

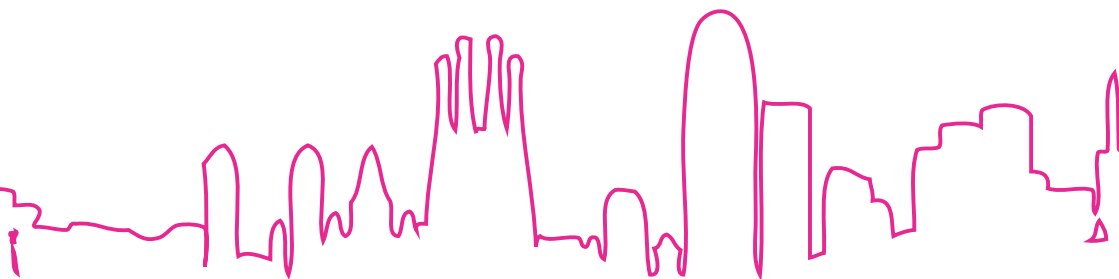


# Chemistry for Life Sciences

5th European Conference

Barcelona | June 10-12 | 2013

## Final Programme



# Summary

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# Welcome

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We are pleased to welcome you to the 5th European Conference on “Chemistry for Life Sciences” (5th ECCLS), the fifth in a series - Rimini (2005), Wroclaw (2007), Frankfurt (2009) and Budapest (2011) - organized by the EuCheMS Division of Chemistry in Life Sciences.

Following the spirit of previous editions of ECCLS, this Barcelona conference will gather an ensemble of scientists at the crossroads between chemistry, biology, biophysics and materials science.

A lot of discussion, disclosure of unpublished results, and a very iterative atmosphere will be the signature of this meeting.

Welcome to Barcelona, welcome to the 5th European Conference on “Chemistry for Life Sciences”.

Ernest Giralt, Chairman

**Institute for Research in Biomedicine (IRB Barcelona) and University of Barcelona - Spain**

# Committees

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## Organizing Committee

### - **Fernando Albericio**

Institute for Research in Biomedicine (IRB Barcelona) and University of Barcelona, Spain

### - **Ramon Eritja**

Institute for Research in Biomedicine (IRB Barcelona) and Consejo Superior de Investigaciones Científicas, CSIC, Spain

### - **Ernest Giralt**

Institute for Research in Biomedicine (IRB Barcelona) and University of Barcelona, Spain

### - **Antoni Riera**

Institute for Research in Biomedicine (IRB Barcelona) and University of Barcelona, Spain

### - **Xavier Salvatella**

Institute for Research in Biomedicine (IRB Barcelona) and ICREA, Spain

## Scientific Committee

Organizing Committee Plus:

### - **Annette G. Beck-Sickinger**

University of Leipzig, Institute für Biochemie, Leipzig, Germany

### - **Muriel Delepierre**

Unité de RMN des Biomolécules, URA 2185 du CNRS: Biologie Structurale et Agents Infectieux, Paris, France

### - **Joachim Engels**

Institute for Organic Chemistry, Goethe Universität, Frankfurt am Main, Germany

### - **Shiroh Futaki**

Institute for Chemical Research, Kyoto University, Kyoto, Japan

### - **Samuel H. Gellman**

University of Wisconsin, Department of Chemistry, Madison, USA

### - **Ivan Huc**

Institut Européen de Chimie et Biologie, Pessac, France

### - **Kai Johnson**

Ecole Polytechnique Fédérale de Lausanne, Institut des sciences et ingénierie chimiques, Lausanne, Switzerland

