

XIII Meeting Paul Ehrlich Euro-PhD Network & COST action OneHealthdrugs

Department of Chemistry & Technology for Drugs
Sapienza University of Rome, June 17-19, 2024



XIII Meeting Paul Ehrlich Euro-PhD Network & COST Action One Health approach to tackle neglected infectious diseases challenges

17-19 June 2024 Rome, ITALY

Venue:

Department of Chemistry and Technology of Drugs
La Sapienza University of Rome

CONFERENCE PROGRAMME



SAPIENZA
UNIVERSITÀ DI ROMA



XIII Meeting Paul Ehrlich Euro-PhD Network & COST action OneHealthdrugs

Department of Chemistry & Technology for Drugs
Sapienza University of Rome, June 17-19, 2024



Day 1: Monday, June 17th

| | |
|---|---|
| 2.00 - 3.00 p.m CU019 building | Registration |
| 3.00 - 3.30 p.m La ginestra (CU014) | Opening and welcome |
| Chair: Elias Maccioni | |
| 3.30 - 4.00 p.m La ginestra (CU014) | Plenary lecture Antivirals testing versus neurotropic viruses in single cell culture and in in vitro models of the blood brain barrier Joachim J. Bugert , Bundeweher Institute of Microbiology, Munich, Germany |
| 4.00 - 4.30 p.m La ginestra (CU014) | Invited lecture Heterocycles Synthesis under Green Processes - Organometallic or Visible-light Catalysis. Philippe Belmont , University Paris Cité, Paris, France |
| 4.30 - 5.00 p.m La ginestra (CU014) | Flash Poster Presentation (FP1-FP12) |
| 5.00 - 5.30 p.m | Coffee break and Poster session |
| 5.30 - 7.00 p.m La ginestra (CU014) | Oral Communication (OC1-OC6) |
| OC-1 | B. Aguiar Optimization and Characterization of Edaravone loaded Nanoparticles for the Treatment of ALS |
| OC-2 | B. Riss Yaw Promising Antagonist for Neupilin Receptor Targeting |
| OC-3 | F. Buonsenso Recent Advances in Stimuli Responsive Iminosugars as Pharmacological Chaperones for Gaucher and Parkinson's Disease Treatment |
| OC-4 | G. Cernicchi Potent 2-Phenyl-7-chloroquinazoline as new Mycobacterium avium Efflux Pump Inhibitors |
| OC-5 | A. Coco Novel σ 1R agonists/HDAC inhibitor codrugs modulating Tau protein |
| OC-6 | M. Coluccia Design, synthesis and human monoamine oxidase inhibitory activity of 2-aryloxybenzofuran derivatives: a new route towards hMAOs inhibition |
| 7.00 - 9.00 p.m CU019 building | Welcome Party |

Day 2: Tuesday, June 18th, Morning session

| | |
|--|---|
| Chair: Serge van Calenbergh | |
| 9.00 - 9.30 a.m La ginestra (CU014) | Plenary lecture Nucleotides as Antivirals - Development of membrane-permeable pronucleotides Chris Meier , Universität Hamburg, Germany |
| Chair: Maria Paola Costi - Daniela Secci | |
| 9.30 - 10.00 a.m La ginestra (CU014) | Invited lecture Rohini R. Roopnarine , School of Vet. Med, St. George's University, Grenada COST Action Workshop "One Health approach to tackle neglected infectious diseases challenges" |
| 10.00-10.30 a.m La ginestra (CU014) | E. Uliassi introduction to COST YRI (young investigator and innovators) Flash poster presentation <i>Cost Action</i> (FP13-FP26) |
| 10.30-11.00 a.m | Coffee break and Poster session |
| 11.00-11.10 a.m La ginestra (CU014) | S. Alcaro The Chemotheca networking tool for the OneHealthDrugs <i>Cost Action</i> |
| Chair: Stefano Alcaro | |
| 11.10 -1.10 p.m La ginestra (CU014) | Oral communication (OC7-OC14) |
| OC-7 | T. Quennesson Design, synthesis and evaluation of reverse β -aza fosmidomycin analogues as 1-deoxy-d-xylulose-5-phosphate reductoisomerase (DXR) inhibitors as antimicrobials |
| OC-8 | L. Tisseur Modulating the 2-position of imidazo[1,2-a]pyrazine lead CTN1122 alters its antileishmanial properties and L-CK1.2 kinase inhibition profile |
| OC-9 | E. Sanna Discovering potential Pan-hCoV inhibitors by targeting Nsp13 Helicase |
| OC-10 | M. Bufano Novel FtsZ inhibitors identified by virtual screening and Adaptive Steered Molecular Dynamics |
| OC-11 | L. Márquez Cantudo Insight into the catalytic mechanism of M17 leucine aminopeptidase through QM/MM computer simulations and selective mutagenesis |
| OC-12 | B. Nunes Tailoring Quaternary Phosphonium Salts: Design, Synthesis, Antimicrobial and Cytotoxicity |
| OC-13 | M. Pacetti Investigation of the Cycloheptathiophene-3-carboxamide Core for the Discovery of Influenza Virus Polymerase inhibitors |
| OC-14 | E. Van de Velde Synthesis and phenotypical discovery of imidazo[2,1-f]triazine ribosides as broad spectrum antitypanosomal agents |
| 1.10 - 2.15 p.m | Long coffee break |

