Biennial Report 2010-2011
# IQAC Biennial Report 2010-2011

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8.2 APPENDIX 2. SCIENTIFIC OUTPUT 139
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The Institute of Advanced Chemistry of Catalonia (IQAC) is one of the research centers of the Consejo Superior de Investigaciones Científicas (CSIC). The Institute is located in Barcelona and it was created to do research of excellence focused on basic chemical sciences, but also addressed to solve specific problems of our society by using tools from the chemistry-biology interface, theoretical chemistry, chemical and biomolecular nanotechnology and sustainable chemistry. In particular, the identification of niches where our expertise can make important contributions is systematically pursued. Equally important to all of us is to be in a permanent attitude to transfer our knowledge and technology results to the industrial sector.

The present Report covers the biennium 2010-2011. It gives an account of our research activity and of the main objectives achieved during this period.

The analysis of the data herein reported permits to conclude that the mission that inspired the creation of our Institute is being successfully accomplished. We deem that the expertise and the intense efforts of all our personnel have contributed to consolidate our scientific project at the international scale.

In addition to the information given here, we invite you to navigate our website (www.iqac.csic.es). There, you will find additional information about the research problems that we face and their results and perspectives. The web page contains also details about the facilities and methodologies that we can offer to the scientific community, both from the public and the private domains, to complement or improve their own projects, or those that can be put in the frame of a joint initiative. In this sense, the research groups and technical services from our Institute will be wide open to attend your inquiries and to offer their best efforts to find adequate responses to your needs, based on their background and expertise.

Yours faithfully,

Àngel Messeguer
Director of IQAC
STRUCTURE AND GENERAL RESULTS
HISTORY

The Institute was created in 2007 to better accommodate the interests of scientists of the Chemistry areas working at the “Center of Investigation and Development” (CID) and to provide a greater external projection of the activities of these scientists within the frame of the Spanish Research Council (CSIC). In spite of its recent creation, the Institute inherits the long and fruitful research tradition in Organic Chemistry initiated by Prof. José Pascual Vila since 1940. After finalizing his activity in the University, in 1967 Prof. Pascual Vila moved with his co-workers of CSIC into the Institute of Organic Chemistry of Barcelona in CID. At the same time, CSIC scientists working on Chemical Technology, such as those related to the textile and leather fields, were also incorporated into CID. During many years the CID has been the referent of the CSIC Chemistry in Catalonia and of the organic and bioorganic chemistry research in our community. Many graduate students and post-docs formed in this Center have moved to relevant positions in academic institutions (Universities, CSIC) and in private sector. In 1996, a joined action of the bioorganic, theoretical and technological groups together with those working in chemical issues related to the environment, led to the creation of the Institute of Chemical and Environmental Research “Josep Pascual Vila” (IIQAB). During the ten-year period of IIQAB, research groups have adapted their objectives to the new demands of society and new groups have also been generated. From these efforts, the Biological Chemistry, Theoretical and Computational Chemistry, Sustainable Chemistry and selected items of Chemical Technology have been reinforced. Concomitantly, potent groups working on Chemical and Biomolecular Nanotechnology have emerged or have been incorporated into IQAC. Actually, this set of scientific interests, in which the apparent heterogeneity of the active research areas is clearly compensated by the wide opportunities of their mutual interaction, justifies the creation of IQAC as a solid and modern Institute that looks at the future leaning on two pillars: the enthusiasm and expertise of its personnel and the robustness of the Chemistry tradition in our Centre.

Although its creation was in 2007, the research groups incorporated into IQAC have a recognized international prestige in their research fields. Among others, it should be highlighted the design, synthesis and evaluation of molecules of therapeutic, pharmacological or biological interest, the chemistry and applications of surfactants, the study of hormones and enzymatic transformations in insects, the development of environmentally friendly technologies, the research in peptides and proteins, the theoretical study in electronic structure, or the application of nanotechnological approaches to the understanding of nanoscale systems and the development of novel nanomaterials and nanodevices, such as bioanalytical tools based on the combination of tailored bioreceptors, new nucleic acid derivatives and well-defined nanostructures and advanced materials.

In addition, our Institute has a set of scientific and technical facilities that offer services to the IQAC research groups as well as to groups or companies from elsewhere: Thermal Analysis and Calorimetry, Magnetic Resonance (NMR and EPR), Organic Microanalysis, Synthesis of High-Added Value Molecules, X-Ray Dispersion at Small Angle (SAXS-WAXS), Characterization of Colloidal Dispersions, Percutaneous Absorption and Skin Efficacy, Monoclonal Antibodies Production and Characterization (CAbS), Biodegradation and Aquatic Toxicity, Proteomics and Technology transfer.
INSTITUTE BOARD MEMBERS

Àngel Messeguer Peypoch  
Rosa Infante Martínez-Pardo  
Joan Ricard Ibáñez Villar  
Jesús Joglar Tamargo  
Gemma Fabriás Domingo  
Mª Pilar Marco Colás  
Jordi Esquena Moret  
Ramón Pons Pons  
Jaume Caelles Balcells  
Avencia Diez Ortego  
Meritxell Martí Gelabert  
Josep Carilla Auguet  
Pilar Domènech Duran

Director  
Deputy Director  
Head of Administration  
Department of Biological Chemistry and Molecular Modelling  
Department of Biomedicinal Chemistry  
Department of Chemical and Biomolecular Nanotechnology  
Department of Chemical and Surfactants Technology  
Personnel Representative  
Personnel Representative  
Personnel Representative  
Invited Services Representative

ADMINISTRATION

Director: Àngel Messeguer Peypoch  
Deputy Director: Rosa Infante Martínez-Pardo  
Head of Administration: Joan Ricard Ibáñez Villar  
Secretaries: Lidia Beltran Fabregat  
Josefina Remembla Solé  
Leonor Moliner Ferrer

«Ad honorem» MEMBERS

M DOLORS DE CASTELLAR BERTRAN  
PILAR ERRA SERRABASA
DEPARTMENTS AND RESEARCH GROUPS

Department of Biological Chemistry and Molecular Modelling
- Nutraceuticals and Free Radicals
- Biotransformation and Bioactive Molecules
- Supramolecular Chemistry
- Ecological Chemistry
- Theoretical and Computational Chemistry
- Biologically Active Phytochemicals

Department of Biomedical Chemistry
- Research Unit on BioActive Molecules
- Synthesis and Biomedical Applications of Peptides
- Unit of Glycoconjugate Chemistry

Department of Chemical and Biomolecular Nanotechnology
- Nanobiotechnology and Molecular Diagnostics
- Nucleic Acids Chemistry
- Colloid and Interfacial Chemistry Group
- Bioorganic Chemistry
- Surface Chemistry Group

Department of Chemical and Surfactants Technology
- Minimization of Industrial Wastes: Isolation of High Added-Value Biopolymers
- Development of Non-contaminant Industrial Processes
- Statistical Modelling and Fibre Physics
- Biocompatible Surfactants
- Environmental Chemistry of Surfactants and Ionic Liquids
- Physical Chemistry of Surfactant Systems
- Biophysics of Lipids and Interphases

IQAC FACILITIES AND TECHNOLOGY TRANSFER
- Characterization of Colloidal Dispersions Service
- Custom Antibody Service (CAbS)
- Organic Microanalysis Service
- Biodegradation and Aquatic Toxicity Service
- Magnetic Resonance Service
- Skin Absorption and Skin Efficacy Services
- SAXS-WAXS Service
- Synthesis of High Added Value Molecules Service
- Thermal Analysis and Calorimetry Service
- Proteomics Service
- Technology Transfer
NUMERICAL SUMMARIES

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<sup>a</sup> in SC.  <sup>b</sup> «ad honorem».

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<sup>†</sup> Common publications in two entries.  <sup>*</sup> Common publications in one department (duplicated or triplicated).  <sup>N</sup> National

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### 2010-2011 JOURNAL PUBLICATIONS SUMMARY

Total number of ISI-journals: 152
- with one **single** paper: 94 (61.84 %)
- with more than one paper: 58 (38.16 %)
  - with **two** or more papers: 31 (2); 10 (3); 7 (4)
  - with **five** or more papers: 10
    - [4 (5); 2 (6); 2 (7); 1 (9); 1 (10)]

Total number of papers: 279
- Papers in Non-ISI journals, international: 13

### PROJECTS

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NP: National Project; EU: European Union; AACC: Autonomous Community; CR: Contracted Research

### TECHNOLOGICAL OUTPUT

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SPA: Spanish patent application; PCT: Patent cooperation treaty; L: licensed
### List of ISI JOURNALS in alphabetical order and number of papers/year

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*See J. Mol. Struct. (since 2011); E: errata; ed: editorial

### Papers in non-ISI JOURNALS international

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SPECIAL EVENTS

15th Félix Serratosa Conference (19/01/2010)
Sulfur ylide epoxidations and applications in synthesis
Varinder K. Aggarwal
Universitat de Bristol, UK.

Amb la química es poden fer diners, ben fets?
Conferences at CID “Josep Pascual Vila” (16, 23, 30/03 and 14/04/2011)
Algunos aspectos determinantes en la creación de una empresa
Dr. José Mª García Antón. Director y fundador de Lipotec Group S.A.
El olor de la química: síntesis industrial de compuestos orgánicos para la creación de fragancias
Dra. Mónica Diaz Sierra. International Flavors & Fragances, IFF
Rendibilitzar experiència i coneixement: asesorament a la indústria
Dr. Octavi Colomina. Director y fundador de TDV Compliance Technologies
BASF: Producción química y medio ambiente en Tarragona.
Dr. Primitivo Gutiérrez-Martin. BASF

Chemistry Celebration at CID “Josep Pascual Vila” (5/07/2011)
Bioglane: del laboratori a la planta pilot, i al mercat?
Josep Lluís Torres
Dpt. Química Biològica i Modelització Molecular
Peptids per al tractament de la SIDA.
Mª Jose Gomara
Dpt. Química Biomèdica
Nous medicaments basats amb el DNA i el RNA.
Montserrat Terrazas
Dpt. Nanotecnologia Química i Biomolecular

INVITED CONFERENCES AT CBN WORKSHOPS

II Workshop CBN’10 (15/10/2010)
Dr. Josep Rocas.
Applied Nanotechnology. From University to technological based Industry. Example: Polymeric Micro and Nanoencapsulation.
Ecopol Tech S.L. (R&D Department)
Dr. Enrique Pérez-Payá.
Playing with chemical biology around apoptosis.
Department of Medicinal Chemistry, Centro de Investigaciones Príncipe Felipe, Valencia
Dr. Ignacio Alfonso.
Constitutional dynamic chemistry as a supramolecular approach to functional pseudopeptidic compounds.
Department of Biological Chemistry and Molecular Modelling, IQAC-CSIC

III Workshop CBN’11 (27/10/2011)
Dr. Ignasi Miquel.
Thrombotargets, the development of procoagulant nanovesicles.
Thrombotargets Europe (Strategic Alliances, Director)
Dr. Nicholas Hud.
DNA folding and assembly in natural and non-natural environments.
Georgia Institute of Technology, USA
Dr. Amadeu Llebaria.
Glycolipids and aminoacyclohexanes.
Department of Biomedical Chemistry, IQAC-CSIC

AWARDS AND NOMINATIONS

A. Meseguer
Advisory Council Member, Chemistry Faculty, Universitat de Barcelona
A. Marsal
Asociación Química Española de la Industria del Cuero Award
BioGlLane
Biotecnología de I+D+i Award (P. Clapés, J. Joglar, J. Ll. Torres founding IQAC members)
DEPARTMENT OF BIOLOGICAL CHEMISTRY
AND MOLECULAR MODELLING
Research interests of this Department are focused on:
Molecules of biological and biomedical interest. Isolation, design, synthesis, biosynthesis, and activity evaluation of drugs, insect pheromones, secondary metabolites, enzymatic inhibitors, biocatalysts, agro-forestry by-products and antioxidants.
Molecular recognition of ions and molecules of biological interest.
Study of non covalent interactions. Modelling of enzymatic catalysis mechanisms.
Modification of the activity and selectivity of biocatalysts by means of genetic engineering.
Mechanisms of action of antioxidant protectors.
Persistent organic free radicals as biochemical sensors.
Study of the electronic structure and reactivity of molecules by means of theoretical chemistry computational techniques. Computational elucidation of reaction mechanisms of interest in atmospheric chemistry. New theoretical methods for exploring potential energy surfaces.

Research groups
- Nutraceuticals and Free Radicals
- Biotransformation and Bioactive Molecules
- Supramolecular Chemistry
- Ecological Chemistry
- Theoretical and Computational Chemistry
- Biologically Active Phytochemicals
Nutraceuticals and Free Radicals

Research at NFR involves the preparation (extraction, synthesis) and evaluation of natural products of plant origin or their derivatives with application as disease preventing agents. In particular, the nutraceuticals (e.g. antioxidant polyphenols) are obtained from agricultural and forest by-products and this gives the Lab an environmental side. The biological activities tested on the nutraceuticals are related to the control of the oxidative stress which is a major damaging process, mediated by free radicals and occurring in many disorders (metabolic syndrome, cardiovascular disease, type 2 diabetes, cancer, Alzheimer, Parkinson). The study of free radicals, their reactivity, their use as probes for antioxidant activity and their control or elimination by natural nutraceuticals is a central focus of our research.

