



Medicinal Chemistry of Tropical Diseases
XIIth SEQT Symposium
IIIrd Spanish/Portuguese/Brazilian Meeting

November, 17-18th 2016

Scientific Program

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Thursday 17 November

- 8:00 Bus from hotel to GSK.
8:30-9:00 **Registration**
9:00-9.15 Opening of XII SEQT Mini-Symposium. IIIrd Spanish/Portuguese/Brazilian Meeting

First Session: Tuberculosis

- 9:15-10:15 Plenary Lecture: **Charles Mowbray**. Head of Drug Discovery, DNDi
"DNDi - catalysing R&D for neglected patients"
- 10:15-10:45 **Benoit Deprez**. Institut Pasteur de Lille, INSERM. Université de Lille
"Smart-1 Overcoming antibiotic resistance by reprogramming bacterial metabolism"
- 10:45-11:15 *Coffee Break*
- 11:15-12:15: Plenary lecture. **David Barros**. Head of Tuberculosis DPU, DDW, GSK
"Development of New drugs for the Treatment of MDR-TB"
- 12:15-12:45: **Julia Castro**. Diseases of the Developing World, GSK
"GSK693 as a novel InhA direct inhibitor: a new antitubercular drug for an old target"
- 12:45-13:20 Flash Poster Presentations
- F1: **Esther Porras**, TB DPU, DDW-GSK. *"Identification of a novel antimycobacterial compound active against non-replicating M. Tuberculosis: from hit to in vivo PoC"*
- F2: **Marta Piquero Martí**, Dpto. Qca. Orgánica y Farmacéutica. Facultad de Farmacia, U. Complutense de Madrid. *"Potential multitarget anti-tuberculosis agents contain pyrrole and isoniazid structural fragments"*
- F3: **M^a Fernanda Rey-Stolle**, CEMBIO. Facultad de Farmacia, U. CEU San Pablo. *"Metabolomics approach to study time trajectory metabolic changes in lung of TB infected mice"*
- F4: **Víctor Sebastián**, Centro de Investigaciones Biológicas (CIB-CSIC). *"Searching for novel drugs to treat schistosomiasis: phenotypic and target-based approaches"*
- F5: **Maria João Gouveia**, ICETA. University of Oporto. *"Estrogen-like metabolites and DNA-adducts in urogenital schistosomiasis-associated bladder cancer"*
- F6: **Pedro J. Llabrés**, Dpto. Qca. Orgánica. Facultad de Farmacia. U. de Valencia. *"Evaluation of the novel antischistosomal activity of [1,2,3]triazolo[1,5-a]pyridine derivatives"*
- F7: **Noelia de la Cruz**, Instituto de Investigaciones Químicas (IIQ-CSIC). *"Multivalent glyconanogels to inhibit viral infections"*
- 13:20-14:30 *Lunch*

Second Session: Malaria

- 14:30-15:30 Plenary Lecture: **María Mota**, Molecular Medicine Institute. University of Lisbon
"The complexity and the simplicity of host-Plasmodium interactions"
- 15:30-16:00 **Esther Fernández**, Malaria DPU, DDW-GSK
"Quinazolindione series identified from TCAMS: a new anti-malarial series with potential for blocking transmission of the disease"

- 16:00-16:30 *Coffee Break*
- 16:30-17:00 **Paula Gomes**, UCIBIO-REQUIMTE, University of Oporto
"When peptide chemistry meets antimalarial drug rescuing"
- 17:00-17:30 **Moni Sharma**, Research Institute for Medicines and Pharmaceutical Sciences, University of Lisbon
"Identification and SAR Evaluation of a Novel Chemotype with dual stage antimalarial activity"
- 17:30-18:00 Flash Poster Presentations
- F8: **Margarita Puente**, Malaria DPU, DDW-GSK. *"Antimalarial pyrazines: from a phenotypic hit to a pre-clinical candidate"*
- F9: **Caterina Pont**, Facultad de Farmacia, U de Barcelona. *"Selective inhibitors of plasmodium falciparum glucose-6-phosphate dehydrogenase as a new class of antimalarial agents"*
- F10: **Gustavo da Silva**, Research Institute of Medicines. University of Lisbon. *"Synthesis and biological evaluation of a novel C2 functionalized indole against blood stage malaria"*
- F11: **Sara Palomo**, Malaria DPU, DDW-GSK *"Malaria bifunctional DHFR-TS enzyme as a target for drug discovery against asexual stages of P. falciparum"*
- F12: **Paul Horrocks**, Institute for Science and Technology in Medicine. Keele University. *"A validated bioluminescence-based assay for the rapid determination of the initial rate of kill for discovery antimalarials"*
- F13: **Rosana Leiva**, Lab. de Química Farmacéutica. U. de Barcelona. *"Novel thiazoles as trypanocidal agents"*
- 18:00-18:30 **Silvia Pérez-Silanes**, Instituto de Salud Tropical, U. de Navarra.
"In vitro and in-vivo anti-trypanosoma cruzi activity of new arylamine mannich base derivatives"
- 18:30 *Bus to hotel (for participants not attending the SEQT General Meeting)*
- 18:30-19:30 **SEQT Members General Meeting**
- 21:00 *Symposium Dinner*

