORILLO**
Università di Napoli "Federico II" (Italy)
Identification of molecular basis of praja2 and TBC1D31 interaction
Supervisor Bruno Catalanotti

15:20 **PENP-5/Jorge GÓMEZ-CARPINTERO**
Universidad Complutense de Madrid (Spain)
Flavonoid-derived acetylcholinesterase inhibitors as multitarget drug ligands for the treatment of Alzheimer's disease
Supervisor José Carlos Menéndez

15:40 **PENP-6/Annachiara TINIVELLA**
Università di Modena e Reggio Emilia (Italy)
LigAdvisor: a unified and easily accessible webserver for polypharmacology and drug repurposing
Supervisor Giulio Rastelli

16:00 **Coffee break and Sponsor Slideshow**

Moderator **Hanoch SENDEROWITZ**
Bar-Ilan University (Israel)

16:10 **PEEPA-6/Javier GARCÍA-MARÍN**
Universidad de Alcalá (Spain)
Strategies against chronic kidney disease: new modulators of PTP1B and ILK

16:25 **PEEPA-7/Francesca MANCUSO**
Università di Messina (Italy)
Targeting carbonic anhydrases (CAs): rational design, synthesis, structural studies and biochemical evaluation

16:40 **PEEPA-8/Francesco MESITI**
Università "Magna Græcia" di Catanzaro (Italy)
Mapping chromone-3-phenylcarboxamide pharmacophore: quid est veritas?

16:55 **PEEPA-9/Katarzyna SZCZEPAŃSKA**
Jagiellonian University Medical College (Poland)
The search for novel histamine H3 receptor ligands in the group of piperazine derivatives

17:10 **PEEPA-10/Serena VITTORIO**
Università di Messina (Italy)
Targeting protein-protein interactions for the treatment of tumors and neurodegenerative disorders

Editor's corner:

a Q&A session on best practices in publishing

Moderator **Rosaria GITTO**
Università di Messina (Italy)

17:30 **Paola BARRAJA (EJMC)**
Maria Laura BOLOGNESI (JMC)
David PERALTA (ChemMedChem)

18:00 **Closing**

#PEVM2021

SCIENTIFIC COMMITTEE
Stefano Alcaro (Coordinator)
Julio Alvarez-Builla (Past Coordinator)
Athina Geronikaki (Elected member)
Elias Maccioni (Elected member)
Serge Van Calenberg (Coordinator Elect)

ORGANIZING COMMITTEE
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PENP Session III - Topic: "Infectious diseases"

Chairs **Maria Paola COSTI**
Università di Modena e Reggio Emilia (Italy)
Athina GERONIKAKI
Aristotle University of Thessaloniki (Greece)
Danijel KIKELJ
Univerza V Ljubljani (Slovenia)
Oriana TABARRINI
Università di Perugia (Italy)

15:00 **PENP-7/Vincenzo Maria D'AMORE**
Università di Napoli "Federico II" (Italy)
Discovery of an Effective Dual avβ6/avβ8 Integrin Ligand as a Herpes Simplex Virus-1 Entry Inhibitor
Supervisor Luciana Marinelli

15:20 **PENP-8/Antoine FRANCHE**
Université de Paris (France)
Amphiphilic azobenzenes: Antibacterial activities and biophysical investigation of their interaction with bacterial membrane lipids
Supervisor Luc Demange

15:40 **PENP-9/Cai LIN**
Ghent University (Belgium)
6-Methyl-7-aryl-7-deazapurine nucleosides as anti-trypanosoma cruzi agents: structure-activity relationship and in vivo efficacy
Supervisor Serge Van Calenbergh

16:00 **PENP-10/Elisa ULIASSI**
Università di Bologna (Italy)
Chimeric small molecules in the search for novel anti-trypanosomatid agents
Supervisor Maria Laura Bolognesi

16:30 **Coffee break and Sponsor Slideshow**

Flash PE Poster Communications (3 min)

Moderator **Agostino MARRAZZO**
Università di Catania (Italy)

16:45 - 17:15
FC-1 PC_7/Carla BARBARACI
University of Catania (Italy)
Haloperidol metabolite II Valproate ester MRJF22 enantiomers as potential multifunctional agents against uveal melanoma

FC-2 PC_17/Valeria CAVALLORO
Università di Pavia (Italy)
An in house library of secondary metabolites as a useful tool for the identification of proteasome activators

FC-3 PC_29/Francesca INTRANUOVO
University of Bari "Aldo Moro" (Italy)
Design, synthesis and biological evaluation of new 4-oxo-1,4-dihydroquinolin-3-adamtilamides derivatives to develop CB2R fluorescent probes

FC-4 PC_42/Emmanuel OROCIO RODRÍGUEZ
Universidad Complutense de Madrid (Spain)
New cytosine-based multitarget compounds for neurodegenerative diseases

FC-5 PC_52/Virginia PONTECORVI
Sapienza University of Rome (Italy)
A novel scaffold for potent and selective inhibition of tumor-related carbonic anhydrase isoforms IX and XII

FC-6 PC_56/Mariagrazia RULLO
University of Bari "Aldo Moro" (Italy)
Hybrid design, synthesis and in vitro biological evaluation of 1H-indazoles as MAO B inhibitors: effect of 1,2,4-oxadiazole bioisosteric replacement of the amide linker

Social Event "PE Alumni meet again"

Moderators **Cosimo ALTOMARE**
Università di Bari "Aldo Moro" (Italy)
Federica MORACA
Università di Napoli "Federico II" (Italy)

Special issue launch & Awards Announcement

17:30 **What about a PE Alumni Association?**

18:00 **Best PENP**
Best POSTER
Best FLASH COMMUNICATIONS

Greetings and Closing Remarks

Next Meeting Announcement