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JUAN ANTONIO MESA DÍAZ
EUNICE MOLINAR TORIBIO

Publications (articles)

Synthesis of a new stable and water-soluble tris(4-hydroxy sulfonfyltetrachlorophenyl)methyl radical with selective oxidative capacity.
Mesa, J.A., Velázquez-Palenzuela, A., Brillas, E., Torres, J.L., Julià, L.
Tetrahedron 67 3119-3123, 2011

An EPR analysis of β-dimerization in α-blocked pyrroles in oxidant conditions.
Julià, L., Rius, J., Torrentes, X.

A lyophilized red grape pomace containing proanthocyanidin-rich dietary fiber induces genetic and metabolic alterations in colon mucosa of female C57BL/6J mice.

Role of galloylation and polymerization in cytoprotective effects of polyphenolic fractions against hydrogen peroxide insult.
Mitjans, M., Ugartondo, V., Martínez, V., Touriño, S., Torres, J.L.; Vinardell, M.P.

Protective effect of structurally diverse grape procyanidin fractions against UV-induced cell damage and death.
Matito, C., Ageil, N., Sánchez-Tena, S., Torres, J.L.; Cascante, M.

Galloylated polyphenols as inhibitors of hemoglobin-catalyzed lipid oxidation in fish muscle.
Iglesias, J., Pazos, M., Maestre, R., Torres, J.L., Medina, I.

Metabolites in contact with the rat digestive tract after ingestion of a phenolic-rich dietary fiber matrix.

Analysis of nonextractable phenolic compounds in foods: the current state of the art.
Pérez-Jiménez, J., Torres, J.L.

Stable radical cores: A key for bipolar charge transport in glass forming carbazole and indole derivatives.
Chem. Commun. 46 5130-5132, 2010

Differential behavior of amino-imino constitutional isomers in nonlinear optical processes.
Latorre, S., de Moreira, I.P.R., Villacampa, B., Julià, L., Velasco, D., Bofill, J.M., López-Calahorra, F.
ChemPhysChem. 11 912-919, 2010
EPR/Spin-trapping study of free radical intermediates in the photolysis of trifluoromethyl ketones with initiators.

Antioxidant activities of hydroxytyrosol main metabolites do not contribute to beneficial health effects after olive oil ingestion.

Absorption and metabolization of cytoprotective epicatechin thio conjugates in rats.
Selga, A., Vinardell, M.P., Martín-Venegas, R., Jáuregui, O., Casas, J., Torres, J.L. Drug Metab. Dispos. 38 2188-2194, 2010

ZmMYB31 directly represses maize lignin genes and redirects the phenylpropanoid metabolic flux.

Proanthocyanidin metabolites associated with dietary fibre from in vitro colonic fermentation and proanthocyanidin metabolites in human plasma.

Impact of thermal processing on the activity of gallotannins and condensed tannins from hamamelis virginiana used as functional ingredients in seafood.

Research highlights

Synthesis of a new stable and water-soluble tris(4-hydroxysulfonyltetrachlorophenyl)methyl radical with selective oxidative capacity
A new stable organic free radical of the PTM (perchlorotriphenylmethyl) series very soluble in water was reported. This free radical is sensitive to electron transfer processes, and the selectivity of these reactions in the presence of ascorbic acid, pyrogallol and catechol as reducing species is described. The electron paramagnetic resonance spectrum and the electrochemical behaviour were also reported. The new radical can be used to evaluate the scavenging activity of antioxidants in water including the antioxidant capacity of biological fluids.

Evolution of the UV-vis spectra of an aqueous basic solution of αH-TSPTM every two hours; generation of the TSPTM radical

Metabolites in contact with the rat digestive tract after ingestion of a phenolic-rich dietary fiber matrix.
By use of HPLC-ESI-MS/MS techniques phenolic metabolites were detected in feces, cecal content, and colonic tissue from rats given grape antioxidant dietary fiber (GADF). During their transit along the digestive tract, proanthocyanidin oligomers and polymers are depolymerized into EC units. Thus, after ingestion of GADF, free EC and its conjugates, as well as free and conjugated microbially derived phenolic metabolites, come into contact with the intestine epithelium for more than 24 h and may be partly responsible for the positive influence of GADF on gut health.
Metabolization of polymeric proanthocyanidins from GADF
Biotransformation and Bioactive Molecules

Carbon-carbon bond formation lies at the core of organic synthesis. Biocatalytic carbon-carbon bond synthesis is an attractive methodology for the asymmetric construction of molecular frameworks, giving access to complex, multifunctional target structures that are difficult to prepare by conventional means. Carbolligases are particularly appropriate to generate innovative molecules and molecular diversity accessible for investigations in drug discovery. Our research is focused on the design, production and evaluation of carboligation biocatalysts and biologically active molecules. This includes the redesign of aldolases by structure-guided site directed mutagenesis and computational models to alter their selectivity properties.

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ANNA SZEKRENYI
KAREL HERNANDEZ SANCHEZ
ANNA SOLER CASAPONSA
RAQUEL ROLDAN

Publications (articles)

Current trends in asymmetric synthesis with aldolases
Clapés, P., Garrabou, X.

Redesign of the phosphate binding site of L-rhamnulose-1-phosphate aldolase towards a dihydroxyacetone dependent aldolase.
Garrabou, X., Joglar, J., Parella, T., Crehuet, R., Bujons, J., Clapés, P.

Structure-guided redesign of D-fructose-6-phosphate aldolase from E. coli: Remarkable activity and selectivity towards acceptor substrates by two-point mutation.
Gutierrez, M., Parella, T., Joglar, J., Bujons, J., Clapés, P.
Chem. Commun. 47 5762-5764, 2011

Direct analysis of glucuronidated metabolites of main olive oil phenols in human urine after dietary consumption of virgin olive oil.
Khymenets, O., Farré, M., Pujadas, M., Ortiz, E., Joglar, J., Covas, M.I., De La Torre, R.
Food Chemistry 126 306-314, 2011

Triazine-based vanilloid 1 receptor open channel blockers: Design, synthesis, evaluation, and SAR analysis.
J. Med. Chem. 54 7441-7452, 2011

Highly Efficient Aldol additions of DHA and DHAP to N-Cbz-Amino aldehydes Catalyzed by L-Rhamnulose-1-Phosphate and L-Fuculose-1-Phosphate Aldolases in Aqueous Borate Buffer.
Garrabou, X., Joglar, J., Parella, T., Bujons J., Clapés, P.
Org. Biomol. Chem. 9 8430-8436, 2011

Chemical modulation of peptoids: synthesis and conformational studies on partially constrained derivatives.

New glucocerebrosidase inhibitors by exploration of chemical diversity of N-substituted aminocyclitols using click chemistry and in situ screening.
Díaz, L., Casas, J., Bujons, J., Llebaria, A., Delgado, A.
J. Med. Chem. 54 2069-2079, 2011

Computational prediction of structure-Activity relationships for the binding of aminocyclitols to β-glucocerebrosidase.

Identification of new ozonation disinfection byproducts of 17β-estradiol and estrone in water.
Chemosphere 84 1535-1541, 2011


Publications (books and book chapters)

Georg Thieme Verlag KG, Stuttgart (Germany)

Applied Biocatalysis Unit (IQAC, CSIC-UAB) Publications


Bioremediation of PAHs-contaminated soil through composting: Influence of bioaugmentation and biostimulation on contaminant biodegradation.

Soil colonization by Trametes versicolor grown on lignocellulosic materials: Substrate selection and naproxen degradation.

Research highlights
Redesign of recombinant aldolases for asymmetric carbon-carbon bond formation
l-Fuculose-1-phosphate aldolase (FucA), l-rhamnulose-1-phosphate aldolase (RhuA) and d-fructose-6-phosphate aldolase (FSA) from E. coli genome are amazing powerful catalysts for asymmetric C-C bond formation. Structure guided redesign of the active center by site-directed mutagenesis furnished a collection of novel aldol addition catalysts with broad substrate selectivity and complementary stereochemistry. Furthermore, RhuA and FSA tolerate unphosphorylated DHA analogues, and this simplifies the synthetic scheme avoiding the use of highly elaborated starting materials. Their selective catalytic properties allow organic chemists to access easily to sugars of the ketose and aldose families and their analogs, difficult to prepare by purely chemical procedures.
Supramolecular Chemistry

Supramolecular chemistry is the “chemistry beyond the molecule” and deals with the interactions between chemical species in an ordered and hierarchical way, leading to the formation of well-defined supramolecules. We mainly work in the fields of molecular recognition, programmed folding and self-assembling processes, using a large variety of experimental and theoretical approaches. The discovery, preparation and study of new synthetic receptors for biologically interesting molecules and ions (especially anions) are our main activities. We also use supramolecular approaches to synthetic procedures, such as templated synthesis, dynamic combinatorial chemistry and constitutional dynamic chemistry. Additionally, we collaborate with several groups (both at IQAC and outside) to study biomolecular and biomimetic systems from a supramolecular point of view.

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ENRICO FAGGI

Ph. D. STUDENTS
JOAN ATCHER UBIERGO

Publications (articles)

Enantioselective triazolium salts: Chemoenzymatic synthesis and applications in organocatalysis.
ChemCatChem 3 1921-1928, 2011

Stimulus responsive self-assembly of Gemini Amphiphilic Pseudopeptides.
Rubio, J., Alfonso, I., Burguete, M.I., Luis, S.V.
Soft Matter 7 10737-10748, 2011

Crystal structure of the N-benzyloxy carbonyl-alanyl-phenylalanyl-methyl ester: the importance of the H-bonding pattern.
Alfonso, I., Bolte, M., Burguete, M.I., Luis, S.V.
Crystals 1 163-170, 2011

Chemical modulation of peptoids: Synthesis and conformational studies on partially constrained derivatives

Polyhydroxylated bicyclic isoureas and guanidines are potent glucocerebrosidase inhibitors and nanomolar enzyme activity enhancers in gaucher cells.
Trapero, A., Alfonso, I., Butters, T.D., Liebaria, A.

Update 1 of: Enantioselective enzymatic desymmetrizations in organic synthesis.
García-Urdiales, E., Alfonso, I., Gotor, V.
Chem. Rev. 111 PR110-PR180, 2011

Structurally disfavoured pseudopeptidic macrocycles through anion templation.
Bru, M., Alfonso, I., Bolte, M., Burguete, M.I., Luis, S.V.

Gemini amphiphilic pseudopeptides: Synthesis and preliminary study of their self-assembling properties.
Rubio, J., Alfonso, I., Bru, M., Burguete, M.I., Luis, S.V.
Tetrahedron Lett. 51 5861-5867, 2010

Optically active macrocyclic hexaazapyridinophanes decorated at the periphery: Synthesis and applications in the NMR enantiodiscrimination of carboxylic acids.
Tetrahedron 66 6070-6077, 2010

Molecular recognition of N-protected dipeptides by pseudopeptidic macrocycles: A comparative study of the supramolecular complexes by ESI-MS and NMR.
Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V., Vicent, C.
Org. Biomol. Chem. 8 1329-1339, 2010

Structural diversity in the self-assembly of pseudopeptidic macrocycles.
Alfonso, I., Bru, M., Isabel Burguete, M., García-Verdugo, E., Luis, S.V.

Chiral molecular receptors based on trans-cyclohexane-1,2-diamine.
Alfonso, I.
The pseudopeptidic macrocycles recently prepared in our group were studied for the molecular recognition of N-protected dipeptides by a combination of ESI-MS and NMR techniques and with the help of molecular modeling. Some of the receptors displayed good selectivity for dipeptides over the corresponding amino acids and a slight preference for the dipeptides containing aromatic side chains. On the other hand, some of these macrocycles were able to self-assemble into hierarchical nanostructures rendering different morphologies depending on the chemical structures of the compound. Thus we observed the formation of fibers or vesicles at the micro/nanometric scale. A deep study using a battery of techniques (SEM, TEM, ATR FT-IR, UV-CD, NMR) allowed us to understand the aggregation process, induced by a combination of polar (H-bonding) and nonpolar (van de Waals and π-stacking) non-covalent interactions. The full understanding of the process led us to fabricate hybrid nanostructures rendering either spheres covered by fibrils or segregated vesicles and fibers. Moreover, the self-assembling capabilities of pseudopeptidic molecules have been exploited one step further. We have synthesized a new family of Gemini Amphiphilic Pseudopeptides (GAPs) which can also aggregate into different nanostructures (fibers, fibrils, spheres, tapes or tubes) depending on the growing conditions (solvent, pH) and the chemical structure of the GAP. A systematic study using a large number of techniques allowed us to fully understand the process and to propose a model for the assembling mechanism. Moreover, the delicate interplay between hydrophobic and hydrophilic interactions served for the design of a new generation of GAPs capable to undergo stimulus-dependent morphological transitions (from fibers to vesicles) in aqueous medium, as well as to form stable supramolecular hydrogels with promising applications in bionanotechnology.
Ecological Chemistry

Our group deals with different aspects related with new insect pheromones, from structural characterization and synthesis of pheromones and analogues to the establishment of the attractant activity in the laboratory, by electrophysiological techniques (EAG and GC-EAD) and behavioral bioassays, and in the field.

We are also engaged in the development of new alternative and non-contaminant methods of pest control, based on inhibition of the enzymes involved in the degradation of pheromone molecules at the insect's antennae.

