

Advancements in Structural and Functional Drug Discovery of Vector-borne Diseases

Working version of the program

Wednesday 3rd to Friday 5th July 2024

Saïd Business School & Diamond Light Source

Wednesday 3rd July 2024		Saïd Business School
09:00	Arrival & registration	
09:45	Welcome	
Session 1: Biology and ecology of parasites (Chairing: <i>Elton Rogozi & Anabela Cordeiro</i>)		
09:30	"Novel insights from animal models into uncharted Leishmania biology" Guy Cajon, University of Antwerp (Belgium)	
10:00	"Unprecedented high-resolution chemical imaging of proteins, surfaces of microbes & histological tissue using mid-IR photo-induced force microscopy" Daniela Trauber, Friedrich Schiller University Jena, (Germany)	
10:30	"Mitochondrial NADH/NAD ⁺ balance in Leishmania survival and its interest for chemotherapy" Margarida Duarte, Instituto de Investigação e Inovação em Saúde (Portugal)	
11:00	Coffee Break	
11:30	<p>Round table: Parasitology. Promoters: <i>Guy Cajon, Jose Maria Alunda, Louis Maes</i>. to discuss the roadmap of <i>in vitro</i> and <i>in vivo</i> laboratory experiments towards high-quality drug leads based on our experiences. Within this round table theme, José María will also pitch his poster about formulation (see attachment).</p> <p>OHD3: Transition from <i>in vitro</i> to <i>in vivo</i> evaluation: recommendations for obtaining high-quality leads against kinetoplastids</p> <p>To initiate the round table and discussion, I would propose to discuss a few items to which everyone can provide input from their expertise:</p> <ul style="list-style-type: none"> • What defines a good antiparasitic hit with NO GO criteria in early discovery – which essential assays are needed? – discuss for the different kinetoplastids • Which pharmacokinetics assays are available and accessible within the network to transition to <i>in vivo</i> studies • What should we consider when formulating a drug for <i>in vivo</i> testing? (pitch José María) • Where we position 'Omics and what are the benefits of MoA studies? • Where do we position ecotoxicology in the discovery process and which assays are accessible? • With which labs can you collaborate to test antiparasitic activity /ecotoxicity? <p>Poster presentation: Drug formulation, bridging the gap from <i>in vitro</i> experiments to <i>in vivo</i> results José María Alunda, Javier Carrión, Juan José Torrado</p>	
12:30	Break	

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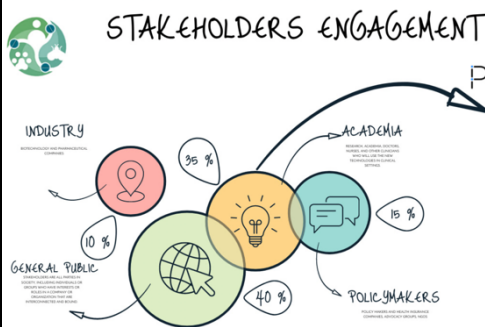
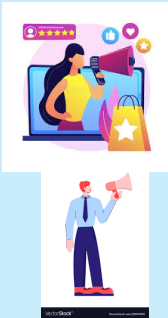

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Session 2: Drug discovery approaches towards VBDs

(Chairing: *Theodora Calogeropoulou & Violeta Valcheva*)

14:00	<p>Invited Speaker Combining AI, phenotypic screening and structure guided drug design to aid discovery of new NTD and VBD therapeutics 'Nick Furnham, London School of Hygiene & Tropical Medicine (UK)</p>
14:30	<p>"Biological Properties and In Silico Studies of Thiazolopyrimidine Derivatives Active Against Visceral and Cutaneous Leishmania spp. Amastigote Forms" Gülşah Bayraktar, Ege University (Türkiye)</p>
15:00	<p>"Identification of novel Leishmania infantum SIR2RP1 inhibitors" Joana Tavares, Instituto de Investigação e Inovação em Saúde (Portugal)</p>
15:30	Coffee Break
16:00	<p>Round table: Compounds database: expanding the knowledge towards low environment impact drugs. Promoters: <i>Theodora Calogeropoulou, Sandra Gemma.</i></p> <div style="display: flex; align-items: flex-start;">  <div style="margin-left: 20px;"> <p><i>Poster flash presentation</i></p> <ol style="list-style-type: none"> 1. New amides of shikimic acid as powerful antimicrobial agents – synthesis, <i>in vitro</i> and <i>in silico</i> studies Violeta Valcheva. 2. Ferrocene conjugates as potential antiparasitic vector-borne lead compounds. David C. Magri </div> </div>
17:00	<p>CA21111 general meeting Stakeholders engagement plan and OHD Objective & Future plan (working together) and – OHD Academy. Maria Paola Costi, Theo Zacharis and Anabela Cordeiro.</p> <div style="display: flex; justify-content: space-around; align-items: center;">    </div>