### - **András Perczel**

Eötvös Loránd University, Institute of Chemistry, Budapest, Hungary

# Scientific Programme

**Monday 10/6/2013**

## AUDITORIUM

9.00	<b>OPENING</b>
9.30-11.15	Chair: Xavier Salvatella
9.30	<b>L-01 - Annette G. Beck-Sickinger</b> New Approaches to Target Metabolic Diseases
10.10	<b>L-02 - Natàlia Carulla</b> Structural Characterization of Soluble and Membrane-Associated A $\beta$ Oligomers
10.50	<b>O-01 - Christian Heinis</b> Directed Evolution of Bicyclic Peptides for Therapeutic Application
11.15	<b>COFFEE</b>
11.45-13.15	Chair: Samuel Gellman
11.45	<b>L-03 - Jesús Jiménez-Barbero</b> Carbohydrate-Protein Interactions. A 3D View by Using NMR
12.25	<b>O-02 - Dietmar Appelhans</b> Glycodendrimer Interactions Against Alzheimer and Prion Peptides and Proteins: Exhibiting Promising Therapeutic and Diagnostic Agents
12.50	<b>O-03 - Luca Gentilucci</b> Opioid Receptor-Targeting Cyclopeptides for Pain Management: New Structures, New Mechanisms
13.15	<b>LUNCH</b>
15.00-16.40	Chair: Paola Turano
15.00	<b>O-04 - Nicholas J. Westwood</b> Allosteric Modifiers of Bacterial Protein Function
15.25	<b>O-05 - Suzanne Peyrottes</b> Optimized Analogues of Albitiazolium (T3/ Sar97276 ) to Target the Phosphatidylcholine Biosynthesis of <i>P. Falciparum</i>
15.50	<b>O-06 - Tao Ye</b> Total Synthesis and Biological Studies of Thiazole/Thiazoline-containing Marine Natural Products
16.15	<b>O-07 - M<sup>a</sup> Carme Fabrega</b> DNA Origami as Potential hAGT Recognition Biosensor

16.40

## POSTER SESSION 1 / COFFEE

### PARALLEL SESSION A - AUDITORIUM

17.40-19.10 Chair: Anna Aviñó

17.40 **SO-01 - Björn Palitzsch**  
The Impact of Glycosylation of Tumor-Associated Muc1 Anti-Cancer Vaccines on the Specificity of the Generated Antibodies In BALB/c Mice.

17.55 **SO-02 - Sebastian Hartmann**  
Synthesis and Immunological Evaluation of Fully Synthetic Polymer Based Multicomponent and Multivalent Muc1 Glycopeptide Antitumor Vaccines

18.10 **SO-03 - Francois Morvan**  
Influence of the Scaffold of Glycoclusters on their Binding to Pseudomonas Aeruginosa Lectin II and Burkholderia Ambifaria Lectin

18.25 **SO-04 - Ana Arda**  
Chemical Glycobiology: Molecular Recognition Features of Small and Complex Glycan Epitopes are Feasible by NMR

18.40 **SO-05 - Nadja Bertleff**  
Galectin-1: Sweet Weapons in The Fight of Cancer

18.55 **SO-06 - Laura Masgrau**  
Mechanism of Glycosidic Bond Formation by Retaining Glycosyltransferases. Insights from QM/MM Calculations.

### PARALLEL SESSION B - ROOM 1

17.40-19.10 Chair: Judit Tulla

17.40 **SO-07 - Sabine Müller**  
Twin Ribozymes for the Correction of Genetic Disorders at the Level of RNA

17.55 **SO-08 - Laura Nevola**  
Remote Control of Protein-Protein Interactions: Photo-Switchable Peptides for the Regulation of Clathrin-Mediated Endocytosis.

18.10 **SO-09 - Sílvia Osuna**  
Exploring the Structural Basis of Improved Catalysis Achieved by Directed Evolution on LovD Mutants: The Importance of Long Scale Molecular Dynamics

18.25 **SO-10 - Dolors Grillo-Bosch**  
Chemical Biology Approaches to Study the Role of PDZ Domain-Mediated Interactions in Glutamate Receptor Trafficking at the Synapse

18.40 **SO-11 - Thomas Laverne**  
Template Assembled Synthetic Quadruplex: Construction, Recognition and Application

18.55 **SO-12 - Zoltan Gaspari**  
Protein Structural Ensembles Reflecting Experimentally Determined Dynamics: Developments and Applications

19.30 **WELCOME COCKTAIL**

**Tuesday 11/6/2013**

**AUDITORIUM**

9.00-11.10 Chair: Fernando Albericio

9.00 **L-04 - Samuel H. Gellman**  
Mimicry of Protein Recognition Surfaces with Peptidic Foldamers

9.40 **L-05 - Paola Turano**  
Solution and Solid State NMR Approaches for Nanocage Proteins

10.20 **O-08 - Tamás Beke-Somfai**  
ATP Synthase: A Complex Biomolecular Machine

10.45 **O-09 - Injae Shin**  
A Synthetic Small Molecule that Inhibits Hsp70 Induces Apoptosis and has Antitumor Activities

