

Tuesday, January 23rd

University of Salamanca Old Building (Patio de Escuelas, C/ Libreros)

17:00	Registration
18:00	OPENING CEREMONY (<i>Parainfo</i>)
18:15	<i>Opening session</i> . Chairperson: Pilar Goya Ginés Morata (CBM, CSIC-UAM, Príncipe de Asturias Prize 2007) <i>Cell competition: killing cells to keep you alive</i>
19:15	SEQT AWARDS
19:30	Welcome cocktail (<i>Salón de Claustros</i>)

Wednesday, January 24th

Main hall, Faculty of Pharmacy (Campus Miguel de Unamuno, C/ Licenciado Méndez Nieto, s/n)

9:00	Session 1. Chairpersons: M^a José Camarasa and Toni Torrens	
9:00	PL1. David K. Smith (Department of Chemistry, University of York)	<i>Supermolecules for self-assembled medicine (Super-SAM)</i>
9:45	OC1. Javier García OC2. Sonia Martínez	<i>Pyrrolo[1,2-a]quinoxalines as new small molecules to modulate PTP1B activity by an allosteric mechanism</i> <i>Novel CDK8 inhibitors</i>
10:25	FL1. Álvaro Lorente FL2. José Clerigué FL3. Miryam Pastor FL4. Sarah Mazzotta FL5. Bruno di Geronimo FL6. Sara del Mazo FL7. Horacio Larqué FL8. Dolores Viña	<i>Amide-controlled, one-pot synthesis of tri-substituted purines generates structural diversity and analogues with trypanocidal activity</i> <i>Alkaloid-like, benzo-fused diazabicyclic compounds as neuroprotective agents</i> <i>Promising HITS as selective MMP13 inhibitors</i> <i>Synthesis of new aminoglycerol derivatives as potential antibacterial agents</i> <i>Towards selective phosphatase inhibition: a new PTPRZ1 binding mode proposal promotes rational design of compounds that increase PTPRZ1/PTP1B selectivity</i> <i>Antimitotic amides based on combretastatin A-4</i> <i>Synthesis of falcarinol-type compounds and in vitro leishmanicidal activity</i> <i>Parkinson's disease: potential therapeutic alternatives based on the coumarin scaffold</i>
11:25	Coffee break	
11:45	VISIT TO THE UNIVERSITY OLD BUILDING AND LIBRARY	
14:00	Lunch: Colegio Mayor "Arzobispo Fonseca" (C/ Fonseca, 4)	
16:00	Session 2. Chairpersons: Francisco Palacios and Javier Rojo	
16:00	KN1. Ignacio García-Ribas (Takeda Pharmaceutical International Co.)	<i>From cytotoxics to immunotherapy: shortening the long story of systemic cancer treatment</i>
16:30	OC3. Amadeu Llebaria OC4. María Marco	<i>Precise control of native GPCRs with light and photoactive molecules</i> <i>Discovery of GSK3494245A as a potential antileishmanial drug</i>
17:10	FL9. Marta Gargantilla FL10. Julia Revuelta	<i>Exploration of the $\alpha\beta$ tubulin interface at the colchicine-domain through cyclohexanedione derivatives</i> <i>Tunable heparan sulfate glycomimetics for promote neural differentiation</i>

	<p>FL11. Ángela P. Hernández <i>New hybrids derived from podophyllic aldehyde and diterpenylhydroquinones selective to osteosarcoma cells</i></p> <p>FL12. Marco Leonardi <i>Diversity-oriented synthesis of pyrrole-related frameworks for lead discovery via high-throughput screening</i></p> <p>FL13. Cristina Blázquez <i>Synthesis and metal chelating properties of aminophenanthridinones as potential therapeutic agents for the treatment of Alzheimer's disease</i></p> <p>FL14. Ángel González <i>Identifying human diamine sensors for death related putrescine and cadaverine molecules</i></p> <p>FL15. Matteo Staderini <i>A robust sensing system for electrochemical detection of proteases</i></p>
18:00	Coffee break
18:30	Session 3. Chairpersons: Rodolfo Lavilla y M ^a Jesús Pérez
18:30	<p>KN2. M^a Ángeles Martínez-Grau (Medicinal Chemistry, DCRT Spain, Lilly, S.A.) <i>Discovery and optimization of the first small molecules targeting GOAT (ghrelin O-acyl transferase) inhibition in vivo</i></p>
19:00	<p>OC5. Oskia Bueno <i>Protein-ligand complex for structure-based design: impact on the affinity and antitumor activity of new tubulin ligands</i> RAMÓN MADROÑERO AWARD</p>
19:20	<p>FL16. Marta Barniol <i>Multitarget directed ligands featuring an NMDA antagonist moiety: new strategies of potential interest for the treatment of Alzheimer's disease</i> ESTEVE AWARD</p> <p>FL17. Alejandro Revuelto <i>First non-peptide dimerization inhibitors of trypanothione reductase with potent in vitro leishmanicidal activity</i> ALMIRALL AWARD</p> <p>FL18. Belén Martínez <i>Modified tryptophan derivatives as dual inhibitors against HIV and enterovirus 71 (EV71) replication</i> JANSSEN-CILAG AWARD</p> <p>FL19. Cristina Chamorro <i>iLab: drug discovery and design research in co-creation</i></p> <p>FL20. Begoña Verdejo <i>Synthesis and platinum (II) complexes of polyazacyclophane receptors as potential therapeutic agents</i></p> <p>FL21. Sheila Abril <i>Synthesis and study of new chiral melatonin-acetylcholinesterase inhibitor hybrids to treat neurodegenerative diseases</i></p>

