

Novel leads and drugs for vector borne diseases: Targets and off targets (toxicity and ecotoxicity) and mechanism of action”

Thursday 19th and Friday 20th September 2024

National Hellenic Research Foundation, Athens, Greece

To attend the workshop on line use the following zoom link

https://us06web.zoom.us/meeting/register/tZwkd-yrqTwtGdZu3mzBVWBejf9FMOMn_yzC

Thursday 19th September 2024	
08:30	Arrival & registration
09:00	Welcome
Session 1: Targets and Mechanism of Action Studies for Vector Borne Diseases Chairing: Anabela Cordeiro da Silva and Cecilia Pozzi	
09:15	“Innovative approaches to target trypanothione reductase an essential enzyme for the survival of trypanosomatids in the host” Andrea Ilari , Institute of Molecular Biology and Pathology, Italian National Research Council, Italy
09:35	“Cyclic AMP signaling and nucleoside activated Protein Kinase A in Trypanosoma and Leishmania: genetic target validation and structure-guided inhibitor design” Michael Boshart , University of Munich (LMU), Germany
09:55	“Chemical tools to decipher the modes of action of antiplasmodial redox-active 3-benzylmenadiones” Elisabeth Davioud-Charvet , CNRS-Université de Strasbourg-Université Haute-Alsace, France
10:15	“Unravelling the mechanism of action of highly potent Pteridine Reductase 1 inhibitors: new insights into dual targeting of PTR1 and DHFR Nuno Santarém , i3S, University of Porto, Portugal.
10:35	Coffee Break
11:05	Promoters: Cecilia Pozzi, Ulrike Wittig and the Team OHD1 - Target database project: the BioTarget DataBase (BioT-DB) Round table discussion: Structural biology approaches to understand and fight VBDs.

Session 2: Novel leads and drugs for Vector Borne Diseases

Chairing: Sandra Gemma and Gulsah Bayraktar

12:00	<p><i>“Phenotypic and target-based screening of nucleoside analogues as antitrypanosomal agents”</i> Ewout Van de Velde, Ghent University, Belgium <i>Recipient of the "Best presentation on vector-borne diseases" from the COST action (CA21111) at the Paul Ehrlich meeting held in Rome on June 2024.</i></p>
12:20	<p><i>“Specialized pro-resolving mediators as leads for resolution pharmacology targeting vector borne diseases.”</i> Trond Vidar Hansen, University of Oslo, Norway</p>
12:40	<p><i>“Robenidine Derivatives As Potential Antischistosomal Drug Candidates”</i> Christian N. Lotz, University of Basel, Switzerland</p>
13:00	Break-Refreshments
14:00	<p><i>“Synthesis and Anti-Parasitic Evaluation of Fused N,S-Heterocyclic Derivatives”</i> Maria João Ribeiro Queiroz, University of Minho, Portugal</p>
14:20	<p><i>“Discovery and preliminary preclinical in vivo evaluation of a dicationic candidate for the oral treatment of leishmaniasis”</i> Christophe Dardonville, Medicinal Chemistry Institute, CSIC. C. Madrid, Spain.</p>
14:40	<p><i>“Arnica tincture is effective against cutaneous Leishmaniasis in human patients: A novel drug for this vector borne disease without toxic or ecotoxicological impact”</i> Thomas J. Schmidt, University of Münster, Germany</p>
15:00	<p>Promoters: Jose Maria Alunda, Anabela Cordeiro da Silva, Guy Caljon and the Team OHD3 project: Transition from in vitro to in vivo evaluation: recommendations for obtaining high-quality leads against kinetoplastids and round table discussion.</p>
16:00	Coffee break