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Ph. D. STUDENTS
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ANNA RODRÍGUEZ RIVERO

Publications (articles)

Enzymatic enantiomeric resolution of phenylethylamines structurally related to amphetamine.
Muñoz, L., Rodríguez, A.M., Rosell, G., Bosch, M.P., Guerrero, A.
Org. Biomol. Chem. 9 8171-8177, 2011

Pheromone synthesis in a biomicroreactor coated with anti-adsorption polyelectrolyte multilayer.
Biomicrofluidics 5 034102, 2011
http://dx.doi.org/10.1063/1.3608138 (12 pages)

Inhibition of electrophysiological response to the pheromone of the fall armyworm, Spodoptera frugiperda.
Perez Luis, C.P., Guerrero, A., Malo, E.A.
J. Pest. Sci. 35 23-26, 2010

Behavioural and electrophysiological responses of the European corn borer Ostrinia nubilalis to host-plant volatiles and related chemicals.
Solé, J., Sans, A., Riba, M., Guerrero, A.
Physiol. Entomol. 35 354-363, 2010

Reactivity versus steric effects in fluorinated ketones as esterase inhibitors: A quantum mechanical and molecular dynamics study.
Rayó, J., Muñoz, L., Rosell, G., Hammock, B.D., Guerrero, A., Luque, F.J., Pouplana, R.
J. Mol. Mod. 16 1753-1764, 2010

Improved microwave-assisted ring opening of 1,1,1-trifluoro-2,3-epoxypropane: Synthesis of new 3-alkoxy-1,1,1-trifluoropropan-2-ols.
Rayó, J., Muñoz, L., Rosell, G., Bosch, M.P., Guerrero, A.
Synthesis 3117-3120, 2010

Synthesis of allylic trifluoromethyl ketones and activity as inhibitors of the sex pheromone of the leopard moth, Zeuzera pyrina L. (Lepidoptera: Cossidae).
Muñoz, L., Bosch, M.P., Batllori, Ll., Rosell, G., Bosch, D., Guerrero, A., Avilla, J.
Pest Manag. Sci. 67 956-964, 2011

(E)-Pityol as aggregation pheromone of Pityophthorus pubescens (Marsham) (Coleoptera: Scolytinae): Biological activity in the laboratory and in the field.
Lopez, S., Quero, C., Iturrondo-beitia, J.C., Guerrero, A., Goldarazena, A.
Can. Entomol. 143 447-454, 2011

Sex pheromone of the Spanish population of the beet armyworm Spodoptera exigua.
Acín, P., Rosell, G., Guerrero, A., Quero, C.

EPR/Spin-trapping study of free radical intermediates in the photolysis of trifluoromethyl ketones with initiators.
Rosa, E., Guerrero, A., Bosch, M.P., Julià, L.
Magn. Reson. Chem. 48 198-204, 2010
The main features accomplished by the Chemical Ecology Group in the period 2010-2011 are the following:

1. The pheromone composition of the Spanish population of the beet armyworm (BAW), Spodoptera exigua (Lepidoptera: Noctuidae), was identified. Analysis of female gland extracts showed the presence of compounds Z\(_9\), E\(_{12-14}:\text{Ac}\) (1), Z\(_9\)-14:Ac (2), Z\(_{11-16}:\text{Ac}\) (3), Z\(_9\), E\(_{12-14}:\text{OH}\) (4), Z\(_9\)-14:OH (5) and Z\(_{11-16}:\text{OH}\) (6) in a ratio of 26:11:1:22:31:9. The amount of compound per gland ranged from 2.08 ng for 5 to 0.09 ng for 3. However, analysis of female volatiles by SPME only revealed the presence of compounds, 1, 2, 3 and 5 in a 34:40:4:22 ratio. In EAG assays, compound 1 elicited the highest response and the C14 acetates evoked higher electrophysiological responses than the corresponding alcohols and the C16 isomers. GC-EAD analysis of PBAN-treated pheromone gland extracts confirmed the presence of compounds 1, 2, 4, 5 and 6 (see Figure 1). In wind tunnel, no behavioral difference was observed between formulations based on the gland extracts and female volatiles. In both cases, males responded similarly to when virgin females were used as the attractant source.

Compound 1 alone elicited upwind flight on males but required the presence of compound 5 in a 80:20 to 40:60 ratio for full activity. Ternary mixtures of 1, 5 and the minor components did not improve the performance of the blend 1+5 in a 60:40 ratio. In the field, the mixture 1+5+3 in a 56:37:7 ratio was the most attractive formulation and is expected to be useful in future pest control strategies (J. Chem. Ecol. 36 778-786, 2010).

2. Carboxylesterases (CEs) are a family of ubiquitous enzymes with broad substrate specificity, and their inhibition may have important implications in pharmaceutical and agrochemical fields. One of the most potent inhibitors both for mammalian and insect CEs are trifluoromethyl ketones (TFMKs), but the mechanism of action of these chemicals is not completely understood. We have examined the balance between reactivity versus steric effects in modulating the activity against human carboxylesterase 1. The intrinsic reactivity of the ketone moiety was determined from quantum mechanical computations, which combined gas phase B3LYP calculations with hydration free energies estimated with the IEF/MST model. In addition, docking and molecular dynamics simulations were used to explore the...

Research highlights

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Characterization of an antennal carboxylesterase from the pest moth Spodoptera littoralis degrading a host plant odorant.


Publications (books and book chapters)


Low-frequency sounds induce acoustic trauma in cephalopods.


Proteomics of toxic oil syndrome in humans: Phenotype distribution in a population of patients.


A diversity of putative carboxylesterases are expressed in the antennae of the noctuid moth Spodoptera littoralis.


Figure 1. a GC-EAD response of a Spodoptera exigua male antenna to a PBAN-treated pheromone extract. b GC of a mixture of synthetic compounds Z\(_9\), E\(_{12-14}:\text{Ac}\) (1), Z\(_9\)-14:Ac (2), Z\(_{11-16}:\text{Ac}\) (3), Z\(_9\), E\(_{12-14}:\text{OH}\) (4), Z\(_9\)-14:OH (5) and Z\(_{11-16}:\text{OH}\) (6) (100 ng each).
binding mode of the inhibitors along the deep gorge that delineates the binding site. The results point out that the activity largely depends on the nature of the fluorinated ketone, since the activity is modulated by the balance between the intrinsic electrophilicity of the carbonyl carbon atom and the ratio between keto and hydrate forms. However, the results also suggest that the correct alignment of the alkyl chain in the binding site can exert a large influence on the inhibitory activity, as this effect seems to override the intrinsic reactivity features of the fluorinated ketone.

Overall, the results sustain a subtle balance between reactivity and steric effects in modulating the inhibitory activity of TFMK inhibitors (*J. Molec. Mod.* 16 1753-1764, 2010).

3. Both enantiomers of several phenylethylamines 4a-i, structurally related to amphetamine, have been prepared in good yields and excellent enantiomeric purity by enzymatic kinetic resolution using CAL-B and ethyl methoxyacetate as the acyl donor (Figure 2). In the case of the 4-hydroxyderivative of amphetamine (compound 4i), the S enantiomer racemized possibly in a dynamic kinetic resolution (DKR) under the enzymatic conditions used (*Org. Biomol. Chem.* 9 8171-8177, 2011)

Figure 2. Enzymatic resolution of racemic amines 4a-i

4. To prepare a biosynthetic module in an infochemical communication project, we have built a silicon-based microreactor coated with an anti-adsorption polyelectrolyte multilayer, containing an immobilized (agarose beads) alcohol acetyl transferase (atf), one of the key biosynthetic enzymes of the pheromone of *Spodoptera littoralis*. The system has been developed to reproduce the last step of the biosynthesis in which the precursor diene alcohol (Z,E)-9,11-tetradecadienol is transformed into the major component of the pheromone (Z,E)-9,11-tetradecadienyl acetate (Figure 3). The microreactor has been built using a polyelectrolyne/dextran sulfate sodium salt-based multilayer as an anti-adsorption coating. The deposition has been implemented layer by layer and the coating has been optimized in terms of thickness, morphology and stability at pH 9.2 and 6.0 and two PEI with molecular weights 750 and 1.2 kDa. Validation of the microreactor functionality was done by evaluation of the acetylation reaction of the diene alcohol to the acetate by gas chromatography coupled to mass spectrometry (*Biomicrofluidics* 5 034102-1-12, 2011).

Figure 3. Bioconversion catalyzed by an alcohol acetyl transferase (atf). In the presence of acetyl-CoA, atf transforms (Z,E)-9,11-tetradecadienol into (Z,E)-9,11-tetradecadienyl acetate, the major component of the pheromone

5. Trifluoromethyl ketones (TFMKs) structurally related to the pheromones are good inhibitors of pheromone communication in insects. To determine their activity on *Zeuzera pyrina* L. (Lepidoptera: Cossidae), a polyphagous pest, we have prepared two diunsaturated TFMK analogues of the major and the minor pheromone components, and two monounsaturated ones. The new prepared chemicals are good inhibitors of the pheromone in electrophysiology (EAG), wind tunnel and in the field. Our results show the importance of two unsaturations at positions 2 and 13 of the trifluorocetyl group in the structure of the analogues, the latter being critical for the inhibitory activity. (*Pest Manage. Sci.* 67 956-964, 2011). In Figure 4 it is shown the disrupting effect exerted by (E,Z)-3,13-octadecadienyl trifluoromethyl ketone on males flying to a virgin female. The ketone was placed in a filter paper 1 cm from the calling female.

Figure 4. Track flights of *Zeuzera pyrina* males towards a calling female (A and C) and a calling female in the presence of (E,Z)-3,13-octadecadienyl trifluoromethyl ketone at 0.1 µg (B) and 1 µg (D). The insect moved upwind from left to right. The insect position at 0.4 s intervals is shown by the dark points.
Theoretical and Computational Chemistry

The Theoretical and Computational Chemistry Group (QTC) studies the structure and reactivity of molecules using the computational methods of Theoretical Chemistry. Special interest is devoted to two main areas: first, the investigation of oxidation reactions playing an important role in atmospheric and environmental chemistry, as well as in biological systems; second, the study of enzyme catalysis, with special interest in the role of protein dynamics in the catalytic cycle.

Publications (articles)

Water effects on atmospheric reactions.
Buszek, R.J., Francisco, J.S., Anglada. J.M.

A new approach to local hardness.
Gál, T., Geerlings, P., De Proft F., Torrent-Sucarrat, M.

Redesign of the phosphate binding site of L-rhamnulose-1-phosphate aldolase towards a dihydroxyacetone dependent aldolase.
Garrabou, X., Joglar, J., Parella, T., Crehuet, R., Bujons, J., Clapés, P.

Effect of the substituents on the reactivity of carbonyl oxides. A theoretical study on the reaction of substituted carbonyl oxides with water.
Anglada, J.M., González, J., Torrent-Sucarrat, M.

Changes in dynamics upon oligomerization regulate substrate binding and allostery in amino acid kinase family members.
Marcos, M., Crehuet, R., Bahar I.

Protonation of water clusters induced by the hydroperoxyl radical surface.
Torrent-Sucarrat, M., Ruiz-López, M.F., Martíns-Costa, M., Francisco, J.S., Anglada, J.M.

The gas phase reaction of carbonyl oxide with hydroxyl radical in presence of water vapor. A theoretical study on the reaction mechanism.
Mansergas, A., González, J., Ruiz-López, M., Anglada, J.M.

Anharmonicity and the Eigen-Zundel dilemma in the IR spectrum of the protonated 21 water cluster.
Torrent-Sucarrat, M., Anglada, J.M.

On the dissociation of ground state trans-HOOO radical: A theoretical study.
Anglada, J.M., Olivella, S., Solé, A.
Gas phase reaction of nitric acid with hydroxyl radical without and with water. A theoretical investigation
Gonzalez, J., Anglada, J.M.

Pentacoordinated phosphorus revisited by high-level QM/MM calculations
Marcos, E., Field, M.J., Crehuet, R.
Proteins 78 2405-2411, 2010

The reactions of SO$_3$ with HO$_2$ radical and H$_2$O--HO$_2$ radical complex. Theoretical study on the atmospheric formation of HSO$_2$ and H$_2$SO$_4$
Gonzalez, J., Torrent-Sucarrat, M., Anglada, J.M.

On the applicability of local softness and hardness
Torrent-Sucarrat, M., De Proft, F., Ayers, P.W., Geerlings, P.

Research highlights

The hydrotrioxyl radical (HOOO$^*$) plays a crucial role in atmospheric processes involving the hydroxyl radical (HO$^*$) and molecular oxygen (O$_2$). The figure shows two potential energy profiles for dissociation of trans-HOOO$^*$ (X $^2$A') to HO$^*$ (X $^2$Π) + O$_2$ (X $^3$Σ$_g^-$) calculated at two different CASPT2 levels along the r(O$_b$O$_c$) coordinate. CASPT2(19,15) calculations predict for trans-HOOO$^*$ (X $^2$A') a central O—O bond length of 1.682 Å, which is in excellent agreement with the experimental value of 1.688 Å (Science 2005, 308, 1885), and give a dissociation energy at 0 K $D_0^*$ = 3.0 kcal/mol. This value of $D_0^*$ is in excellent agreement with the recent experimentally determined $D_0^*$ = 2.9 ± 0.1 kcal/mol by Le Picard et al. (Science 2010, 328, 1258).