Thursday, January 25th

Main hall, Faculty of Pharmacy (Campus Miguel de Unamuno, C/ Licenciado Méndez Nieto, s/n)

9:00	Session 4. Chairpersons: Beatriz de Pascual-Teresa and José Ignacio Andrés	
	9:00	PL2. Christa Müller (PharmaCenter, Bonn Pharmaceutical Institute) <i>Medicinal chemistry of purinergic signalling in inflammation and cancer</i>
	9:45	OC6. F. Javier Rojo <i>Glycodendropeptides including a PRU P 3 epitope induce tolerance to peach allergy in mice</i> OC7. M ^a José Lorite <i>Lilly Open Innovation Drug Discovery Program (OIDD)</i> OC8. Rocío V. Paucar <i>Preclinical development of Mannich base derivatives as potent antichagasic agents</i>
	10:45	FL22. Asier Selas <i>Design, synthesis and biological evaluation of novel Top I inhibitors</i> FL23. Jorge Gómez-Carpintero <i>Design and synthesis of novel m-terphenylamine-tacrine hybrids compound as potential multitarget agents for the treatment of Alzheimer's disease</i> FL24. Sonia de Castro <i>Discovery of 1,4,4-trisubstituted piperidines as dual inhibitors of influenza and human corona viruses</i> FL25. Javier Recio <i>Synthesis and study of non-hepatotoxic acetaminophen analogs</i> FL26. Marta Piquero <i>Novel mitochondria-targeted, leishmanicidal derivatives of 4-aminostyrylquinolines</i> FL27. Concepción López <i>AOX properties and cytotoxicity of 1,5-benzodiazepin-2-ones</i> FL28. Myriam González <i>Modifying the methoxy groups of new tubulin inhibiting sulfonamides</i>
11:35	Coffee break	
12:00	Session 5. Chairpersons: David K. Smith and José Fiandor	
	12:00	KN3. Gabriele Costantino (Department of Food and Drugs, Università di Parma) <i>Non essential targets for the discovery of new potential antibacterial agents</i>
	12:30	OC9. Daniel Plano <i>As-10: Pre-clinical data of a very promising cancer drug candidate</i> OC10. Javier García <i>A positive allosteric modulator of the serotonin 5-HT_{2C} receptor for obesity</i>
	13:10	FL29. Pablo Duarte <i>Design, synthesis and biological evaluation of new multitarget compounds for the treatment of Parkinson's disease</i> FL30. Regina Martínez <i>CK2/HADAC1 dual inhibitors: new strategy for the design of antitumoral agents</i> FL31. Carolina Estarellas <i>Molecular dynamics simulations of AMPK mechanism of allosteric</i>

