



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

**November, 17-18th 2016**

**Scientific Program**

## Thursday 17 November

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- 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  
*Title to be confirmed*
- 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  
*"Decaprenylphosphoryl- $\beta$ -D-ribose oxidase (DprE1) as a promising target of Mycobacterium tuberculosis inhibitors"*
- 12:45-13:20 Flash Poster Presentations
- F1: **Ester Porras**, TB DPU, DDW-GSK. *"Identification of a novel anti-mycobacterial compound active against non-replicating M. Tuberculosis: fro 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<sup>a</sup> 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  
*Title to be confirmed*

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

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- 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 Tecnologia 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 leishmanicidal 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, U. de Alcalá  
*“ $\alpha/\beta^3$ -peptide foldamers with cell-penetrating capacity targeting the dimerization interface of leishmania infantum trypanothione reductase”*

12:00-12:30 **Tim Miles**, DDW-GSK.  
*Title to be confirmed*

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

13:00-13:30 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: **Rosana Leiva**, Lab. de Química Farmacéutica. U. de Barcelona. *“Novel thiazoles as trypanocidal agents”*

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”*

13:30 Closing. Concluding remarks

14:00 Lunch



**Venue:**

-The XIIth SEQT Mini Symposium. IIIrd Spanish/Portuguese/Brazilian Meeting will be held at GlaxoSmithKline

C/Severo Ochoa, 2, 28760 Tres Cantos, Madrid

- Accommodation will be provided at Hotel Exe Puerta Castilla

Paseo de la Castellana, 191, 28046 Madrid

**Scientific Committee**

Dr. José María Fiandor (GSK, Madrid, Spain) (Chairman)

Prof. Rui Moreira (U. Lisbon, Lisbon, Portugal)

Prof. Aurea Echevarría (U. Federal Rural do Rio de Janeiro, Rio de Janeiro, Brazil)

Prof Pilar Goya (Instituto de Química Médica, CSIC, Madrid, Spain)

Dr. Antoni Torrens (Esteve, Barcelona, Spain)

**Organizing Committee**

Ana Merino (GSK, Madrid, Spain)

Dra. Eva-María Priego (Instituto de Química Médica, CSIC, Madrid, Spain)

Dra. Ana San Félix (Instituto de Química Médica, CSIC, Madrid, Spain)

Elena Santos (BCD Travel Spain, Madrid, Spain)

Isabel Pérez (BCD Travel Spain, Madrid, Spain)

[jornadas\\_seqt@iqm.csic.es](mailto:jornadas_seqt@iqm.csic.es)

