

July 8-11<sup>th</sup>  
**seqt**  
**2019**  
vitoria-gasteiz



8-11 julio  
**seqt**  
**2019**  
vitoria-gasteiz



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- **Javier Vicario, University of the Basque Country UPV/EHU, Vitoria-Gasteiz, Spain**

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- **Barbara Noverges, Faes Farma, Bilbao, Spain**
- **Javier Fernandez Gadea, Janssen-Cilag, Toledo, Spain**
- **Antoni Torrens, Esteve Farma, Barcelona, Spain**

# SCIENTIFIC PROGRAMME

MONDAY, JULY 8th

16:00 **Registration**

18:00 **OPENING CEREMONY**

## *Opening session*

Chairpersons: J. Fernández Gadea and Francisco Palacios

18:15-19:15 PL-01 **Yvette van Kooyk** "The function of glycans in cancer-immunology"

19:15 **SEQT AWARDS**

20:00 **Welcome cocktail.** Vitoria Museum of Fine Arts

# SCIENTIFIC PROGRAMME

TUESDAY, JULY 9th

## Session 1

Chairpersons: Joaquín Pastor and Joaquín C. García-Martínez

- 09:00-09:35 KN-01 **Catherine Llorens-Cortes** "Central-acting aminopeptidase A inhibitors for new treatment of hypertension: from discovery to clinical trial"
- 09:35-09:50 OC-01 **Álvaro Lorente** "Optimization of kinase inhibition and metabolic stability of pyrazolopyridine inhibitor of Yeast Kinase YCK2"
- 09:50-10:05 OC-02 **Carmen Escolano** "Preclinical data on (2-imidazolin-4-yl)phosphonates"
- 10:05-10:20 OC-03 **Alejandra Rodríguez** "Discovery and development of a novel nanomolar F508-del CFTR corrector for the treatment of cystic fibrosis"
- 10:20-10:25 FL-01 **Javier García-Marín** "New tools in medicinal chemistry: design, synthesis & evaluation of new molecules for the modulation of integrin linked kinase: a new target for chronic kidney disease"
- 10:25-10:30 FL-02 **M. Dolores Moya-Garzón** "Dual GO/LDHA inhibitors for the treatment of primary hyperoxaluria type 1"
- 10:30-10:35 FL-03 **Carolina Izquierdo** "Chemical tools to modulate KChIP3 signaling"
- 10:35-10:40 FL-04 **Silvia M. Barolo** "Synthesis of novel conformationally restricted sulfonamides as antiproliferative agents"
- 10:40-10:45 FL-05 **Mario De Juan** "Synthesis of 1*H*-1,2,3-triazoles from heterochalcones as potential antiproliferative agents"
- 10:45-10:50 FL-06 **Xabier del Corte** "Synthesis and evaluation of the cytotoxic activity of 3-amino-1,5-dihydro-2*H*-pyrrol-2-ones"

11:00-11:30 **Coffee break**

## Session 2

Chairpersons: Rosario González Muñoz and Eddy Sotelo

- 11:30-12:05 KN-02 **GianLuca Sbardella** "Sympathy for the methyl: a library-on-library screening approach to identify small-molecule ligands of methyl-lysine reader proteins"
- 12:05-12:20 OC-04 **Joaquín C. García** "Anti-biofilm activity of new oligostyrylbenzene compounds over sessile cells of *Candida tropicalis*"
- 12:20-12:35 OC-05 **Sara del Mazo** "Tetrazoles as analogs of combretastatin A-4"
- 12:35-12:50 OC-06 **Concepción Alonso** "Design, synthesis and biological evaluation as antiproliferative agents of heterocyclic fused [1,5]naphthyridines"
- 12:50-13:05 OC-07 **Fernando Herranz** "Bioorthogonal Chemistry for the *in vivo* diagnosis of cardiovascular diseases"
- 13:05-13:10 FL-07 **Bruno Di Geronimo** "A proposed protac binding mode in kinases. Is an allosteric binding mode possible?"
- 13:10-13:15 FL-08 **Victor Carramiñana** "Probing the anticancer potential of new phosphorylated aziridine derivatives"

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|-------------|-------|---|
| 13:15-13:20 | FL-09 | <b>Irene Fernández-Barahona</b> "Cu-doped iron oxide nanoparticles with large longitudinal relaxivity; one-pot synthesis and <i>in vivo</i> tumour detection by magnetic resonance imaging"   |
| 13:20-13:25 | FL-10 | <b>Marta Gargantilla</b> "Chalcone-mimetics as Nocht inhibitors: synthesis, conformational studies and biological effects in an <i>in vitro</i> model of T-cell acute lymphoblastic leukemia" |
| 13:25-13:30 | FL-11 | <b>María Fuertes</b> "Synthesis of phosphorylated quinolines and biological evaluation as topoisomerase I inhibitors"   |