Understanding the hydrated proton is of paramount importance for the knowledge of fundamental processes in chemistry and biology, and the investigation of protonated water clusters has been proven to be essential for understanding the nature of protons in solution. The computed anharmonic IR spectra of protonated water clusters show that the Eigen signature covers a wide range of frequencies. In the case of the magic number cluster these signatures are predicted to appear close to 2000 cm$^{-1}$.

Miquel Torrent-Sucarrat, and Josep M. Anglada

Josep M. Anglada, Santiago Olivella, and Albert Solé,
Species having Möbius and Hückel topologies have promising applications in the manufacture of Hückel-to-Möbius topological optical switches with high nonlinear optical properties. We have evaluated the electronic and vibrational contributions to static and dynamic nonlinear optical properties of the CS Hückel and C2 Möbius topologies synthesized by Herges and co-workers (Ajami, D. et al. Nature 2003, 426, 819).

Miquel Torrent-Sucarrat, Josep M. Anglada, and Josep M. Luis

Enzymes catalysing phosphoryl transfer reactions are extremely efficient and are involved in crucial biochemical processes. The reaction can proceed through a pentacoordinated phosphorus species that is either a stable intermediate or a transition state. Because of this, the first X-ray structure of a pentacoordinated phosphorus intermediate in the beta-phosphoglucomutase enzyme aroused great interest when published in Science. To provide new insights into the nature of that structure, we determined the reaction path of the phosphorylation step using high-level QM/MM calculations. We conclude that the pentacoordinated phosphorus formed in this enzyme is not a stable species but a transition state. We have confirmed the idea of some authors that questioned the presence of the pentacoordinated phosphorus in the crystal and proposed the presence of a MgF3- salt as a transition state analogue.

Marcos, E.; Field, M. J.; Crehuet, R.
Proteins 2010, 78, 2405-2411.

The dynamical basis underlying the increased thermal stability of thermophilic proteins remains uncertain. We have challenged the new paradigm established by neutron scattering experiments in solution, in which the adaptation of thermophilic proteins to high temperatures lies in the lower sensitivity of their flexibility to temperature changes.

By means of multi-scale simulations we reported a reinterpretation of those experiments and showed evidence that under crowding conditions, thermophilic and homologue mesophilic proteins have diffusional properties with different thermal behavior. The more intense electrostatic potential at the surface of the thermophilic protein entails stronger electrostatic inter-protein interactions in solution that affect the diffusional behavior. This work opens up opportunities to further studies to ascertain whether this is a general trend and, if so, which biological implications might have.

Marcos, E.; Mestres, P.; Crehuet, R.
Water vapor is one of the most important species in the Earth atmosphere. It plays and important role as a greenhouse gas but it has also a very significant impact on the processes that occur in the Earth’s atmosphere. Because of its ability to be both a hydrogen bond donor and acceptor, it can form very stable complexes. The formation of these complexes can dramatically affect the chemistry in the atmosphere, including heterogeneous removal and alteration of the photochemical properties of the atmospheric species, the formation of water droplets and aerosol particles, as well as the participation of these complexes in chemical reactions. Along eight different publications we have investigated different effects that water vapor play in atmospheric reactions.

Biologically Active Phytochemicals

The BAP research group has a long-standing interest in the structural elucidation of new natural compounds of plant origin (sesquiterpenoids related to insect juvenile hormones and the associated chromene antagonists or precocenes; diterpenes as insect anti-feedants; insect molting hormone agonist or antagonist steroids or ecdysteroids) and their biological activities. Other research has involved rotenoids, furanocoumarins, triterpene glycosides, anthraquinones, bibenzyls, sterols...

Nowadays, the main goals are the prospective development of new eco-friendly and sustainable insect pest-control agents from plants and to provide basic knowledge for new applications, safety and quality-control procedures for other secondary metabolites components of aromatic and medicinal plants.

Publications (articles)

neo-Clerodane diterpenoids from *Ajuga bracteosa*
Castro, A., Coll, J., Arfan, M.

Phytotoxic activity of flavonoids from *Dicranostyles ampla*.

Research highlights

A different set of neo-clerodane diterpenoids were isolated depending on the isolation procedure used, owing to the labile nature of tetrahydrofurufuran metabolites. From a dichloromethane extract of *Ajuga bracteosa* both clerodin- and dihydroclerodin-type diterpenes were obtained under “hydroxyl-free” purification conditions (four new compounds, ajubractins A-D (1-4), along with the known 5-11).

Epimeric (15'R and 15'S) mixtures of 14-hydro-15'-hydroxyclerodin derivatives (15'-hydroxyajubractin C (13), 14-hydro-15'-hydroxyajugachin A (14), and 14'-hydro-15'-hydroxyajugapitin (15)), were obtained instead, along with 15'-epi-lupulin B (16).

In addition to the importance of the isolation procedure highlighted above, the isolation and characterization of small amounts of molecules difficult to monitor due to their nonspecific UV/Vis absorption, such as the neo-clerodane diterpenes of plant origin, was reported for the first time from *Teucrium luteum* subsp. *flavovirens*. Three new neo-clerodane diterpenes, 3β-hydroxyteucroxylepin (1) and teuluteumin A (2) and teuluteumin B (3), were reported.
3

DEPARTMENT OF BIOMEDICINAL CHEMISTRY
DEPARTMENT OF BIOMEDICINAL CHEMISTRY

Head: Gemma Fabriàs Domingo

The Department of Biomedical Chemistry conducts multidisciplinary research focused on the biomedical applications of peptides, lipids and glycoconjugates. The early detection, markers discovery and treatment of serious human diseases, such as amyloidosis related to the protein transthyretin, chronic pain, sphingolipidosis, cancer, neurodegeneration, autoimmune and infectious diseases, are emphasized. The investigations encompass the rational design of active molecules (peptides, glycoconjugates and small molecular entities) based on the knowledge of specific cell signalling routes, metabolic pathways, mechanisms of ligand-protein interactions, etc., as well as the concept of chemical modulation for optimising hit compounds based upon the modern medicinal chemistry technologies (combinatorial chemistry, in silico design and screening, solid phase organic synthesis, delivery systems).

Research groups
  Research Unit on BioActive Molecules
  Synthesis and Biomedical Applications of Peptides
  Unit of Glycoconjugate Chemistry
The Research Unit on BioActive Molecules works on the discovery of small molecules with activity on biologically relevant processes, with special interest on sphingolipid metabolism and functions. Sphingolipids play essential roles in the outcome and progression of diseases, including both rare diseases (sphingolipidosis) and diseases of high socio-economic impact (cancer, infectious diseases, diabetes 2, neurodegenerative diseases, etc.) thereby providing attractive targets to develop tools of use in diagnosis and prognosis, and leads in drug discovery. The research conducted encompasses from the design and synthesis of molecules and libraries to their biological study in cell lines, including sphingolipidomics.

**Staff**

Gemma Fabrias Domingo, Group Leader  
Jose Luis Abad Saiz  
Josefin Casas Brugulat  
Antonio Delgado Cirilo  
Amadeu Llebaria Soldevila, Group Leader

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Lucia Diaz Bueno  
Maria Garrido Martinez  
Jose M. Munoz Olaya  
Fabio Simbari  
Ana Trapero Puig  
Francesca Cingolani  
Ingrid Nieves Calatrava  
Xavier Gomez Santacana

**Publications (articles)**

- An unexpected access to a new sphingoid base containing a vinyl sulfide unit. Nieves, I., Garrido, M., Abad, J. L., Delgado, A. Synlett 2950-2952, 2010

Inhibition of acid ceramidase by a 2-substituted aminoethanol amide synergistically sensitizes prostate cancer cells to N-(4-hydroxyphenyl) retinamide. Gouazé-Andersson, V., Flowers, M., Karimi, R., Fabiáns, G., Delgado, A., Casas, J., Cabot, M.C. Prostate 71 1064-1073, 2011


The myo-1,2-diaminocyclitol scaffold defines potent glucocerebrosidase activators and promising pharmacological chaperones for Gaucher disease.

Trapero, A., Llebaria, A. 

Medicinal chemistry of aminocyclitols

Díaz, L., Delgado, A. 

Research highlights

Dihydroceramide Desaturase as Therapeutic Target in HIV-1 Infection. The lateral organization of lipids in cell membranes is thought to regulate numerous cell processes. Most studies focus on the coexistence of two fluid phases, the liquid crystalline (l(d)) and the liquid-ordered (l(o)), the putative presence of gel domains (s(o)) is not usually taken into account. In our article in Chem. Biol. 17 766-775, 2010, we show that in phospholipid:sphingolipid: cholesterol mixtures, in which sphingomyelin promoted fluid l(o) domains, dihydrosphingomyelin tended to form rigid domains. Genetic and pharmacological blockade of the dihydroceramide desaturase, which replaced sphingomyelin with dihydrosphingomyelin in cultured cells, inhibited cell infection by replication-competent and -deficient HIV-1. Increased dihydrosphingomyelin levels gave rise to more rigid membranes, resistant to the insertion of the gp41 fusion peptide, thus inhibiting viral-cell membrane fusion. These results clarify the function of dihydrosphingolipids in biological membranes and identify dihydroceramide desaturase as a potential target in HIV-1 infection.

Aminocyclitols

Pharmacological Chaperones in Gaucher Disease.

Different libraries containing the aminoaminocyclitol core have been synthesized and tested against glucocerebrosidase, the defective enzyme in Gaucher disease, with the aim of identifying pharmacological chaperones of further therapeutic usefulness. In some of the libraries, the aminocyclitol N-alkyl substituent contains a triazole moiety. Some of the library members have shown biochemical data similar or superior to those reported for N-propargylaminocyclitols. Some of the triazole and the aminocyclitol core.

Bioassays of compounds with potential juvendoic activity on Drosophila melanogaster: Juvenile hormone III, bisexode juvenile hormone III and methyl farnesatoes.

Hardshman, L.G., Song, K.-D., Casas, J., Schuermanns, A., Kuwano, E., Kachman, S.D., Riddiford, L.M., Hammock, B.D. 
J. Insect Physiol. 56 1465-1470, 2010

On the other hand, four diastereomeric series of N-alkylated [6+5] bicyclic isoureas having hydroxyl substituents mimicking glucose hydroxyl groups have been synthesized. One of the series of isoureas exhibited strong inhibition of recombinant glucocerebrosidase activity with Ki values in the 2-42 nM range. Furthermore, the [6+5] bicyclic guanidine derivatives with a substitution pattern analogous to the most active isoureas were also found to be potent inhibitors of glucocerebrosidase with Ki values between 3 and 10 nM. Interestingly, the active bicyclic isoureas and guanidines also behaved as glucocerebrosidase inhibitors in wild-type human fibroblasts at nanomolar concentrations. Importantly, some of the compounds exhibited the capacity of increasing glucocerebrosidase activity in Gaucher disease lymphoblasts derived from N370S and L444P variants. These results describe a promising series of potent glucocerebrosidase ligands having the cellular properties required for pharmacological chaperones.

Immunomodulatory agents.

A new class of α-galactosylceramide (αGC) nonglycosidic analogues bearing galacto-configured aminocyclitols as sugar surrogates have been obtained. Natural Killer T (NKT) cellular assays have resulted in the identification of an active compound able to promote NKT cell expansion in vitro in a similar fashion but more weakly than αGC. These compounds have been described in a paper (J. Med. Chem. 2011, 54, 6445-6448) showing that produce stimulation of the release of Interferon-γ (IFNγ) and Interleukin-4 (IL-4) in Invariant Natural Killer T (iNKT) cell culture but with lower potency than αGC. The activation of iNKT cells by this compound has been confirmed in flow cytometry experiments. Remarkably, when tested in mice, this compound selectively induced a very strong production of IFN-γ indicative of a potent Th1 cytokine profile. Overall, these data confirm the agonist activity of αGC lipid analogues having charged amino-substituted polar heads and their capacity to modulate the response arising from iNKT cell activation vivo. This discovery has been abstracted in SCIBx (SciBx, July 28 2011, vol 4, issue 29) outlining the potential of galactoaminocyclitols as vaccine adjuvants. SciBx is a Nature group weekly journal providing analysis of the scientific content and commercial potential of the most important translational research papers from across the life science literature. SciBx selects weekly the 25 published papers of basic life sciences with higher potential for commercial exploitation.
Synthesis and Biomedical Applications of Peptides

The Unit of Synthesis and Biomedical Applications of Peptides (USiBAP) interests focus on peptide chemistry from three different points of view: design, synthesis and therapeutic value of peptide molecules. The overall objectives of the USiBAP research summed up in the use of synthetic peptides in the field of Biomedicine both in improving diagnosis systems and in the design of new therapeutic targets. More specifically, work is being carried out on the design of immunopeptides, on the use of peptides for the development of new biosensors for the diagnosis of human illnesses and on the selection of therapeutic agents of peptide origin through biophysical testing.

Publications (articles)

Effect of synthetic peptides belonging to E2 envelope protein of GB virus C on human immunodeficiency virus type 1 infection.
J. Med. Chem. 53 6054-6063, 2010

A langmuir monolayer study of the interaction of E1(145-162) hepatitis G virus peptide with phospholipid membranes.
Sánchez-Martin, M.J., Haro, I., Alsina, M.A., Busquets, M.A., Pujol, M.