Day 2: Tuesday, June 18th, Afternoon session

| Chair: Athina Geronikaki | |
|---|---|
| 2.15 - 3.15 p.m Room A (CU019) | Meeting of PE Coordinators/ Free time |
| 3.15 - 5.15 p.m La ginestra (CU014) | Oral Communication (OC15-OC22) |
| OC-15 | F. Falbo Synthesis of new benzanilide derivatives as HDAC1 selective inhibitors for CRC treatment |
| OC-16 | A. Fanizzi Rational optimization of the N-adamantyl-anthranil amide structural core for the development of new selective ligands for the Cannabinoid subtype 2 Receptor (CB2R) |
| OC-17 | A. Fontana Semisynthetic usnic acid-based compounds as promising antifungal agents |
| OC-18 | R. Purgatorio Investigating the multi-target potential for complex diseases of the alkaloidcontaining pyrrolo[2,1-a]isoquinoline scaffold |
| OC-19 | P. Sciò Benchmarking a Deep Generative Model for the Optimization of 3-Aroyl-1,4-diarylpyrroles (ARDAP) |
| OC-20 | A.R. Gomes Discovery of a potent steroidal oxime against breast and lung cancers |
| OC-21 | R. Astolfi Quantitative Composition-Activity Relationships Through Machine Learning Algorithm. Application to Essential Oil Tested as Acetylcholinesterase Inhibitors |
| OC-22 | L. Lombardo Designing an Effective Pharmacophore Model for Sigma 1 Receptor |
| 5.15 - 5.30 p.m La ginestra (CU014) | Flash Poster communication (FP27-FP34) |
| 5.30 - 6.00 p.m | Coffee break and Poster session |
| Chair: Romano Silvestri | |
| 6.00 - 7.15 p.m La ginestra (CU014) | Oral communication (OC23-OC27) |
| OC-23 | E. Marchese Revealing Polyphenols' Therapeutic Potential in Multiple Myeloma: Insights from Computational Studies on 20S Proteasome |
| OC-24 | G. Buttitta Scalable microfluidic method for tunable liposomal production by a rational approach |
| OC-25 | I. Sardo Natural F-series Pyrrolomycins: Microwave-assisted total synthesis, anticancer activity, and mechanism of action |
| OC-26 | C. Sarnari Progresses in targeting mono-ADP ribosylating enzymes: towards selective inhibitors |
| OC-27 | B. Serambeque Photodynamic therapy for endometrial cancer: can aldehyde dehydrogenase play a key role in eliminating cancer stem cells? |
| 8.30 p.m | Social Dinner at Casale di Tor di Quinto |

