

SEQT · 2011



XVI Congress of the SEQT

From a Classical to a New Age in
Medicinal Chemistry

Centro de Investigación Príncipe Felipe • Valencia 18-21 September, 2011

Scientific Program

Sunday, September 18th, 2011

- 15:30 Registration
- 17:30 Opening
- SEQT awards. **Dr. Antoni Torrens**, Esteve
- Inaugural lecture: **Dr. Tim Gallagher**, Bristol University
- “Natural products as leads to nicotinic agonists. Exploring the chemistry of cytisine”*
- 20:00 Cocktail

Monday, September 19th, 2011

Morning Session (Chairs: **M.L. López-Rodríguez/M.J. Vicent**)

- 09:00 IS1: **Rosario González-Muñiz**, IQM-CSIC
“Looking for innovative bioactive compounds: underexplored approaches, creative synthesis”
- 09:30 IS2: **Andrés Trabanco**, Janssen
“Discovery of a potent and orally bioavailable positive allosteric modulator of mGluR2 for the treatment of CNS disorders”
- 10:00 Ramón Madroñero SEQT Award
IS3: **Valle Palomo**, IQM-CSIC
“Design, synthesis, enzymatic and cellular evaluation of novel neurogenic ATP-non competitive GSK-3 inhibitors”
- 10:30 Coffee Break

- 11:00 IS4: **Stephan A. Sieber**, TU Munich
"Natural products and their biological targets"
- 11:30 IS5: **Jesús Martínez**, Instituto de Nanociencia de Aragón
"Gold nanoparticles for gene therapy and photo-thermal ablation"
- 12:00 Oral Communications (OC1-OC4)
OC1: **Jordi Quintana**, Parc Científic de Barcelona
"The ChEMBioBank and EU-OPENSREEN initiatives in Chemical Biology: Current status and case studies"
OC2: **Joaquín Campos**, Universidad de Granada
"Increased phosphorylation of the translation initiation factor eIF2 α is associated with G2/M cell-cycle arrest and apoptosis in breast cancer cells"
OC3: **Inmaculada Conejos**, Centro de Investigación Príncipe Felipe
"Polymer-drug conjugates for the treatment of Familial Amyloidotic Polyneuropathy (FAP)"
OC4: **Miriam Corredor**, IQAC-CSIC
"Chemical modulation of cellular signalling routes relevant to the control of apoptosis"
- 13:00 Lunch

Afternoon Session (Chair: Enrique Pérez-Payá)

- 15:00-16:00 Poster Session and Coffee
- 16:00 IS6: **Antonio Ferrer-Montiel**, Universidad Miguel Hernández
"TRPducins: a novel paradigm to modulate ion channel activity"
- 16:30 Oral Communications (OC5-OC7)
OC5: **Gianni de Fabritiis**, Universitat Pompeu Fabra
"Reconstructing an enzyme-inhibitor binding process by molecular dynamics simulations"
OC6: **Óscar Delgado**, Janssen
"Design, synthesis and biological evaluation of novel fluorinated ethanolamines"
OC7: **Rafael Gozalbes**, Centro de Investigación Príncipe Felipe
"Development and validation of QSAR-based ADME models for drug-like compounds"

Tuesday, September 20th, 2011

Morning Session (Chairs: Javier Rojo/Silvia Ortega)

- 09:00 IS7: **Félix Calderón**, GSK
"Open innovation in malaria: breaking the ice with Tres Cantos Antimalarial Set (TCAMS)"
- 09:30 IS8: **Paul Finn**, InhibOx Ltd
"The future of computer-aided drug design"

- 10:00 IS9: **Juan Granja**, Universidad de Santiago de Compostela
"Peptide nanotubes, a supramolecular approach for membrane targeting drugs"
- 10:30 Coffee Break
- 11:00 IS10: **Juan Miguel Jiménez**, Vertex Pharmaceuticals
"Discovery of orally active GSK-3 inhibitors for the treatment of neurodegenerative diseases"
- 11:30 Oral Communications (OC8-OC9)
OC8: **Mónica Sancho**, Centro de Investigación Príncipe Felipe
"Minocycline inhibits cell death and decreases mutant Huntingtin aggregation by targeting Apaf-1"
OC9: **María Jesús Pérez-Pérez**, IQM-CSIC
"Multivalent compounds based on 1,3,5-triazines targeting gp120: Anti-HIV evaluation and binding analysis with Surface Plasmon Resonance"
- 12:00 SEQT Meeting
- 13:00 Lunch

Afternoon Session (Chair: Rodrigo J. Carbajo)

- 15:00-16:00 Poster Session and Coffee
- 16:00 Oral Communications (OC10-OC14)
OC10: **Silvia Ortega-Gutiérrez**, Universidad Complutense de Madrid
"Development of a chemical toolset for the study of the endogenous cannabinoid system"
OC11: **Rafael Peláez**, Universidad de Salamanca
"Conformationally restricted macrocyclic analogues of combrestatins"
OC12: **Renato Márcio Ribeiro-Viana**, IIQ-CSIC
"Glyconanoparticles: Virus-like particle construction and anti-viral activity"
OC13: **Hugo Gutiérrez-de-Terán**, FPGMX
"Structure-based ligand design on adenosine receptors"
OC14: **Pilar Serra**, Universidad San Pablo CEU
"Molecular modeling studies for the design of new selective MMP2 inhibitors"
- 21:00 Gala Dinner

Wednesday, September 21th, 2011

Morning Session (Chair: María José Camarasa)

- 10:00 Round Table
"The new paradigm in the academy-industry collaborations"
- 11:00 Coffee Break

- 11:30 IS11: **Martin Drysdale**, The Beatson Institute for Cancer Research
"Fragment-based approaches to cancer drug discovery"
- 12:00 IS12: **Marc Marti-Renom**, Centro de Investigación Príncipe Felipe
*"Comparative docking for predicting molecular targets of known drugs. A
"kernel" for the tropical disease initiative"*
- 12:30 Concluding Remarks
- 13:00 Lunch

CONTACT

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