11.10 **COFFEE**

11.10-13.15 Chair: Annette Beck-Sickinger

11.40 **L-06 - Ivan Huc**  
Foldamers: Expanding the Chemical Space

12.20 **O-10 - Tamas Kiss**  
Metal Ion Homeostatic Therapy in Alzheimer's Disease

12.45 **O-11 - Gonalo Bernardes**  
Chemically Defined Therapeutic Proteins

13.15 **LUNCH**

**PARALLEL SESSION C - AUDITORIUM**

15.00-16.30 Chair: Xavier Verdaguer

15.00 **SO-13 - St phanie Vandekerckhove**  
Synthesis and Antimalarial/Antifungal Evaluation of Novel Functionalized Quinolines

15.15 **SO-14 - Marcin Ziemniak**  
Interactions of Chemically Modified Cap Analogues with Yeast Decapping Complex Dcp1/2

15.30	<b>SO-15 - Miriam Corredor</b> Optimizing the Control of Apoptosis by Amide/Triazole Isosteric Substitution in a Constrained Peptoid
15.45	<b>SO-16 - Raphael Stoll</b> Structural and Functional Studies on Cp*Rh Derivatives of GPCR Peptide Ligands
16.00	<b>SO-17 - Chiara Nardon</b> Cutting-Edge Anticancer Agents: Gold-Based Peptidomimetics Targeting Peptide Transporters
16.15	<b>SO-18 - Marta Pelay-Gimeno</b> First Total Synthesis of the "Head-To-Side-Chain" Cyclodepsipeptide Pipecolidepsin A: Overcoming the AHDMHA Sterical Hurdle

#### PARALLEL SESSION D - ROOM 1

15.00-16.30	Chair: Meritxell Teixidó
15.00	<b>SO-25 - Laurence Raehm</b> Functionalized Mesoporous Silica Nanoparticles for Two-Photon Photodynamic Therapy
15.15	<b>SO-26 - Cristina Fornaguera</b> Dendronized Polymeric Nanoparticles from Nano-Emulsion Templating as Gene Delivery Systems
15.30	<b>SO-27 - Giulio Chiesa</b> A Study of the Mechanism of Fibril Formation in Spinal Bulbar Muscular Atrophy
15.45	<b>SO-28 - Shai Rahimipour</b> Self-Assembled Cyclic D,L- $\alpha$ -Peptide Nanotubes with Potent Anti-Amyloidogenic Activity.
16.00	<b>SO-29 - Omar Boutureira</b> Chemical Approaches to Well-Defined Fluoroglycoproteins and Radiolabelling Strategies
16.15	<b>SO-30 - Benjamí Oller-Salvia</b> From Venoms to BBB Shuttles. Synthesis, Protease Stability and Blood-Brain Barrier Transport of Apamin and a Non-Toxic Analogue.
16.30	<b>POSTER SESSION 2 - COFFEE</b>

#### PARALLEL SESSION E - AUDITORIUM

17.30-19.00	Chair: Agustí Lledó
17.30	<b>SO-19 - Laura Mendieta</b> Plants as a Source of New Dpp-IV Inhibitors for the Treatment of Type 2 Diabetes Mellitus



17.45	<b>SO-20 - Susana Liébana</b> Novel Promising Bionanomaterial for Biosensing: The Bacteriophages
18.00	<b>SO-21 - Filippo Favretto</b> NMR Study of HLFABP in Complex with Hydrophobic Molecules of Biological Relevance
18.15	<b>SO-22 - Bernat Guixé</b> Beyond Phage Display Limitations: Mass Spectrometry Tools for Identification and Quantification of Peptide Blood-Brain Barrier shuttle Libraries.
18.30	<b>SO-23 - Gemma Triola</b> Site-Specific, Reversible and Fluorogenic Immobilization of Proteins on Flash-Modified Surfaces
18.45	<b>SO-24 - Ádám Hadházi</b> Synthesis of Fullerene - Sugar Hybrids Against Influenza Virus