Day 3: Wednesday, June 19th

| Chair: Fernanda Borges | |
|--|---|
| 9.30 - 10.00 a.m La ginestra (CU014) | Plenary lecture Kick-start new drug design projects using computer-aided drug design Andrea Brancale , University of Chemistry and Technology Prague, Czech Republic |
| 10.00-10.45 a.m La ginestra (CU014) | Oral communication (OC28-OC31) |
| OC-28 | M. Garbagnoli Discovery of SMol acting on HuR-RNA complexes. STD-NMR competition studies using Peptide Nucleic Acids |
| OC-29 | A. Gargano Drug discovery of natural agents endowed with anticancer properties |
| OC-30 | R. Rocca Targeting TERRA G-quadruplex: Design and Biophysical Evaluation of Chromene Scaffold Derivatives |
| OC-31 | E. L. Citriniti Lithospermic Acid: Unveiling Its Potential as a Pancreatic Lipase and hCA V Inhibitor through In Silico and In Vitro Studies |
| 10.45- 1.15 a.m | Coffee break |
| 11.15-12.45 a.m La ginestra (CU014) | PE MedChem Euro-PhD Label communications PEA1-PEA6 |
| PEA-1 | C. Gratteri Development of multi-target agents with anti-cancer activity |
| PEA-2 | A. Olejarz-Maciej Multidirectional activity of new histamine and adenosine receptor ligands |
| PEA-3 | A. Onali Application of computational and synthetic techniques for the identification of compounds with potential antitumour and antiviral activity |
| PEA-4 | V. Pontecorvi From Hypoxia to Human Carbonic Anhydrases: design, synthesis, and evaluation of novel pyran-2-one based derivatives as anti-tumour and anti-inflammatory agents |
| PEA-5 | F. Procopio Molecular Modelling for medicinal chemistry: Development and application |
| PEA-6 | P. Stępnicki Optimization of virtual hits D2AAK3 and D2AAK2 in the search for new drugs for the treatment of schizophrenia |
| 12.45 - 1.15 p.m | Closing remarks |

Organised by:



Sponsored by:



Flash poster presentation List

| | | | |
|----------------------------|------|--------------------------|------|
| L. Acosta Benavides | FP1 | G. Malpezzi | FP18 |
| P. Pyka | FP2 | M. Msanif | FP19 |
| B. Bogdańska | FP3 | L. Tagliazucchi | FP20 |
| J. Bošković | FP4 | J. Traen | FP21 |
| L. Carosella | FP5 | E. Tumminelli | FP22 |
| C. El Hadri | FP6 | M. Fesatidou | FP23 |
| J. Ceramella | FP7 | A. Speroni | FP24 |
| F. Chiera | FP8 | R. Listro | FP25 |
| E. Fabbrizi | FP9 | H. Akkari | FP26 |
| M. Bilotta | FP10 | R. Ghanem Kattoub | FP27 |
| M. Fois | FP11 | A. Gil Rivas | FP28 |
| A. Fossati | FP12 | S. Gulino | FP29 |
| E. Uliassi | FP13 | M. Papadrakaki | FP30 |
| A.R. Alfenim | FP14 | M. Sapeta | FP31 |
| G. Atzeni | FP15 | K. Czarnota-Łydka | FP32 |
| L. Demuru | FP16 | D. Secci | FP33 |
| C. Lima | FP17 | P. Wójcik | FP34 |

Poster contributions number

| | | | |
|-----------------------|------|----------------------------|------|
| A. Albano | PC1 | E. Patacchini | PC14 |
| M. Casciari | PC2 | G. Pitasi | PC15 |
| M. Castelôa | PC3 | M. Crevar | PC16 |
| M. Chieffallo | PC4 | A. Raucci | PC17 |
| D. Ciampoli | PC5 | G. Ruggieri | PC18 |
| A. Grudzińska | PC6 | M. Santelli | PC19 |
| E. D'Intino | PC7 | K. Sdougkou | PC20 |
| M. Guida | PC8 | J. Sokolowska-Duda | PC21 |
| M. Jastrzębski | PC9 | J.L.Sousa Janela | PC22 |
| S. Krols | PC10 | K. Toufas | PC23 |
| P. Kuropka | PC11 | A. Van Hauwermeiren | PC24 |
| C. Lambona | PC12 | A. Zięba | PC25 |
| M. Marra | PC13 | | |