	<p>regulation by direct activators</p> <p>FL32. Hee-Doo Kim <i>D-Ring opened oxime analogues of 17-beta estradiol as estrogen receptor subtype selective ligands</i></p> <p>FL33. Juan F. González <i>New synthetic approach to quinoxaline di-N-oxide containing a peptide side chain with in vitro anti-leishmanial activity</i></p> <p>FL34. Pilar M^a Luque <i>Design, synthesis and biological evaluation of bioisosteric inhibitors of choline kinase</i></p> <p>FL35. Tiziana Ginex <i>Natural (poly)phenols and Alzheimer's disease: theoretical elucidation of the structural determinants for covalent amyloid beta (Aβ) inhibition</i></p>
14:00	Lunch: Residencia Universitaria "Colegio de Oviedo" (Campus Miguel de Unamuno)
16:00	Session 6. Chairpersons: Guillermo de la Cueva and Bárbara Noverges
16:00	<p>KN4. Juan Carlos Morales (Inst. Parasitology & Biomedicine "López Neira", CSIC, Granada) <i>From food ingredients to effective drugs?</i></p>
16:30	<p>OC11. Clara Herrera <i>Design, synthesis, and functional characterization of new photoswitchable neuromuscular ligands</i></p> <p>OC12. Concepción Alonso <i>Anticancer activity of novel phosphorylated quinolines</i></p>
17:10	<p>FL36. José Manuel Méndez <i>Triazolopyrimidine derivatives and complexes: Synergic effect of metal ions against parasitic neglected diseases</i></p> <p>FL37. Lucía Mayán <i>Curcumin-coumarin analogues: new MAO-B inhibitors with neuroprotective activity</i></p> <p>FL38. Raquel Álvarez <i>Replacement of trimethoxyphenyl ring of combretastatin analogues by pyridine moieties. Study of the biological effect</i></p> <p>FL39. Sofía de la Puente <i>Aminophenol derivatives as antibiotic alternatives</i></p> <p>FL40. Ricardo Escarcena <i>Design, synthesis and antiparasitic activity of phthalazinones</i></p> <p>FL41. Martín Estrada <i>New neurogenic and neuroprotective donepezil-flavonoid hybrids as multitarget drugs for Alzheimer's disease</i></p> <p>FL42. Ana Carolina Ruberte <i>Synthesis and biological evaluation of selenocompounds as antioxidant and antiproliferative agents</i></p>
18:00	Coffee break
18:30	SEQT MEETING
21:00	Conference dinner : Gran Hotel Corona Sol (C/ Víctor García de la Concha, s/n)

Friday, January 26th

Main hall, Faculty of Pharmacy (Campus Miguel de Unamuno, C/ Licenciado Méndez Nieto, s/n)

9:00	Session 7. Chairpersons: Gabriele Costantino and Víctor Segarra	
	9:00	KN5. Fernanda Borges (Department of Chemistry, University of Porto) <i>Shifting from single to multitarget drugs. Is pharmacological promiscuity a herald for neurodegenerative diseases?</i>
	9:30	OC13. Patrycja Michalska <i>Novel multitarget Nrf2 inducers with potent antiinflammatory properties and neurogenic effect for the treatment of Alzheimer disease</i> OC14. Ouldouz Ghashghaei <i>Unexplored chemistry of isocyanides: modular access to N-heterocyclic scaffolds with applications in Medicinal Chemistry</i> OC15. Claire Coderch <i>In silico identification and in vivo characterization of small molecule therapeutic hypothermia mimetics</i>
	10:30	FL43. José Manuel Espejo <i>Design and synthesis of HA-CD44 interaction inhibitors as antiproliferative compounds</i> FL44. José Luis Lavandera <i>Citotoxicity and neuroprotective effects of N,C-diaryl-1,2,3-triazoles</i> FL45. Francisco Muñoz <i>Anion receptors based on pirazolones</i> FL46. M ^a Eugenia González <i>New polyamine derivatives as antiproliferative compounds</i> FL47. Alba Gigante <i>Hit selection from the GSK Tres-Cantos anti-kinetoplastid set (TCAKS) using a rapid in vivo assay</i> FL48. Pedro J. Llabrés <i>Controlled release of molecules using macroscopic IRMOF-10 crystals</i> FL49. M ^a Dolores Moya <i>Structural modulation of salicylates reducing oxalate production in hyperoxaluric mouse hepatocytes</i> FL50. Francisco Javier García <i>Novel DDR1/2 inhibitors: from hit identification (HTS) to hit generation by drug design</i>
11:35	Coffee break	
12:00	Session 8. Chairpersons: Fernanda Borges and Belén Abarca	
	12:00	OC16. Alba Vicente <i>Design, synthesis and evaluation of sulphonamide-based microtubule disruptors causing mitotic arrest</i>
	12:20	FL51. José Carlos Menéndez <i>Leishmanicidal activity of 2-acylquinolines and their hydrazones</i> FL52. Olmo Martín <i>Multiple target directed ligands derived from a rho-associated kinase (ROCK) inhibitor for the potential treatment of neurodegenerative disorders</i> FL53. Olaia Martí <i>Tryptophan dendrons as potent HIV and enterovirus A71 entry inhibitors. SAR in the focal point</i> FL54. Belén Rubio

	<p><i>Gold-triggered release of histone deacetylase inhibitor panobinostat from a biorthogonal precursor</i></p> <p>FL55. Maite Docampo</p> <p><i>Glucuronidated flavonoids in neurological protection: approaches to their chemical and biochemical synthesis</i></p>
13:00	<p><i>Closing session.</i> Chairperson: Marina Gordaliza</p> <p>PL3. Sergio Moreno (Inst. of Functional Biology and Genomics, CSIC-USAL)</p> <p><i>Using chemical-genomics to identify new targets for cancer and aging</i></p>
14:00	MEETING CLOSURE