



Organized by Ulrike Wittig, Theodora Calogeropolou, Cecilia Pozzi, Katarzyna Goździk, Guy Caljon, Elisa Uliassi, Gülşah Bayraktar, Anabela Cordeiro da Silva and Maria Paola Costi

Monday, 25 November 2024

Medicinal chemistry and structural biology

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Moderators: Cecilia Pozzi and Theodora Calogeropoulou

14.30: Welcome (Action Chair: Maria Paola Costi)

14.40: Andrea Ilari, National Research Council of Italy (CNR), Rome, Italy

Exploring the Ubiquitin-Proteasome System for Structure-Based Design of Effective PROTACs targeting Trypanothione Reductase

15.00: Thomas J. Schmidt, University of Münster, Germany

Natural Products against Neglected Diseases

15.20: John Igoli, Joseph Sarwuan Tarka University, Nigeria

Novel scaffolds from African medicinal plants for antiparasitic drug discovery

15.40: Ineta Meldaikytė, Kaunas University of Technology, Lithuania.

Investigation of bipyrazole derivatives

16.00: Break

16.10: Ieva Bartkeviciute, Kaunas University of Technology, Lithuania

Synthesis of substituted oxadiazoles and evaluation of anthelmintic properties

16.30: David C. Magri, University of Malta, Malta

Molecular Logic Gates Derived from Fluorescent Natural Products

16.50: Maria Paola Costi, University of Modena and Reggio Emilia, Italy

High Throughput screening deselection of Leishmania dihydrofolate reductase for highly selective pteridine reductase inhibitors

17.10: Maria Laura Bolognesi, University of Bologna, Italy

Opportunities and challenges in the discovery of PROTACS for Vector-borne Parasitic Diseases.

17.30: Elisa Uliassi, University of Bologna, Italy



Exploring the chemical space of small molecules targeting trypanothione reductase for parasitic diseases

17.50: Closing remarks

Tuesday, 26 November 2024

Integration of Ecotoxicology in drug discovery

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Moderators: Maria Paola Costi and Crtomir Podlipnik

10.00: Welcome (Action Chair: Maria Paola Costi and Anabela Cordeiro)

10.10: Dominga Evangelista, University of Bologna, Italy

Characterisation of persistence, bioaccumulation and toxicity of biologically active compounds with deep learning-based methods

10.30: Daniele Aiello (STSM), University of Modena and Reggio Emilia, Italy

Integrating Ecotoxicological Profiling and Computational Approaches for Sustainable Drug Discovery Against Neglected Parasitic Diseases

10.50: Lorenzo Raffellini, Department of Pharmacy, University of Pisa, Italy

Waste of Punica Granatum: a source of bioactive components to develop new anti-infective treatments

11.10: Črtomir Podlipnik, University of Ljubljana, Slovenia

Machine learning models for assessing toxicity of aquatic model organisms

11.30: Break

11.40: Bianca Martinengo, University of Bologna, Italy

Green chemistry strategies for vector-borne parasitic disease drug discovery: design, synthesis and biological evaluation of cashew nut shell liquid derivatives

12.00: Tahira Iftakhar, University of Agriculture Faisalabad, Punjab, Pakistan, KBCMA College of Veterinary and Animal Sciences (CVAS) Narowal, Punjab, Pakistan

Participatory And Molecular Surveillance Of Tick-Borne Theileriosis, And Anaplasmosis In District Bahawalpur, Punjab, Pakistan

One Health drugs against parasitic vector borne diseases in Europe and beyond
OneHealthdrugs **Cost Action CA21111**



- 12.20:** **Daniel Sojka**, Institute of Parasitology, Biology Centre of The Czech Academy of Sciences (IoP BC CAS), Czech Republic
ASP3a/b - the promising druggable plasmepsin IX/X analogues from Babesia
- 12.40:** **Closing remarks**



Wednesday, 27 November 2024
Parasitology and pharmacology

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Moderators: Guy Caljon and José Maria Alunda

14.30: Welcome (Action Chair: Maria Paola Costi and Guy Caljon)