Session 3: Flash Poster Presentations

Chairing: George Magoulas, Daniele Aiello

16.30	<p>Targets and Mechanism of Action Studies for Vector Borne Diseases</p> <ul style="list-style-type: none"> <i>“Comparative analysis of activated cysteine residues in human and parasitic enzymes: potential for covalent inhibition”</i> Črtomir Podlipnik, University of Ljubljana, Slovenia <i>“Molecular modelling on antiparasitic nucleoside drugs: revealing mechanism of drug action”</i> Alexandar Cvetkovski, Goce Delcev University, Republic of Northern Macedonia <i>“Plasmodium falciparum type-II NADH:ubiquinone:oxidoreductase as a possible target for bioreductively activated antiplasmodial agents”</i> Narimantas Čėnas, Vilnius University, Lithuania <p>Questions</p>
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17:00	Novel leads and drugs for Vector Borne Diseases
17:00	<ul style="list-style-type: none"> • <i>“Antitrypanosomal activity of D-ring modified steroid derivatives”</i> Jovana Ajdukovic, University of Novi Sad, Serbia • <i>“Novel Naphthyl Indolyl maleimides (NIM’s) as inhibitors of kinase and new leads in the treatment of Leishmaniasis”</i> Florence McCarthy, University College Cork, Ireland • <i>“Adamantane Nitro-Heterocyclic Derivatives with Activity against L. infantum”</i> Konstantina Stavropoulou, National Kapodistrian University of Athens • <i>“Activity of novel heterocyclic compounds against promastigote and amastigote-like Leishmania infantum and Leishmania tropica”</i> Gulsah Bayraktar, Ege University, Turkey <p>Questions</p>
17:45	Diagnostics-Epidemiology of Vector Borne Diseases
	<ul style="list-style-type: none"> • <i>“Molecular Detection Of Filarial Nematode Parasites In Mosquitoes From Albania”</i> Elton Rogozi, Institute of Public Health, Albania • <i>“Analyzing High Throughput Malaria Rapid Diagnostic Test Effectiveness and Genetic Diversity in Dominican Republic: Considerations for Elimination Efforts”</i> Claudia Federo, University of Minho, Portugal • <i>“A stochastic model for spread of Malaria under insecticide-treated nets and possible treatments”</i> Jasmina Djordjevic, University of Niš, Serbia • <i>“Vivax malaria cases imported from Greece during 2010-2016”</i> Teita Myrseli, Institute of Public Health, Albania <p>Questions</p>
18.30	<i>End of 1st day</i>
20:30	<i>Dinner</i>

Friday 20th September

Session 4: Medicinal chemistry and One Health principle integration: expanding the concepts of selectivity in drug discovery

Chairing: Ioannis Papanastasiou & Ulrike Wittig

09:00	<p><i>"Integration of AI Assisted Toxicity Assessment framework across All Life Forms in Green Chemistry Principles while Designing New Pharmaceuticals and Chemicals"</i></p> <p>Nikolaos Thomaidis, National and Kapodistrian University of Athens, Greece</p>
09:20	<p><i>"G.A.I.A. A computational platform for ecotoxicity predictions of chemical compounds"</i></p> <p>Evangelos Tsoukas, CLOUDPHARM, Athens, Greece</p>
09:40	<p><i>"In silico Ecotoxicological Assessment of Compounds and their Metabolites: A Lesson from Curcumin"</i></p> <p>Simone Brogi, University of Pisa, Italy</p>
10:00	<p><i>"Optimizing Trypanothione Reductase Inhibitors for Leishmania Treatment: A Multiparametric Prediction Approach to Enhance Solubility and Biodegradability"</i></p> <p>Sandra Gemma, University of Siena, Italy</p>
10:20	<p><i>"Development of NMT-A004-loaded biodegradable nanocarriers"</i></p> <p>Theano Fotopoulou, National Hellenic Research Foundation, Greece</p>
10:40	Coffee Break
11:10	<p><i>"One Health Approach in Drug Discovery for Leishmaniasis by Targeting Calpain cys-protease"</i></p> <p>Daniele Aiello, University of Modena and Reggio Emilia, Italy</p>
11:30	<p><i>"Innovative Therapeutic Strategies for Vector-Borne Diseases: Exploring Novel Drug Targets and Addressing Off-Target Toxicity"</i></p> <p>Lori Doko, University of natural sciences and biological sciences, Albania</p>
11:50	<p><i>"Drug Discovery and preclinical Development for Human and Animal African Trypanosomiasis: Profiling of a collection of Natural Compounds with ADME-(Eco)Toxicity properties"</i></p> <p>Laura Bertarini, University of Modena and Reggio Emilia, Italy</p>
12:10	<p><i>"Bioethical and human security approaches on evolution of drugs for vector borne diseases"</i></p> <p>Serghei Sprincean, Moldova State University, Moldova</p>
12:30	<p>Promoters: Sandra Gemma, Gulsah Bayraktar and the Team</p> <p>OHD2 – Compound Database project: Antiparasitic drug discovery and emerging scaffolds with predictive low environmental impact. Round table discussion</p>
13:10	Break-Refreshments
14:00	<i>COST CA21111 General Meeting (Planning Action activities and YRI)</i>
17:00	Closing remarks