Assessment of synthetic chimeric multiple antigenic peptides for diagnosis of GB virus C infection.
Anal. Biochem. 396 51-58, 2010

Effects of smoking on disease activity and radiographic progression in early rheumatoid arthritis.
J. Rheumatol. 38 2536-2539, 2011

The use of chimeric vimentin citrullinated peptides for the diagnosis of rheumatoid arthritis.
Malakoutikhah, M., Gómar, M.J., Gómez-Puerta, J.A., Sanmartí, R., Haro, I.
J. Med. Chem. 54 7486-7492, 2011

Biophysical investigations of GBV-C E1 peptides as potential inhibitors of HIV-1 fusion peptide.
Sánchez-Martín, M.J., Urbán, P., Pujol, M., Haro, I., Alsina, M.A., Busquets, M.A.

Carbon nanotube composite peptide-based biosensors as putative diagnostic tools for rheumatoid arthritis.

Effect of E1(64-81) hepatitis G peptide on the in vitro interaction of HIV-1 fusion peptide with membrane models.
Sánchez-Martín, M.J., Busquets, M.A., Girona, V., Haro, I., Alsina, M.A., Pujol, M.
BBA-Biomembranes 1808 2178-2188, 2011

Diagnostic value of anti-GBV-C antibodies in HIV-infected patients.

Analysis of HIV-1 fusion peptide inhibition by synthetic peptides from E1 protein of GB virus C.
Sánchez-Martín, M.J., Hristova, K., Pujol, M., Gómara, M.J., Haro, I., Alsina, M.A., Busquets, M.A.
Study of the inhibition capacity of an 18-mer peptide domain of GBV-C virus on gp41-FP HIV-1 activity.
Haro, I., Gómara, M.J., Galatola, R., Domènech, O., Prat, J., Girona, V., Busquets, M.A.
BBA-Biomembranes 1808 1567-1573, 2011

Research highlights

**Effect of Synthetic Peptides Belonging to E2 Envelope Protein of GB Virus C (GBV-C) on Human Immunodeficiency Virus Type 1**
Recent years have seen the publication of numerous works in which co-infection with GB virus C (GBV-C) and HIV has been associated with slower progression of the illness and a higher survival rate of patients once AIDS has developed. The mechanism by which the GBV-C virus has a “protective effect” in patients with HIV has still not been defined. 124 synthetic sequences of the GBV-C E2 envelope protein have been obtained by SPPS and published in J. Med. Chem. 53, 6054, 2010. The interaction of certain GBV-C peptide sequences with the HIV-1 fusion peptide has been proven through the use of biophysical techniques. We also show how GBV-C E2 domains notably decrease cellular membrane fusion and interfere with the HIV-1 infectivity in a dose-dependent manner highlighting their potential utility in future therapies anti-HIV-1.

**The Use of Chimeric Vimentin Citrullinated Peptides for the Diagnosis of Rheumatoid Arthritis.**
Anti-citrullinated protein/peptide antibodies (ACPAs) are considered the most specific serologic markers of rheumatoid arthritis (RA). ACPAs recognize proteins or peptides with arginine residues converted to citrulline by a post-translational modification and have diagnostic and prognostic significance. ACPAs can be detected using enzyme-linked immunoabsorbent assays with different citrullinated protein or peptide substrates. The most widely used in clinical practice is the cyclic citrullinated peptide 2 assay (CCP2). In our group we have obtained three chimeric fibrin/filaggrin peptides and evaluated the diagnostic yield of the ELISA tests based on these peptides to compare their sensitivity and specificity in RA and other disease groups with the commercial CCP2 test. Our results published in J. Med. Chem. 54, 7486, 2011, highlight the putative application of chimeric peptides for the design of RA diagnosis systems and imply that more than one serological test is required to classify RA patients based on the presence or absence of ACPAs. Each of the target molecules reported (fibrin, vimentin, filaggrin) has a specific utility in the identification of a particular subset of RA patients.
Unit of Glycoconjugate Chemistry

The focus of the Unit is to apply chemical tools to the study of biochemical or medicinal chemistry problems. These tools first involved peptide synthesis, latter carbohydrate chemistry and more recently, study of halogenation reagents and biaryl compounds preparation by C-C bond forming cross coupling reactions. The fields of interest started with the study of enzyme catalysis, pain and immunity related mechanisms and compounds up to the more recent topics of transthyretin fibrillogenesis inhibitors and imaging diagnostics for neurodegenerative diseases using radiotracers. The current research activities fall mainly into three areas: 1) Synthesis and biological study of antinociceptive drugs. 2) Application in peptide chemistry of the iodinating reagent IPy$_2$BF$_4$ (Barluenga’s reagent). 3) Synthesis of transthyretin amyloidosis inhibitors. 4) Development of radiotracer probes for the imaging diagnostics of neurodegenerative diseases.

Publications (articles)

**Synthesis, biological evaluation and structural characterization of novel glycopeptide analogues of nociceptin N/OFQ.**

**Ligand-binding properties of human transthyretin.**
Pinto, M., Blasi, D., Nieto, J., Arsequell, G., Valencia, G., Planas, A., Quintana, J., Centeno, N.B.
*Amyloid* 18 (SUPPL. 1) 51-54, 2011

Drug discovery targeted at transthyretin cardiac amyloidosis: Rational design, synthesis, and biological activity of new transthyretin amyloid inhibitors
Blasi, D., Pinto, M., Nieto, J., Arsequell, G., Valencia, G., Planas, A., Centeno, N.B., Quintana, J.
*Amyloid* 18 (SUPPL. 1) 55-57, 2011

**Retrospective mapping of SAR data for TTR protein in chemico-biological space using ligand efficiency indices as a guide to drug discovery strategies.**
Research highlights

1) As part of our SAR studies on opioid ligands and of pain mechanisms and because glycosylation causes important changes in the native conformation, stability, activity and processing of many proteins we have been exploring the glycoconjugate approach for the rational drug design of new opioids. In applying this strategy to the N/OFQ peptide which is the native ligand of the pain related drug target NOP receptor, we have synthesized three N/OFQ analogues. In testing them in competition binding assays using cloned zebrafish NOP receptor preparations the glycopeptide which was glycosylated at Thr\(^5\) showed a remarkably reduced binding affinity compared to the other two analogues and the parent compound. In aqueous solutions these peptides were mainly populated by random coil conformers as seen by NMR and circular dichroism. However, in membrane mimic environments these peptides exhibited certain proportion of alpha helix structure as measured by NMR. Interestingly, under these conditions only the Thr\(^5\) glycosylated peptide also presented a population of folded hairpin like geometries which make us to speculate that linear helical structures are more complementary to the NOP receptor than folded ones that may account for the reduced binding affinity of this analogue.

2) Transthyretin (TTR) is a homotetrameric plasma protein that functions as the backup transporter for thyroxin hormone. Hereditary mutations on TTR are in the cause of a group of rare and always fatal systemic amyloid diseases. One of the most advanced and best studied possible pharmacological treatments relies on the use of small molecule compounds that bind into the channel formed by the tetramer and kinetically stabilize its dissociation into monomers thus preventing future aggregation events. During 2011 we have published three computationally based contributions to the above outlined drug discovery effort. The Molecular Informatics article deals with the implementation and application of the concept of Ligand Efficiency Indexes (LEIs) to a family of 80 salicylates with a diflunisal core structure that we have previously prepared with the aim to optimize the biological properties of this series of TTR aggregation inhibitors. After retrospectively prioritize the compounds on the nBEI SEI plane we have undertaken a prospective LEI analysis based in theoretical potency calculations using docking protocols on a 2300 compounds selected from the MMpINC database that has led to propose 12 new analogues that are in the process of being synthesized and biologically tested to validate this optimization strategy.
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DEPARTMENT OF CHEMICAL AND BIOMOLECULAR NANOTECHNOLOGY
Nanoscience and Nanotechnology is a multidisciplinary wide field, defined as the study of entities with dimensions in the nanometer range and the search for its technological applications. Our Department is focused on the understanding of bioactive molecules (oligonucleotides, macrobiomolecules, antibodies, organic molecules and drugs), self-organized supramolecular colloidal systems, nanostructured materials and devices. The research outcome may have useful applications in diagnostics (biosensors for disease prevention), therapeutics (protection against diseases), formulation of new products (pharmaceutical, cosmetics, agrochemicals, food products, etc.), preparation of new advanced materials (nanoparticles and porous materials for novel applications) and in bioorganic synthesis (development of new high added value products). The Department has a deep expertise in chemistry of oligonucleotides, developing novel biosensors with improved features, controlling self-aggregation of amphiphilic molecules, the formation of new nanostructured materials and chemistry of drugs and bioactive substances, among others. The methodologies used imply: the synthesis using combinatorial chemistry tools and designing and screening virtual libraries; the rational design of molecules with affinity to dsDNA and investigating the processes controlled by RNAi; the controlled production of selective antibodies and integrating such biomolecules with nanomaterials and devices; the formation of complex supramolecular structures (micelles, liquid crystals, microemulsions, nano-emulsions, highly concentrated emulsions, etc.); and the use of these systems as templates for formation of materials (organic, inorganic, hybrid) with controlled size and morphology, as well as new drug delivery systems. The Department is formed by consolidated multidisciplinary research teams, with a strong capacity to secure funds from Spanish public institutions, foundations, European programs and contracts of technology transfer to the private sector.

Research groups
Nanobiotechnology and Molecular Diagnostics
Nucleic Acids Chemistry
Colloid and Interfacial Chemistry Group
Bioorganic Chemistry
Surface Chemistry Group
The Nanobiotechnology and Molecular Diagnostics Group has focused on the development of novel molecular diagnostic tools to provide alternatives to the actual limitations existing in several fields, but particularly in the clinical and food safety areas. The combination of nanotechnological and biotechnological advances has given rise to novel molecular diagnostic approaches to improve efficiency and/or to refine and extend the limits of detection. Nanostructured surfaces and nanoparticles may be the basis for the construction of functional hybrid materials consisting of both organic (biomolecules) and inorganic components. Biosensors are among the potential applications of these new immunosensors using antibodies as biorecognition elements displaying fascinating features such as the possibility to respond selectively to biological or bioactive substances and the ability to respond in a physiological manner. The unique properties of certain nanomaterials combined with the excellent features of the antibodies allow for envisaging novel exquisitely sensitive chemical and biological sensors.

Publications (articles)

Recent advances in analytical and bioanalysis applications of noble metal nanorods.
Mannelli, I., Marco, M.P. 

Determination of atrazine residues in red wine samples. A conductimetric solution.
Valera, E., Ramón-Azcón, J., Barranco, A., Alfaro, B., Sánchez-Baeza, F., Marco, M.P., Rodríguez, A. 
Food Chem. 122 888-894, 2010

Gel-based immunotest for simultaneous detection of 2,4,6-trichlorophenol and ochratoxin A in red wine.

Competitive multi-immunosensing of pesticides based on the particle manipulation with negative dielectrophoresis.
Ramón-Azcón, J., Yasukawa, T., Lee, H.J., Matsue, T., Sánchez-Baeza, F., Marco, M.P., Mizutani, F. 

Electronic anabolic steroid recognition with carbon nanotube field-effect transistors.
Martínez, M.T., Tseng, Y.-C., Salvador, J.P., Marco, M.P., Ormategui, N., Loinaz, I., Bokor, J. 
ACS Nano 4 1473-1480, 2010

A high-throughput screening (HTS) immunochemical method for the analysis of stanozolol metabolites in cattle urine samples.
Salvador, J.P., Sánchez-Baeza, F., Marco, M.P. 
J. Chromatogr. B 878 243-252, 2010

Evaluation of immunoassays as an alternative for the rapid determination of pesticides in wine and grape samples.
Argarate, N., Arestin, M., Ramón-Azcón, J., Alfaro, B., Barranco, A., Sánchez-Baeza, F., Marco, M.P. 
J. AOAC Int. 93 2-11, 2010

Intracellular silicon chips in living cells.
Small 6 499-502, 2010
Validation of an enzyme-linked immunosorbent assay for detecting sulfonamides in feed resources.
Jiménez, V., Adrián, J., Guiteras, J., Marco, M.P., Comaño, R.
J. Agric. Food Chem. 58 7526-7531, 2010

Juvenile hormone and allatostatins in the German cockroach embryo.
Maestro, J.L., Pascual, N., Treiblmayr, K., Lozano, J., Bellés, X.

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Reisewitz, S., Schroeder, H., Tort, N., Edwards, K.A., Baeumner, A.J., Niemeyer, C.M.
Small 6 2162-2168, 2010

Mass spectrometric characterization of urinary toremifene metabolites for doping control analyses.

Preliminary study for simultaneous detection and quantification of androgenic anabolic steroids using ELISA and pattern recognition techniques.
Calvo, D., Tort, N., Pablo Salvador, J., Marco, M.P., Centi, F., Marco, S.
 Analyst 136 4045-4052, 2011

Development of a cellular biosensor for the detection of 2,4,6-trichloroanisole (TCA).
Varelas, V., Sanvicens, N., Marco, M.P., Kintzios, S.
Talanta 84 936-940, 2011

Quantum dot-based array for sensitive detection of Escherichia coli

A label-free and portable multichannel surface plasmon resonance immunosensor for on site analysis of antibiotics in milk samples.
Fernández, F., Hegnerová, K., Piliarik, M., Sánchez-Baeza, F., Homola, J., Marco, M.P.
Biosens. Bioelectron. 26 1231-1238, 2010

Portable surface plasmon resonance immunosensor for detection of fluoroquinolone antibiotic residues in milk.
Fernandez, F., Pinacho, D.G., Sánchez-Baeza, F., Marco, M.P.