14.40: André Lopes, Centre of Chemistry, University of Minho, Portugal

Recent Structural Optimizations of Pyrimido[5,4-d]pyrimidines Exhibiting Antileishmanial Activity

15.00: Sener Cintesun, Yildiz Technical University, Turkiye

Investigation of the bifunctional enzyme dihydrofolate reductase-thymidylate synthase (DHFR-TS) from Leishmania major

15.20: Cassandra Present, University of Antwerp, Belgium

A drug discovery journey: exploring N6-Methyltubercidin as an alternative antileishmanial drug treatment in a cutaneous Leishmania amazonensis mouse model

15.40: Lori Doko, eCampus University, Albania

Robotic Workflow for Antiparasitic Screening: Streamlined Cell Culture and Data Analysis in Pharmacology

16.00: Break

16.10: Estefania Calvo Alvarez, University of Milan, Italy

The role of NOD2 in macrophage activation and its therapeutic targeting in Leishmania infections

16.30: Tomilola Akingbade, Computer-Aided Therapeutic Discovery and Design Platform, Federal University of Technology, Nigeria

Synergistic inhibition of Plasmodium's vital proteins: A multi-target strategy using Buxus sempervirens

16.50: Rokaya Ahmad, University of Antwerp, Belgium

Towards knowing your target in Leishmania: establishment of validated in situ assays for antileishmanial drug discovery

17.10: Gaia Mazza, University of Milan, Italy

One Health drugs against parasitic vector borne diseases in Europe and beyond
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Immunomodulatory effects of Helicobacter pylori Neutrophil Activating Protein (HP-NAP) on human and canine macrophages infected with Leishmania infantum

17.30: Stephanie A. Blandin, Inserm U1257, CNRS UPR9022, University of Strasbourg, IBMC, Strasbourg, France

Plasmodium antimalarial activity is partially mediated by the NADH dehydrogenase PfNDH2

17.50: Closing remarks



Thursday, 28 November 2024
YRI presentations + STSM presentations & @13:00 Awards

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Moderators: Elisa Uliassi and Gulsah Bayraktar

9.30: Welcome (Action Chair: Maria Paola Costi and Elisa Uliassi)

9.40: Rodrigue Keumoe (STSM), Inserm U1257, CNRS UPR9022, University of Strasbourg, IBMC, Strasbourg, France
Imaging of Fe²⁺ gradients as a ferroptosis marker in malaria parasites using a fluorogenic labile heme reporters

10.00: Lorenzo Tagliazucchi (STSM), Unimore, Italy
Revealing the Mechanism of Action of the innovative antileishmanial agent H80 through fractionated MS Proteomics, untargeted metabolomics, and fluorescence imaging

10.20: Aleksandar Cvetkovski (STSM), Goce Delcev University, Faculty of medical science, Stip, N. Macedonia
Molecular docking study on antiparasitic nucleoside drugs

10.40: Theano Fotopoulou (STSM), National Hellenic Research Foundation, Institute of Chemical Biology, Greece
Synthesis and biological evaluation of new antiparasitic 4-thiazolidinone bioisosters of alkylphosphocholines

11.00: Break

11.10: Giulia Saporito, Unimore, Italy
Addressing the drug resistance issue by targeting the folate cycle proteins in Trypanosoma brucei and Leishmania major parasites

11.30: Graikioti Dafni (STSM), University of Patras, Greece
Libraries of analogues of Eucalyptus G-endoperoxides, antiparasitic activities, mechanisms of action

11.50: Roberta Listro, University of Pavia, Italy
Towards the discovery of novel Sortase A inhibitors as potential antibiofilm agents

12.10: Cristina Sanz Cuesta, University of Salamanca, Spain

One Health drugs against parasitic vector borne diseases in Europe and beyond
OneHealthdrugs **Cost Action CA21111**



Sulfonamides as antitrypanosomatid agents: A preliminary study

12.30: **Clara Lima**, University of Porto, Portugal

Preparedness of veterinarians to face emergency of animal leishmaniosis in urban settings of Morocco

12.50: **YRI awards and closing**