Friday 18 November

- 8:30 Bus from hotel to GSK

Third Session: Leishmania

- 9:00-10:100 Plenary Lecture: **Aurea Echevarria**, Chemistry Department. Federal University of Rio de Janeiro
"Some Brazilian studies of medicinal chemistry in anti-leishmanial drugs"
- 10:00-10:30 **Concepción Alonso**, Dpto. Qca. Orgánica. Facultad de Farmacia, U. del País Vasco
"Design and synthesis of novel indeno[1,5]naphthyridine derivatives, topoisomerase I inhibitors with antileishmanial activity"
- 10:30-11:00 Flash Poster Presentations
- F14: **Carmen Sanmartín**, Dpto. de Qca. Orgánica y Farmacéutica. U. de Navarra. *"Selenocompounds with potent and selective activity towards leishmanial in vitro"*
- F15: **Edinéa Mendes**, Instituto de Tecnología em Imunobiológicos. Fundação Oswaldo Cruz. *"Synthesis and antileishmanial activity of novel chalcone derivatives"*

F16: **Javier García Marín**, Dpto. de Qca. Orgánica e Inorgánica. U. de Alcalá. *“Pyridazino[2,3-a]pyrrolo[1,2-c]quinoxalinium salts: potent and selective leishmanicidals that show inhibition of L. infantum trypanothione reductase and human protein tyrosine phosphatase 1B”*

F17: **Daniel Plano**, Dpto. de Qca. Orgánica y Farmacéutica. U. de Navarra. *“Topological and quantum molecular descriptors as effective tools for analysing antileishmanial activity achieved by a series of alkyl, aryl and heteroaryl diselenide derivatives”*

F18: **Raquel Rodrigues**, Lab. de bioquímica de Tripanosomatídeos. Instituto Oswaldo Cruz-Fiocruz. *“Arginase and nitric oxide synthase studies on leishmanial infantum and their relation with infectivity and drug sensibility”*

F19: **Ángela P. Hernández**, Dpto. Ciencias Farmacéuticas. Facultad de Farmacia, U. de Salamanca. *“New antineoplastic and antileishmanial hybrids derived from natural products”*

11:00-11:30 Coffee break

11:30-12:00 **Héctor de Lucio**, Dpto de Biología de Sistemas, Universidad de Alcalá
“ α/β^3 -peptide foldamers with cell-penetrating capacity targeting the dimerization interface of leishmania infantum trypanothione reductase”

12:00-12:30 **Tim Miles**, DDW-GSK.
“Collaboration makes us better: BA05 series as a novel class of anti-leishmanial”

12:30-13:00 **Enmanuele Amata**, Department. of Drug Science, University of Catania
“Identification of novel lead compounds for sleeping sickness via preferred lead repurposing”

13:00-13:35 Flash Poster Presentations

F20: **Marta Ruiz-Santaquiteria**, Instituto de Química Médica (IQM-CISC). *“Design and synthesis of proteomimetics to inhibit the dimerization interface of trypanothione reductase of leishmania infantum”*

F21: **Verónica Alcolea**, Dpto. de Qca. Orgánica y Farmacéutica. U. de Navarra. *“Early preclinical studies of new selenocyanate and diselenide compounds as leishmanial agents”*

F22: **Pilar Manzano**, DDW-GSK. *“GSK-Kineto boxes-Discovering new targets, mechanism and purposes. A collaborative challenge”*

F23: **Belén Martínez-Gualda**, Instituto de Química Médica (IQM-CSIC). *“Amino acids dendrimers as a novel type of HIV and Enterovirus 71 inhibitors”*

F24: **Christophe Dardonville**, Instituto de Química Médica (IQM-CSIC). *“Mitochondrion-targeted trypanosome alternative oxidase inhibitors as chemotherapeutic agents against T. brucei”*

F25: **Alba Gigante**, Instituto de Química Médica (IQM-CSIC). *“Chikungunya virus: further steps among triazolopyrimidines inhibitors to improve potency and microsomal stability”*

F26: **Maria Penzo**, London School of Hygiene & Tropical Medicine and Malaria DPU, GSK. *“High-Throughput Screening to develop new inhibitors against P. falciparum Protein Kinase G”*

13:35 Closing. Concluding remarks

14:00 Lunch