Development of stable, water dispersible and biofunctionalizable superparamagnetic iron oxide nanoparticles.
Chem. Mat. 23 2795-2802, 2011

Development of an immunoassay for terbutryn: Study of the influence of the immunization protocol.
Sanvicens, N., Varela, B., Ballesteros, B., Marco, M.P.
Talanta 89 310-316, 2011

A novel free radical scavenger rescues retinal cells in vivo.
O’Driscoll, C., Doonan, F., Sanvicens, N., Messeguer, A., Cott, T.G.
Exp. Eye Res. 93 65-74, 2011

Publications (books and book chapters)
Sanvicens, N.; Fernández, F.; Salvador, J.P.; Marco, M. P.,
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in Nanoplatform-Based Molecular Imaging, John Wiley & Sons, Inc.: 2011; pp 781-813.
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http://dx.doi.org/10.1117/12.876456
Research highlights

In the last two years, the Nanobiotechnology and Molecular Diagnostics Group has continued studying novel micro and nano(bio)technological approaches to improve the efficiency of the diagnostic tools, particularly in the food safety and clinical fields. In this context, the group has published relevant results addressed to develop immunochemical techniques (ELISA) for the broad detection of antibiotics such as sulfonamides and fluoroquinolones or the detection of bacteria such as *Escherichia coli*, pesticides such as paraquat, antiestrogenic hormones such as toremifene or stanozolol, as well as a multianalyte immunoassays for the detection of up to 25 different antibiotics. Several of these immunoassays have been used for the analysis of different matrices such as environmental samples (river and sea water, wood), milk, honey, wine, grape juice, human and cattle urine, blood and hair.

Interesting results were obtained within the electrochemical immuno-sensors research line showing the potential of different configurations, such as the CNTFET (carbon nanotube field-effect transistors) arrays for the immunochromatographic determination of biomarkers at low concentrations (Martinez et al. ACS Nano). Moreover, in collaboration with Prof. Kintzios (Agricultural University of Athens) a cellular biosensor has been developed for the detection of TCAs, a contaminant of the wine. In the field of optical devices, a SPR immunosensor for the simultaneous determination of a panel of antibiotics has been developed, using a novel technology that could lower the price of these devices, in addition to offer the possibility to be used on site (Fernandez et al, Biosens. Bioelectronics). The ability to internalize conveniently biofunctionalized chips for biomonitoring of intracellular processes has been demonstrated (Gomez-Martinez et al. Small). Moreover, the possibility of capturing living cells on substrates for subsequent growth using antibody arrays, prepared by DNA-directed strategies, has been shown (Reisewitz et al, Small) in collaboration with Prof. Niemeyer (Dortmund, Germany). An interesting microarray approach based on labeling antibodies with QDs has been developing allowing detecting down to 2 CFU/ml of *E. coli* (Sanvicenis et al., ABC). The group has also collaborated with Prof. Santamaría (Zaragoza, Spain) on the demonstration of the biofunctionality of novel water-dispersable superparamagnetic iron oxide nanoparticles (Miguel-Sancho et al., Chem. Mat.).

The group is currently involved in projects for the development of systems for the early detection and quantification of biomarkers for diseases such as Alzheimers and cardio-vascular diseases. In the case of Alzheimers the early detection of 4 known biomarkers will allow for the precocious treatment for the disease. Biosensors are being developed for the detection of cardiovascular diseases. This research is being performed within the context of two INNPACTO projects (IPT-2011-1337-010000 and IPT-2011-1055-900000, MEC, Spain) and the CAJAL4EU projects (EC-FP7-ICT-JU-ENIAC-120215), all of them characterized by a high participation from enterprises and involving the development and application of new nanoelectronic devices for diagnostics.

Pharmasan Laboratories Inc (USA) have commissioned the Nanobiotechnology and Molecular Diagnostics Group for the development of point of care test (POCT) systems related to neurological disorders. Similarly, a collaboration contract has been signed with UNISENSOR SA (Belgium) addressed to the development of test-kits for food safety.

In respect to the food safety research line it is relevant the result obtained within the CONFIDENCE project (FP7-KBBE-2007-1) with the objective of improving food safety in Europe by the development of fast and cost-efficient methods for the detection of a wide range of chemical contaminants in different food products, based on an electrochemical magneto immunosensor assay. Several patents have been awarded (PCT/ES2009/000578 and P200702623) and new ones have been requested in relation to new transducers (PCT/ES2020/070824) and antibodies (P201031721) for diagnostics. Moreover some of these patents have been licensed to the private sector.

The Custom Antibody Service (Cabs), whereby antibodies can be custom produced and technical assistance is offered to companies and research institutes in respect to the preparation of immunoreagents, bioconjugates and immunochemical methods, is gaining acceptance and novel services are being incorporated.

During this period, the Nanobiotechnology and Molecular Diagnostics Group has participated in a variety of International Congresses e.g.in the World Congress on Biosensors (Glasgow, UK) with 8 communications. The Food Integrity and Traceability Conference (Belfast, UK) where the development of immunosensors for pesticides was well received or the IMAGINENANO (Bilbao, Spain) presenting the latest advances of the group in the nanobiotechnology research line.

Finally, the Nanobiotechnology and Molecular Diagnostics group continues to work on new strategies for the screening of small organic molecules, including condumetric sensors, optical biosensors, quantum-dot based arrays, microarrays and the standard ELISA etc.
Nucleic Acids Chemistry

Synthetic oligonucleotides are convenient tools for a large number of studies. The aim of our group is the study of the methodology used for the synthesis of DNA and RNA derivatives in order to obtain new compounds with new and/or improved properties. The projects undertaken along 2008-2009 deal with 1) conjugation of small molecules to DNA and RNA for a potential use in DNA/RNA therapeutics, 2) the effect of modified bases in the structural and biological properties of oligonucleotides, and 3) the use of modified oligonucleotides in the assembly of nanomaterials and biosensors.

Publications (articles)

Acridine and quindoline oligomers linked through a 4-aminoproline backbone prefer G-quadruplex structures.
Ferreira, R., Artali, R., Farrera-Sinfreu, J., Albericio, F., Royo, M., Eritja, R., Mazzini, S.

Synthesis and properties of oligonucleotides carrying isoquinoline imidazo[1,2-a]azine fluorescente units.
Pérez-Rentero, S., Kielland, N., Terrazas, M., Lavilla, R., Eritja, R.
Bioconjugate Chem. 21 1622-1628, 2010

Synthesis, cell-surface binding and cellular uptake of fluorescently labelled glucose-DNA conjugates with different carbohydrate presentation.
Bioconjugate Chem., 21 1280-1287, 2010

Synthesis and structural properties of oligonucleotides covalently linked to acridine and quindoline derivatives through a threoninol linker.
Aviñó, A., Mazzini, S., Ferreira, R., Eritja, R.
Bioorg. Med. Chem. 18 7348-7356, 2010

Stepwise synthesis of oligonucleotide-peptide conjugates containing guanidinium or lipophilic groups in their 3’-termini.
Grijalvo, S., Terrazas, M., Aviñó, A., Eritja, R.

Modified siRNAs for the study of the PAZ domain.
Somoza, A., Terrazas, M., Eritja, R.
Chem. Commun. 46 4270-4272, 2010

Triplex-stabilizing properties of parallel clamps carrying LNA derivatives at the Hoogsteen strand.
Alvira, M., Eritja, R.
Chem. Biodivers. 7 376-382, 2010

Fabrication of patterned surfaces by photolithographic exposure of DNA-hairpins carrying a novel photolabile group.
Manning, B., Leigh, S.J., Ramos, R., Preece, J., Eritja, R.
J. Exp. Nanoscience 5 26-39, 2010

Synthesis of oligonucleotides carrying amino lipid groups at the 3’-end for RNA interference studies.
Grijalvo, S., Ocampo, S.M., Perales, J.C., Eritja, R.
J. Org. Chem. 75 6806-6813, 2010

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Pérez-Rentero, S., Garibotti, A.V., Eritja, R.
Molecules 15, 5692-5707, 2010

Highly polar carbohydrates stack onto DNA duplexes via CH/π interactions.
A direct, efficient method for the preparation of siRNAs containing ribo-like North bicyclo[3.1.0]hexane pseudosugars.
Terrazas, M., Aviñó, A., Siddiqui, M., Márquez, V., Eritja, R.

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Chemical equilibria studies using multivariate analysis methods.
Jaumot, J., Eritja, R., Gargallo, R.

Synthesis and properties of small interfering RNA duplexes carrying 5-ethyluridine residues.
Terrazas, M., Eritja, R.

Synthesis and in vitro inhibition properties of siRNA conjugates carrying glucose and galactose with different presentation.
Aviñó, A., Ocampo, S. M., Lucas, R., Reina, J.J., Morales, J.C., Perales, J.C., Eritja, R.
Mol. Divers. 15, 751-757, 2011

Evaluation of the structure-activity relationship of thrombin binding aptamers by voltammetry and atomic force microscopy.
Diculescu, V.C., Chiorcea-Paquim, A.M., Eritja, R., Oliveira-Brett, A.M.
J. Electroanal. Chem. 656, 159-166, 2011

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Manning, B., Gallego, I., Tintoré, M., Fàbrega, C., Aviñó, A., Eritja, R.

Influence of pH, temperature and the cationic porphyrin TMPyP4 on the stability of the i-motif formed by the 5’-(C3TA2)4-3’ sequence of the human telomere.
Fernández, S., Eritja, R., Aviñó, A., Jaumot, J. Gargallo, R.

Functionnalization and self-assembly of DNA bidimensional arrays.
Garibotti, A.V., Pérez-Rentero, S., Eritja, R
Int. J. Mol. Sci. 12, 5641-5651, 2011

Use of oligonucleotides carrying photolabile groups for the control of the deposition of nanoparticles in surfaces and nanoparticle association.
Manning, B., Eritja, R.
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Synthesis of lipid-oligonucleotide conjugates for inhibition of gene expression.
Grijalvo, S., Ocampo, S. M., Perales, J. C., Eritja, R.

Synthesis and structural properties of G,T-parallel clamps carrying 5-aminopurine residues.
Aviñó, A., Cubero, E., Gargallo, R., González, C., Orozco, M., Eritja, R.

G-quadruplex Nucleic Acids.
Eritja, R., Mergny, J.L., Montesarchio, D., Spindler, L., Webba da Silva, M.

Synthesis and G-quadruplex binding properties of defined acidine oligomers.
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Thrombin binding aptamer quadruplex formation: AFM and voltammetric characterization.
Diculescu, V.C., Chiorcea-Paquim, A.M., Eritja, R., Oliveira-Brett, A.M.

Development of a novel fluorescence assay based on the use of the thrombin binding aptamer for the detection of O6-alkylguanine-DNA alkyltransferase activity.
Tintoré, M., Aviñó, A., Ruiz, F.M., Eritja, R., Fàbrega, C.

Branched RNA: a new architecture for RNA interference.
Aviñó, A., Ocampo, S.M., Perales, J.C., Eritja, R.
PMID: 21461398.

Synthesis and properties of oligodeoxynucleotides carrying 2-aminopurine.
Fàbrega, C., Grijalvo, S., Eritja, R.

Functionally enhanced siRNA targeting TNFα attenuates DSS-induced colitis and TLR-mediated immunostimulation in mice.
Mol. Ther. 20, 382-390, 2011
type conformation. Several authors have focused on characterized by 3'-endo or “North” (N) pucker of N-ring. In standard B-DNA, the pucker is 2'-endo or in DNA/RNA structure is the pucker of the furanose pseudosugars. A structural parameter that is crucial stability against nucleases has been addressed by

1.- Stability of siRNA in serum. The matter of

achieved by the group are summarized below.

luciferase by chemiluminescence. The results measure the inhibition of gene expression of one inhibited by specific siRNA duplexes while the other

the firefly luciferase gene and the other carrying

cells are transfected with two plasmids: one with

chemiluminescence. In the dual luciferase assay

hand, luciferase production can be measured by

a wide spectrum of human diseases. On the other

modulation of the affinity of siRNA to RISC has been addressed by synthesizing siRNA duplexes with guide strands carrying several groups designed to fit on an hydrophobic pocket of RISC. We observed that the inhibitory properties of siRNA duplexes carrying modified guide strands are being affected by the size of the group at the 3’-end, while the same modification on the passenger strand did not yield any change of activity.

3.- siRNA and RISC interactions. The modulation

of target genes. TNF-α was selected because is a major mediator of apoptosis as well as inflammation and immunity, and it has been implicated in the pathogenesis of a wide spectrum of human diseases. On the other hand, luciferase production can be measured by chemiluminescence. In the dual luciferase assay cells are transfected with two plasmids: one with the firefly luciferase gene and the other carrying the Renilla luciferase gene. One of the genes was inhibited by specific siRNA duplexes while the other is used as control. Using this assay it is possible to measure the inhibition of gene expression of one luciferase by chemiluminescence. The results achieved by the group are summarized below.