### PARALLEL SESSION F - ROOM 1

17.30-19.15	Chair: Juan Bautista Blanco
17.30	<b>SO-31 - Christoph Denk</b> Kinetics of Tetrazine Ligations: From Organic to Biological Media
17.45	<b>SO-32 - Francesco Sansone</b> Guanidinium and Arginine Clustering on Calixarene Macrocyclic Scaffolds as a Novel Strategy for Improved Cell Transfection
18.00	<b>SO-33 - Nora Ventosa</b> A Novel Platform of Nanovesicle-Bioactive Conjugates Prepared by a One-Step Scalable Method
18.15	<b>SO-34 - Pierre Maisonneuve</b> Allosteric Regulation of the Phosphatase PTPN4
18.30	<b>SO-35 - Miryana Hémadi</b> Efficient Cellular Internalization of a Holotransferrin-Maghemite Construct by the Iron Acquisition Pathway
18.45	<b>SO-36 - Laia Miret Casals</b> The Search of Mitofusin 2 Modulators Identifies a Link Between Mitochondrial Fusion and Fission Proteins and the Novo Synthesis of Pyrimidines
19.00	<b>SO-37 - Ferial Tera</b> Newly Synthesized Amphoteric Starch as a Flocculant in the Treatment of Raw and Industrial Waste Water

**Buses leave to the restaurant**

**CONFERENCE DINNER**

Wednesday 12/6/2013

AUDITORIUM

9.00-11.00	Chair: Antoni Riera
9.00	<b>L-07 - Shiroh Futaki</b> CXCR4 Stimulates Macropinocytosis: Implications for Cellular Uptake of Arginine-Rich Cell-Penetrating Peptides and HIV
9.40	<b>L-08 - Xavier Salvatella</b> Conformational Ensembles as a Tool to Understand Protein Behavior
10.20	<b>O-12 - Luca Domenico D'Andrea</b> Insight on the Structural and Receptor Recognition Properties of a Proangiogenic Peptide
10.45	<b>O-13 - Rodolfo Lavilla</b> Fluorinated Thiazolines, a New Scaffold for P53-Independent Pro-Apoptotic Antitumorals. Chemical and Biological Insights.
11.10	<b>COFFEE</b>
11.40-13.10	Chair: Jesús Jiménez-Barbero
11.40	<b>L-09 - Christian Griesinger</b> Small Molecule Interference with Neurodegeneration: An NMR Spec- troscopic View and More
12.20	<b>O-14 - Oliver Zerbe</b> Properties of Split Armadillo Repeat Proteins Investigated by NMR Spectroscopy
12.45	<b>O-15 - Joachim Engels</b> RNA Labeling by Pd-Catalyzed Cross-Coupling and Distance Measure- ments in Vitro and In-Cell
13.10	<b>LUNCH</b>
15.00-16.30	Chair: Ramon Eritja
15.00	<b>SO-38 - Juan Bautista Blanco Canosa</b> Synthesis of C-Terminal Modified N-Acylurea Peptides Using a Novel Linker and Their Application to Native Chemical Ligation and Cyclic Protein Synthesis.
15.15	<b>SO-39 - Pablo Martin-Gago</b> Fine-Tuning the Aromatic Interactions in Somatostatin Analogues
15.30	<b>SO-40 - Alessandra Romanelli</b> Interactions of Antimicrobial Peptides with Bacterial Membrane Mod- el Systems and with Whole E. Coli Bacterial Cells

15.45	<b>SO 41 - Arne Berthelmann</b> Exploring Multivalency in Protein-Protein Interaction Using Synthetic Peptides
16:00	<b>SO-42 - Slawomir Potocki</b> IRT1 Metal Transporter and Zinc - What is the Impact of Glu Residues on Metal Complex Stability?
16.15	<b>SO-43 - Ferran Feixas</b> The Role of Cis-Prenyl Diphosphate Synthases in Bacterial Cell-Wall Biosynthesis: Chain Length Control and its Implications for Drug Discovery
16.30	<b>CLOSING</b>

## General Information

### Venue

Auditorio AXA  
Av. Diagonal, 547  
08029 Barcelona (Spain)

### Dates

10th - 12th June

### Internet

Free WIFI in all the areas

### Language

All the sessions will be presented in English. No Spanish translation will be provided.

### Coffe-breaks & Lunch

Coffee-breaks and lunch are included in the registration fee. Coffee-breaks will be served in the Poster Area – WIN Room in AXA Auditorium. Lunchs will be served in the Hotel NH Constanza in the Nhube Restaurant

### Speakers

Presentation shall be delivered at least one hour before your schedule presentation time. Please refer to the reception desk for more information at your arrival.

### Posters

Posters should be displayed on the Poster Area on Monday 10<sup>th</sup> June from 09:00 h and removed on Wednesday 12<sup>th</sup> June after the coffee-break.

## Major Sponsor

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## Gold Sponsor

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## Contributors

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## Other Collaborations

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## Exhibitors

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Booth 11