13:30-15:30 **Lunch**

### **Session 3**

Chairpersons: Juan J. Vaquero and Javier Luque

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|-------------|-------|---|
| 15:30-16:05 | KN-03 | <b>Maria Laura Bolognesi</b> "Harnessing polypharmacology with medicinal chemistry in Alzheimer's Disease drug discovery"                     |
| 16:05-16:20 | OC-08 | <b>Diego Muñoz-Torrero</b> "Revolving around the antioxidant lead CR-6: a new class of multitarget compounds against Alzheimer's Disease"     |
| 16:20-16:35 | OC-09 | <b>Antonio Viayna</b> "On the bioactive species of azocine-based AChE inhibitors: interplay between activity and tautomerism"                 |
| 16:35-16:40 | FL-12 | <b>Clara Herrera-Arozamena</b> "New neurogenic inducers with combined activities in key targets related to Alzheimer's Disease"               |
| 16:40-16:45 | FL-13 | <b>Paloma Mayo</b> "New GSK3 $\beta$ inhibitors and L-VDCCs blockers with neuroprotective potential for the treatment of Alzheimer's Disease" |
| 16:45-16:50 | FL-14 | <b>Carlota Tosat-Bitrian</b> "Neurodots: a novel approach for drug discovery in neurodegenerative diseases"                                   |
| 16:50-16:55 | FL-15 | <b>Andrea L. Turcu</b> "Open-channel blockers of the NMDA receptor in the Alzheimer's Disease"  |

17:00-17:30 **Coffee break**

### **Session 4**

Chairpersons: María José Camarasa and Jordi Quintana

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|-------------|-------|---|
| 17:30-18:05 | KN-04 | <b>Modesto J. Remuiñán</b> "Teaching new tricks to an old dog: reprogramming ethionamide to fight multidrug resistant tuberculosis"           |
| 18:05-18:20 | OC-10 | <b>Mónica Cacho</b> "Decaprenylphosphoryl-b-D-ribose oxidase (DprE1) as a promising target of mycobacterium tuberculosis inhibitors"          |
| 18:20-18:25 | FL-16 | <b>Mikel Etxebeste-Mitxelorena</b> "Selenocyanate and diselenide derivatives as novel antileishmanial drugs"                                  |
| 18:25-18:30 | FL-17 | <b>Asier Selas</b> "Antileishmanial activity of phosphorylated novel quinoline derivatives"   |
| 18:30-18:35 | FL-18 | <b>Victor Sebastián-Pérez</b> "Discovery of novel <i>s. mansoni</i> phosphodiesterase inhibitors as potential agents against schistosomiasis" |

18:45 **Guided walking tour of the old city (group 01 · Spanish)**

# SCIENTIFIC PROGRAMME

WEDNESDAY, JULY 10th

## Session 5

Chairpersons: Bárbara Noverges and Fernando Herranz

- 09:00-09:35 KN-05 **Gonçalo L. Bernardes** "Chemical physiology of antibody conjugates and natural products"
- 09:35-09:50 OC-11 **Jordi Quintana** "EU-OPENSOURCE drive: building the European academic chemical library"
- 09:50-10:05 OC-12 **Javier Rojo** "Peptide-adjuvant conjugates to modulate the immune response in allergic diseases"
- 10:05-10:10 FL-19 **Alejandro Revuelto** "Dimerization modulators of trypanothione reductase as innovative potent and selective leishmanicidal agents"
- 10:10-10:15 FL-20 **Carme Masdeu** "A new functionalized DNA-based nanostructure as antileishmanial agent"
- 10:15-10:20 FL-21 **Olaia Martí-Marí** "Tryptophan trimers and tetramers: extremely potent and selective entry inhibitors of HIV and EV71"
- 10:20-10:55 KN-06 **Ignacio Alfonso** "Supramolecular approaches to Chemical Biology"