1.- Stability of siRNA in serum. The matter of stability against nucleases has been addressed by modifying siRNA duplexes with bicyclohexane pseudosugars. A structural parameter that is crucial in DNA/RNA structure is the pucker of the furanose ring. In standard B-DNA, the pucker is 2’-endo or “South” (S) whereas A-DNA and RNA are characterized by 3’-endo or “North” (N) pucker of N-type conformation. Several authors have focused on

Research highlights

Control of the gene expression inhibitory properties of nucleic acids by chemical modification. The use of synthetic oligonucleotides to control gene expression has triggered the search for new oligonucleotide derivatives with improved therapeutic potential. In these cases nucleic acids are used for the inhibition of a specific gene by blocking gene translation or gene transcription or by stimulating the degradation of a particular messenger RNA. Different strategies are possible. In the antisense strategy synthetic oligonucleotides complementary to the messenger RNA of a given gene are used to inhibit translation of messenger RNA to protein. In the siRNA strategy, small RNA duplexes complementary to messenger RNA bind to a protein complex named RISC. siRNA duplexes contains two strands: the antisense or guide strand that binds to RISC and the sense or passenger strand that is released as a result of the interaction of the siRNA duplex with RISC. The complex formed by the antisense or guide RNA strand and the protein complex RISC is able to catalyze the efficient degradation of a specific messenger RNA, lowering the amount of target protein.

During these years we have concentrated our efforts in the development of novel derivatives of RNA to enhance RNA interference. We used the luciferase and the TNF-α as target genes. TNF-α was selected because is a major mediator of apoptosis as well as inflammation and immunity, and it has been implicated in the pathogenesis of a wide spectrum of human diseases. On the other hand, luciferase production can be measured by chemiluminescence. In the dual luciferase assay cells are transfected with two plasmids: one with the firefly luciferase gene and the other carrying the Renilla luciferase gene. One of the genes was inhibited by specific siRNA duplexes while the other is used as control. Using this assay it is possible to measure the inhibition of gene expression of one luciferase by chemiluminescence. The results achieved by the group are summarized below.

1.- Stability of siRNA in serum. The matter of stability against nucleases has been addressed by modifying siRNA duplexes with bicyclohexane pseudosugars. A structural parameter that is crucial in DNA/RNA structure is the pucker of the furanose ring. In standard B-DNA, the pucker is 2’-endo or “South” (S) whereas A-DNA and RNA are characterized by 3’-endo or “North” (N) pucker of N-type conformation. Several authors have focused on
modifications in the passenger strand. This siRNA was selected for a preclinical study in a mouse model of inflammatory bowel disease (IBD). Anal administration of the modified siRNA resulted in extraordinary anti-inflammatory activity. A gene array study on siRNA treated animals confirmed that anti-inflammatory activity is the result of a reduced inflammatory process caused by the specific action of the siRNA targeting TNF-alpha. The unmodified siRNA was toxic due to the stimulation of the immune system. This work was carried out in collaboration with Dr. J.C. Perales (UB) and Dr. E. Fernández (UAB).

Oligonucleotides and Nanotechnology. A remarkable development in the DNA nanotechnology field was the use of stable DNA Holliday junctions with addressable sticky ends to form two-dimensional DNA crystals. The principles of construction described by Seeman have been used and adapted to generate systems with fine control of shape and function. For example, large DNA lattices have been transformed into highly regular two-dimensional DNA networks on surfaces that provide templates for the deposition of gold nanoparticles in a regular square network by using biotin-streptavidin recognition system. We became interested in the preparation of thiolated 2D DNA arrays because the special reactivity of the thiol group will allow the functionalization of 2D DNA arrays. Thiol groups have a strong affinity for gold surfaces and they can also be used to introduce peptides and proteins as well as large number of molecules that have been functionalized with maleimido groups or bromo- and iodo-acetyl groups. We inserted reactive thiol groups at the nucleobase at specific sites of a well-characterized bidimensional DNA lattice to study the formation of the DNA lattices on gold, a surface that allows electrical contacts. We demonstrated that DNA lattices carrying a single thiol derivative in each topological hairpin sites of a well-characterized bidimensional DNA lattice to study the formation of the DNA lattices on gold, a surface that allows electrical contacts. We demonstrated that DNA lattices carrying a single thiol derivative in each topological hairpin react with small drugs. Moreover, we studied the interaction of DNA-binding drugs with G-quadruplex structures is being studied, as well as, the synthesis of new quadruplex binding drugs. We have developed a method that allows the rapid and efficient synthesis of oligomers consisting of several intercalating drugs. Interestingly, the oligomers produced in this manner have a remarkable affinity for biologically relevant quadruplex, such as telomeric sequences and oncogene promoters. The reagents developed in this project were also used to synthesize oligonucleotides with enhanced hybridization properties, as well as more stable quadruplexes.

Design of inhibitors of DNA repair mechanism in cancer chemotherapy. Chemotherapy still constitutes the major pharmacological approach against cancer. Antiproliferative drugs are highly cytotoxic and aggressive agents. Under attack, the biochemical repair systems of the cancer cell machinery respond, trying to mitigate the cellular damage induced by these agents. As a result, their clinical efficacy is often limited. High doses are required and as a consequence serious secondary effects are commonplace. Recent advances in the molecular biology of cancer have identified key pathways involved in the DNA repair pathways induced by chemotherapeutic agents. As methylating agents are concerned, two main mechanisms have been envisaged. One involves the O6-methylguanine-DNA-methyltransferase (hAGT), which removes the methyl/alkyl group from the O6 position of guanine. A second important mechanism is the base excision repair (BER) pathway, which is involved in the repair of adducts resulting from methylation of the N7 position of guanine (N7-MGs). The objective of this project is the development of potent inhibitors of hAGT and APE1, a key endonuclease in the BER pathway. To this end, a combination of X-ray crystallography and in silico virtual screening of chemical libraries is being used. This research line of the group is supervised by Dr. Carme Fàbrega.

In addition we have developed a new photolithographic method that uses photolabile DNA hairpins to make patterns on silicon oxide and gold surfaces. The method described offers an attractive option for the fabrication of patterned surfaces with potential interest in electronics and biosensors.

G-quadruplex. Guanine-rich sequences capable of forming G-quadruplex structures have been found in telomeres and in transcriptional regulatory regions of important oncogenes, such as c-myc, and c-kit.
The main objectives of the group are the study of surfactant self-aggregation processes to contribute in the development of nanotechnological applications. The knowledge on basic aspects of surfactant aggregates (micelles, liquid crystals, vesicles) and colloidal dispersions (microemulsions, nano-emulsions, etc.) allows their use as nanoreactors for the preparation of novel nanostructured materials and as controlled drug delivery systems.

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Publications (articles)

Surface and self-aggregation properties of bis-benzimidazolones derivatives of D-glucose.
Lakhrissi, B., Lakhrissi, L., Massoui, M., Essassi, E.M., Comelles, F., Esquena, J., Solans, C., Rodríguez-Abreu, C.
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Nonaqueous foam with outstanding stability in diglycerol monomyrystate/olive oil system.
Shrestha, R.G., Shrestha, L.K., Solans, C., González, C., Aramaki, K.

Solution behavior of aqueous mixtures of low and high molecular weight hydrophobic amphiphiles.

Nano-emulsions prepared by the phase inversion composition method: Preparation variables and scale up.
Colloid Interface Sci. 344 417-423, 2010

Effect of alkyl chain asymmetry on catanionic mixtures of hydrogenated and fluorinated surfactants.
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Synthesis of CeO₂, ZrO₂, Ce₅.₂Zr₀.₈O₂, and TiO₂ nanoparticles by a novel oil-in-water microemulsion reaction method and their use as catalyst support for CO oxidation.
Current-voltage characteristic of electrospray processes in microfluidics.

Preparation of ultra-light magnetic nanocomposites using highly concentrated emulsions.

Formation of polymeric nano-emulsions by a low-energy method and their use for nanoparticle preparation.

A combination of hard and soft templating for the fabrication of silica hollow microcoils with nanostructured walls.

Surfactants based on bis-galactobenzimidazolones: Synthesis, self-assembly and ion sensing properties.

Surface versus volume effects in luminescent ceria nanocrystals synthesized by an oil-in-water microemulsion method.

Chromonic liquid crystalline phases of pinacyanol acetate: Characterization and use as templates for the preparation of mesoporous silica nanofibers.

Identification and characterization of organic nanoparticles in food.

Influence of a mixed ionic/nonionic surfactant system and the emulsification process on the properties of paraffin emulsions.

Phase behaviour of a mixed ionic/nonionic surfactant system used to prepare stable oil-in-water paraffin emulsions.

Stability of oil-in-water paraffin emulsions prepared in a mixed ionic/nonionic surfactant system.

Synthesis of Pt nanoparticles in oil-in-water microemulsions: Phase behavior and effect of formulation parameters on nanoparticle characteristics.

Characterization of perylene diimide dye self-assemblies and their use as templates for the synthesis of hybrid and supermicroporous nanotubules.

Tuning high aqueous phase uptake in nonionic water-in-oil microemulsions for the synthesis of Mn-Zn ferrite nanoparticles: Phase behavior, characterization, and nanoparticle synthesis.

Relaxation dynamics in the columnar liquid crystal phase of hard platelets.

Spectrally and temporarily resolved luminescence study of short-range order in nanostructured amorphous ZrO2.
Tiseanu, C., Parvulescu, V.I., Sanchez-Dominguez, M., Boutonnet, M. J. Appl. Phys. 110 103521, 2011

Reference materials for measuring the size of nanoparticles.
Publications (books and book chapters)


Research highlights

Amphiphile self-assembly

Self-assembly studies of amphiphilic molecules are conducted in the group as a bottom up approach for the development of well-defined nanostructures in view of their use as nanocarriers (e.g. controlled drug delivery systems), nanoreactors (e.g. synthesis of advanced materials), tailor-made formulations, etc. During this period, the self-organizing structures formed by a water soluble perylene diimide dye (PDI) have been studied as potential templates for the preparation of hybrid nanomaterials (C. Rodríguez Abreu, ACS Appl. Mater. Interfaces, 2011). This PDI dye forms nematic and hexagonal chromonic liquid crystals in water, consisting of stacks of long aggregates with a diameter close to the size of one PDI molecule (Figure 1).

The use of π-π stacked chromonic aggregates brings new possibilities for the template fabrication of pores with sizes below the mesoporous range. The obtained materials could find applications in photovoltaics as well as in shape selective catalysis and adsorption.

Self-assembly properties of sugar-derived surfactants, such as new nonionic amphiphiles based on bis-galactobenzimidazolones, have also been investigated. These surfactants were synthesized by grafting alkyl bis-benzimidazolones units as hydrophobic tail on hydroxypropyloxygalactopyranose moiety as hydrophilic moiety (B. Lakhrissi, J. Surfactants Deterg., 2011) Evaluation of self-aggregation properties in water showed very low critical micellar concentrations (CMCs) and the formation of hexagonal liquid crystals for a certain range of hydrophobic tail lengths. Furthermore, the new amphiphiles showed characteristic UV-vis absorption and fluorescence emission bands associated with the benzimidazolone moiety. All these properties make these new amphiphiles appropriate candidates as self-assembling chemosensors.

Emulsions: Formation by low-energy methods and properties

Emulsification by low-energy methods produce, generally, emulsions with smaller and more uniform droplets. New knowledge on low-energy emulsification methods has been acquired by studying nano-emulsion formation in systems with a polar solvent containing a preformed polymer as dispersed oil phase. Polymeric O/W nano-emulsions with size below 100 nm were obtained by the phase inversion composition (PIC) method using a non-toxic solvent (G. Calderó, J Colloid Interface Sci., 2011). Conductivity measurements performed along dilution paths of mixtures with different oil-to-surfactant (O/S) ratios confirmed that nano-emulsions were produced by phase inversion (Figure 2).

The results of this study showed that the low-energy emulsification methods are not only valid for aliphatic and semipolar oils, but also for a highly polar solvent such as ethylacetate containing a preformed polymer.
Other research lines developed in the field of emulsions by the group deal with the study of drug release from highly concentrated emulsions (G. Calderó, *J. Pharm. Sci.*, 2010) and on the use of these emulsions as templates for the preparation of ultralight porous materials (G. Ghosh, *Mater. Chem. Phys.*, 2011). Biocompatible highly concentrated water-in-oil (W/O) emulsions suitable for cutaneous and transdermal administration of drugs were successfully prepared (Figure 3). To study the factors influencing drug release, two model drugs, clindamycin hydrochloride and theophylline, with different characteristics (chemical nature, molecular weight, water solubility, acid-base dissociation) were selected and incorporated in the dispersed phase of the emulsions.

![Figure 3](image)

**Figure 3.** Region of formation of highly concentrated emulsions (striped area) at 25°C in the systems: (a) water/Cremophor W07/soybean oil and, (b) water/Cremophor W07/liquid paraffin.

The release of clindamycin hydrochloride, which is freely soluble in water, was very slow, regardless of the emulsion system, while the release of theophylline, which is slightly soluble in water, was faster. By changing the pH of the dispersed phase of highly concentrated emulsions, which in turn affects solubility, drug release could be modulated. These results suggested that with freely soluble drugs, the solubility, rather than interfacial properties of the emulsion system, is the main factor controlling its release. In contrast with slightly soluble drugs, release can be controlled by the interfacial properties of the HIPRE and by inducing solubility changes in the drug.