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Thursday 4th July 2024		Saïd Business School
Session 3: Structural biology and biochemistry (Chairing: Ulrike Wittig & Harry De Koning)		
10:00	Invited Speaker <i>'Structure-guided design of blood stage malaria vaccines'</i> Matt Higgins, University of Oxford (UK)	
10:30	Invited Speaker <i>'Structural characterisation of Trypanosoma cruzi antigens for diagnostic and therapeutic applications'</i> Ivan Campeotto, University of Nottingham (UK)	
11:00	<i>"Structural investigation of Trypanosoma folate enzymes for the development of new antiparasitic agents"</i> Cecilia Pozzi, University of Siena (Italy)	
11:30	Break	
12:00	Round table: Combining structural and functional knowledge to understand and fight VBDs. Promoters: Ulrike Wittig, Harry De Koning OHD1 - Target database project: the BioTarget DataBase (BioT-DB) (promoter Cecilia Pozzi, Marco Mazzorana, Ulrike Wittig) Advancements in Structural and Functional Drug Discovery of Vector-borne Diseases. Poster flash presentation: 1. Leishmania infantum ribose 5-phosphate isomerase a validated drug target. A. Cordeiro 2. The Peroxiredoxins of Leishmania revisited. A. Thomas.	
13:00	Lunch Break	
Session 4: Ecotoxicology and One-Health (Chairing: Elisa Uliassi & Ioannis P. Papanastasiou)		
14:00	Invited Speaker <i>'Pharmaceuticals, Environment, and One Health'</i> Brian Brooks, Baylor University (USA)	
14:30	Invited Speaker <i>Swimming in medicated waters: Understanding and mitigation the impacts of pharmaceutical pollutants on aquatic wildlife'</i> Eli Thoré, Swedish University of Agricultural Sciences (Sweden)	

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15:00	<p><i>"Exploring new frontiers in fighting animal trypanosomiasis: assessing antitrypanosomal and (eco)toxicological characteristics of novel nucleoside-based leads"</i></p> <p>Kayhan Ilbeigi, University of Antwerp (Belgium)</p>
15:15	<p><i>"Advancing sustainable drug development: comparative preclinical study of H80 and Miltefosine using imaging and proteomics"</i></p> <p>Giulia Malpezzi, University of Modena and Reggio Emilia (Italy)</p>
15:30	<i>Coffee Break</i>
16:00	<p>Round table: Sustainable integration of people and animal's health within the ecosystem. Promoters: Clara Lima, Eli Thorè, Harry de Koning, Brian Brooks and Team</p> <p>OHD-4 Review of veterinary pharmaceuticals against Parasitic Vector-Borne Diseases and their environmental impacts</p> <p>Poster presentation</p> <ol style="list-style-type: none"> 1) "Malaria, a parasitic mosquito-borne disease; from imported cases re-emerge, to the presence of primarily Anophelinae vectors population in Albania" by Elton Rogozi 2) "Review of veterinary pharmaceuticals against Parasitic Vector-Borne Diseases and their environmental impacts", by Clara Lima, on behalf of OHD4 collaborators
17:00	<p><i>Poster Session: All poster presenters will present their flash 5 minute.</i></p> <ul style="list-style-type: none"> • Ioannis Papanastasiou, Adamantane imidazolines with trypanocidal activity • Dijana Blazhekovikj, Possibilities For Treating Parasites In Fish With Essential Oils And Plant Extracts • Aleksandar Cvetkovski, Survey on repurposing of anti-parasitic drugs in babesiosis treatment • Elisa Uliassi, Fostering Innovation in Vector Borne Parasitic Diseases through Young Researcher Innovators within CA21111 OneHealthdrugs • Rokaya Ahmad, Discovery of novel drug action mechanisms by studying antileishmanial Aminopyrazoles <p>CA21111 general part 2. MPaolaCosti</p> <ul style="list-style-type: none"> • <i>Next events YEAR 2 (Training school in Warsaw 27-28 September 2024; Athens meeting 19-20 September 2024).</i> • <i>Presentation of the next events and next year planning (WG meeting in Tirana, Albania; annual conference in Antwerp).</i> • <i>Academy ambassadors' proposal discussion.</i> • <i>Next year plan.</i>
18:30	<i>Drinks & Conference Dinner</i>

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Thursday 5th July 2024		Diamond Light Source
Session 5: Visit to Diamond Light Source		
09:00	Private bus transfer from Saïd Business School to Diamond Light Source	
09:00	Welcome to Diamond Light Source	
09:30	Life Sciences at Diamond	
10:00	Tour of the Diamond Light Source life-sciences laboratories and beamlines	
12:00	Closing remarks and private bus transfer back to Saïd Business School	
	Visit to Diamond HRIZON2020 Instruct.eric.eu Introduction director of the center Lecture Martin Walsh First scientific users from 2007 iNEXT Discovery consortium 30 partners and 14 European consortium.	