11:00-11:30 **Coffee break**

## Session 6

Chairpersons: Diego Muñoz-Torrero and Javier Rojo

- 11:30-12:05 KN-07 **José Ignacio Andrés** "Chemical Biology and proteomics in drug discovery: beyond target identification and target validation"
- 12:05-12:20 OC-13 **Ouldouz Ghashghaei** "Near infrared fluorogenic Trp-bodipy cyclopeptide for *in vivo* imaging of carcinomas selectively targeting keratin 1"
- 12:20-12:35 OC-14 **María Muñoz-Hernando** "Enzyme-driven multimodal detection of atherosclerosis with iron oxide nanoparticles"
- 12:35-12:50 OC-15 **Ana Mallo** "A multicomponent approach enabled the discovery of D2 ligands simultaneously exhibiting receptor subtype and biased selectivity"
- 12:50-12:55 FL-22 **Martín Estrada-Valencia** "Surface plasmon resonance for the discovery of new non-electrophilic inhibitors of Keap1-Nrf2 protein-protein interaction"
- 12:55-13:00 FL-23 **Joaquín C. García-Martínez** "Chemodosimeters based on PPV dendrimers as fluoride anion sensor"
- 13:00-13:05 FL-24 **Claudia Gioé** "Multicomponent-assisted GPCR modulation: adenosine receptors as a case study"
- 13:05-13:10 FL-25 **Gloria Tobajas** "New chemical tools to investigate protein misfolding diseases"
- 13:10-13:15 FL-26 **Belén Rubio-Ruiz** "Development of Pd-loaded exosomes for targeted bioorthogonal catalysis"
- 13:15-13:20 FL-27 **Adrián Monteiro** "Ugi-based assembly of peripheral selective rimonabant analogues"

13:30-15:30 **Lunch**

### **Session 7**

Chairpersons: Guillermo de la Cueva and Rodolfo Lavilla

- 15:30-16:30 PL-02 **Erik M. Carreira** "Discovery and surprises with natural products and their connection to human Biology"
- 16:30-16:45 OC-16 **María Majellaro** "A<sub>2B</sub> Antagonists as anticancer drugs: enantioselective recognition, optimization and ligand profiling"
- 16:45-16:50 FL-28 **Myriam González** "A privileged scaffold in the search for new tubulin binding drugs: the sulfonamide"
- 16:50-16:55 FL-29 **Aitor Maestro** "Synthesis and biological evaluation of hybrid bis-(3-indolyl)methane phosphonate derivatives as antiproliferative agents"
- 16:55-17:00 FL-30 **Sarah Mazzotta** "*In vitro* anti-proliferative effect of novel small molecules with acyl piperazine moiety"

17:00 **Coffee break**

17:30 **SEQT MEETING**

17:30 **Guided walking tour of the old city** (group 02 · English)–(group 03 · Spanish)

21:00 **Conference dinner.** Restaurant "El Portalón"

# SCIENTIFIC PROGRAMME

THURSDAY, JULY 11th

## Session 8

Chairpersons: Manuel Medarde and Antonio Pineda-Lucena

- 09:30-10:05 KN-08 **Benoit R. Gauthier** "LRH-1/NR5A2 a novel drug target for Diabetes therapeutics"
- 10:05-10:20 OC-17 **Alba Vicente-Blázquez** "Novel tubulin ligands: design, synthesis and characterization of the antitumor mechanism of action"
- 10:20-10:25 FL-31 **Rubén Prieto** "Discovery of potent and highly selective A<sub>2B</sub> antagonist chemotypes"
- 10:25-10:30 FL-32 **Karim Tighilet** "Phytochemical composition, antiproliferative and antioxidant activities of *retama monosperma*"
- 10:30-10:35 FL-33 **Loganathan Rangasamy** "Pharmacophore hybridization to discover novel CK2/HDAC dual inhibitors"
- 10:35-10:40 FL-34 **Carlos Rodríguez** "Novel series of A<sub>2A</sub> antagonists: design, synthesis and SAR studies"

11:00-11:30 **Coffee break**

## Session 9

Chairpersons: Beatriz de Pascual-Teresa and Víctor Segarra

- 11:30-12:05 KN-09 **Kristof van Emelen** "New and emerging technologies for modern day's medicinal chemistry"
- 12:05-12:10 FL-35 **Ana Carolina Ruberte** "Seleno-heteroaryl derivatives as selective antitumoral agents"
- 12:10-12:15 FL-36 **Endika Martín-Encinas** "Synthesis and biological evaluation of fused [1,5]naphthyridines by intramolecular HDA reaction"

## Closing session

- 12:15-13:15 PL-03 **Luis M. Liz-Marzán** "Diagnosis and therapy based on gold nanoparticles"

13:15 **MEETING CLOSURE**

PL: Plenary Lecture

KN: Keynote

OC: Oral communication

FL: Flash communication