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-OPENSCREEN initiatives in Chemical Biology: Current status and case studies”

OC2: **Joaquín Campos**, Universidad de Granada  
“Increased phosphorylation of the translation initiation factor eIF2α 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

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**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”

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**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”

www.seqt.org  Email: seqt11@cipf.es  Phone: (+34)963289681, ext. 1102, 1104
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 Márício 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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