The knowledge on the use of highly concentrated emulsions as templates for the preparation of porous materials was applied to obtain hybrid magnetic nanocomposite materials. These materials were prepared by polymerization in the continuous oil phase of styrene-divinylbenzene mixtures incorporating magnetite (Fe₃O₄) nanoparticles. Ultra-light porous nanocomposites were obtained with the nanoparticles distributed homogeneously in the polymer walls (Figure 4) giving a uniform magnetic moment over the entire material.

![Figure 4](image)

**Figure 4.** Solid foams (porous nanocomposites) with magnetic nanoparticles of 3 nm. Images by scanning (top) and transmission (bottom) electron microscopy.

These materials are about 20 times lighter than the non-porous nanocomposite material with similar magnetic properties (superparamagnetic behaviour), and stronger particle-particle interaction.

**The Microemulsion Reaction Method**

Among wet chemistry methods for the synthesis of inorganic nanoparticles, the Microemulsion Reaction Method (MRM) has been found to be a suitable option in order to control size and shape in mild reaction conditions. In this context, the formation of w/o microemulsions with high aqueous phase uptake in a nonionic surfactant system was investigated as potential media for the synthesis of magnetic nanoparticles (C. Aubery, *Langmuir*, 2011). Three microemulsions with three different dynamic behavior (non-percolated and percolated w/o, as well as bicontinuous microemulsions) were selected for the synthesis of Mn-Zn ferrites (Figure 5). The aqueous phase content ranged from 5 wt% to 50 wt%.

![Figure 5](image)

**Figure 5.** Microemulsion region in an aqueous solution/surfactant/oil system and TEM images of Mn-Zn ferrite nanoparticles obtained in microemulsions with different dynamic behavior.

Differences were observed in the characteristics of the synthesized nanoparticles depending on the type of microemulsions used, and in all cases spinel nanocrystalline particles with superparamagnetic properties were obtained, directly in the microemulsion, without the need for calcination. A novel approach based on the use of O/W microemulsions for the synthesis of inorganic nanoparticles has been developed in the group since our first report on the subject in 2009. The synthesis of metallic (Pt, Pd, and Rh) as well as metal oxide (CeO₂) nanoparticles were first reported as a proof of concept of the O/W microemulsion reaction method. It was followed by the synthesis of mesoporous nanocrystalline oxides such as ZrO₂, Ce₅₋₂Zr₆₋₂Oₓ, and TiO₂ (M. Sanchez-Dominguez, *Catalysis Today*, 2010). Small particle size (3 nm), and high specific surface area (200-380 m² g⁻¹) was obtained for all materials. The materials were evaluated as catalyst supports in the CO oxidation reaction and showed a good activity in CO oxidation at low temperature.
Bioorganic Chemistry Group

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Publications (articles)

Protein-protein interaction antagonists as novel inhibitors of non-canonical polyubiquitylation.
PLoS ONE 5 e11403, 2010

Peptoids bearing tertiary amino residues in the n-alkyl side chains: synthesis of a potent inhibitor of Semaphorin 3A.
Messeguer, J., Masip, I., Montolio, M., del Rio, J.A., Soriano, E., Messeguer, A.
Tetrahedron 66 2444-2454, 2010

Nanoconjugates as intracorporeal neutralizers of bacterial endotoxins.
Vicent, M.J., Cascales, L., Carbajo, R.J., Cortés, N., Messeguer, A., Pérez-Payá, E.

Antioxidant CR-6 protects against reperfusion injury after a transient episode of focal brain ischemia in rats.

A fluorescent polarization-based assay for the identification of disruptors of the RCAN1-calcineurin A protein complex.
Mulero, M.C., Orzáez, M., Meseguer, J., Messeguer, A., Pérez-Payá, E., Pérez-Riba, M.

Triazine-based vanilloid 1 receptor open channel blockers: Design, synthesis, evaluation, and SAR analysis.
J. Med. Chem. 54 7441-7452, 2011

Chemical modulation of peptoids: Synthesis and conformational studies on partially constrained derivatives.

Molecules that modulate Apaf-1 activity.

A novel free radical scavenger rescues retinal cells in vivo.
O’Driscoll, C., Doonan, F., Sanvicens, N., Messeguer, A., Cotter, T.G.
Exp. Eye Res. 93 65-74, 2011

Improved therapeutic responses for liposomal doxorubicin targeted via thrombospondin peptidomimetics versus untargeted doxorubicin.
Rivera-Fillat, M.P., Reig, F., Martínez, E.M., Grau-Oliete, M.R.

We use the modern medicinal chemistry techniques (combinatorial chemistry, in silico design and construction of chemical libraries, solid phase synthesis, drug delivery methods) for the identification of hit compounds against targets of pharmacological interest. Complementarily, the chemical modulation of these hits for their conversion into lead compounds for further development in collaboration with pharma and biotech companies is intensively pursued. The group has filed four patent applications in 2010-2011 and licensed one patent to a biotech company.
Concerning combinatorial chemistry in drug discovery, our group became interested in this field in 1998. Through the establishment of collaborative projects with different laboratories, the group has been pioneer in Spain in the design and construction of combinatorial libraries of organic molecules, in particular of libraries of controlled mixtures of small organic molecules. In this period, libraries of peptoid mixtures (5,000 and 11,000 N-alkylglycine trimers, and 625 pentamers, respectively) and four libraries of individual components (peptidomimetics bearing heterocyclic moieties) have been prepared. In addition, libraries of peptidomimetics attached to microplates (Chem Chips) have been also constructed.

Along this period, our group has incorporated the required expertise for handling the different methodologies to work on Combichem (solid-phase organic synthesis, synthesis of libraries in solution, libraries of individuals or mixtures, use of microwave activation of organic reactions, in silico methodology for the design and screening of virtual libraries etc.). By using this general strategy, our group has obtained highly interesting results. Thus, we identified two peptoids that exhibit high in vitro and in vivo activity as blockers of the TRPV1 vanilloid receptor. In addition, and also in collaboration with the same partners, we identified a family of molecules exhibiting potent antagonist activity against the NMDA receptor. Moreover, the identification of a peptoid capable of inhibiting Sema-3 and thus interesting for studying the axonal regeneration problem, has been recently achieved.

More recently, in collaboration with the group of Dr. E. Pérez-Payá (CIPF, Valencia), two compounds that neutralise bacterial endotoxins have been identified. In a parallel study in collaboration with the same group, peptoids capable of inhibiting the formation of apoptosome have been discovered. These compounds have been intellectually protected and the patent has been licensed to a pharmaceutical company for co-development. This result represents the first example of a small molecule as inhibitor of apoptosis operating by this mechanism and it also constitutes an interesting example of how small molecules can perturb and even modulate protein-protein interactions. A further conversion of the initial hit into a peptidomimetic exhibiting improved activities in vitro and in vivo has been also carried out. The co-development of this compound in the organ transplant field is currently under contracted research with the above pharmaceutical company.

In a collaboration established with the group of Dr. Timothy Thomson (IMBM-CSIC, Barcelona), we have also identified peptoids capable of perturbing protein-protein interactions (UBC13-UEV) of interest in cancer and inflammation. What is interesting of this example and of some other commented above (for instance, the inhibitor of apoptosome), is that we have done already a step ahead in order to convert the identified hits into compounds exhibiting more friendly pharmacological profiles. Our goal is the selection of a lead candidate. This structural conversion has been carried out by an initial study of the conformational preferences of the peptoid skeleton followed by the design of conformationally restricted analogues bearing different types of heterocyclic scaffolds. At this moment, we have one peptidomimetic showing high inhibitory activity of the apoptosome in intact cells. Moreover, a new generation of apoptosis inhibitors bearing a novel heterocyclic skeleton,
already patented, has been also developed. Likewise, two peptidomimetics have been prepared following a molecular modelling study for improving the properties of the initial hit discovered in the above commented modulation of UBC13-UEV interaction. It should be remarked that this discovery represents the development of the first modulators of this protein-protein interaction that can show a highly promising activity in cancer treatment. Finally, our group has also been interested in expanding the expertise of experimental combinatorial libraries to those designed and screened \textit{in silico}.

Our work on compounds that exhibit bioactive activity has been complemented by research on free radicals quenchers, either from oxygen (ROS) and/or nitrogen (RNS). Some years ago we discovered a tocopherol surrogate (CR-6) bearing a simple structure and potent activity as lipid peroxidation inhibitor. More recently, its activity as inhibitor of RNS species (NO and peroxynitrite) was also shown. Our laboratory participates with a biotech company, the Lipotec Group, in the industrial development of this antioxidant. This compound is now in Phase II clinical trials in antitumour therapy, specifically in preparations containing liposomes that encapsulate doxorubicin. CR-6 is embedded in these liposomes and reduces the side-effects produced by the anticancer drug. Moreover, CR-6 is being commercially used in the dermopharmacy area as antiageing agent. On the other hand, recent work has shown the ability of CR-6 to inhibit apoptosis in photoreceptor cells (collaboration with T. Cotter, Univ. of Cork, Ireland). Likewise, in a collaboration established with the group of A. Planas (IIBB-CSIC, Barcelona), very interesting results on the potential neuroprotective activity of CR-6 have been obtained.

Taken together, all these results show the high therapeutic potential of this radical inhibitor. Currently, we are working on analogues capable of eliciting a higher penetration through the blood brain barrier. In parallel, physicochemical studies concerning interactions between this compound and phospholipids have been performed in order to know how the molecules insert and locate in the bilayers.

Finally, it is worth of mentioning the intense activity of our group in two additional fields. First, we are members of a Consolider Consortium focused on Ion Channels and financed up to 2013 and coordinated by Prof. Antonio Ferrer-Montiel (Univ. Miguel Hernández). Our main task is to provide with molecules (libraries or individuals) to more than 20 research groups working on ion channels and interested in the identification of compounds that can modulate the function of these channels. On the other hand, our group is working intensively in two research projects supported by private pharma or biotech companies. In both cases it is intended to discover lead compounds active in front of highly interesting pharmaceutical targets.
The main objective is to study the formation and characterization of structured materials, and their applications in novel technological processes. This includes: a) Surface modification of materials by chemical and physical (plasma) methods, b) Surface characterization of textile and polymeric materials, c) Formation and characterization of hydrogels, d) Development of stimuli-responsive textiles by incorporation of advanced nanostructured materials, and e) Preparation and characterization of organic and inorganic porous materials.

**Publications** (articles)

**Improved properties of oxygen and argon RF plasma-activated polyester fabrics loaded with TiO2 nanoparticles.**
Mihailovic, D., Saponjic, Z., Molina, R., Puac, N., Jovancic, P., Nedeljovic, J., Radetic, M.
*ACS Appl. Mater. Interfaces* 2 1700-1706, 2010

**Surface and self-aggregation properties of bis-benzimidazolones derivatives of D-glucose.**
Lakhirssi, B., Lakhrissi, L., Massoui, M., Essassi, E.M., Comelles, F., Esquena, J., Solans, C., Rodríguez-Abreu, C.

**Use of hydrophobically modified inulin for the preparation of polymethyl methacrylate/polybutyl acrylate latex particles using a semicontinuous reactor.**
*Langmuir* 26 7717-7724, 2010

**A liquid-crystalline single-molecule magnet with variable magnetic properties.**

**Interfacial processes in textile materials: Relevance to adhesion.**
Molina, R., Esquena, J., Erra, P.

**Influence of chitosan on the effects of proteases on wool fibers.**
Vílchez, S., Jovancic, P., Erra, P.

**Nano-emulsions prepared by the phase inversion composition method: Preparation variables and scale up.**
Solè, I., Pey, C.M., Maestro, A., González, C., Porras, M., Solans, C., Gutiérrez, I.M.
*J. Colloid Interf. Sci.* 344 417-423, 2010

**Preparation of ultra-light magnetic nanocomposites using highly concentrated emulsions.**
Ghosh, G., Vílchez, A., Esquena, J., Solans, C., Rodríguez-Abreu, C.

**Aqueous phase behaviour of choline carboxylate surfactants: Exceptional variety and extent of cubic phases.**
Klein, R., Tiddy, G.I.T., Maurer, E., Touraud, D., Esquena, J., Tache, O., Kunz, W.
*Soft Matter* 7 6973-6983, 2011
Multifunctional properties of polyester fabrics modified by corona discharge/air RF plasma and colloidal TiO2 nanoparticles.
Mihailović, D., Šaponjić, Z., Molina, R., Radojičić, M., Esquena, J., Iovančić, P., Nedeljković, J., Radetić, M.
Polyim. Compos. 32 390-397, 2011

Macroporous polymers obtained in highly concentrated emulsions stabilized solely with magnetic nanoparticles.
Vílchez, A., Rodríguez-Abreu, C., Esquena, J., Menner, A, Bismarck, A.
Langmuir 27 13342-13352, 2011

Influence of a mixed ionic/nonionic surfactant system and the emulsification process on the properties of paraffin emulsions.
Vilasau, J., Solans, C., Gómez, M.J., Dabrio, J., Mújika-Garai, R., Esquena, J.

Novel properties of PES fabrics modified by corona discharge and colloidal TiO2 nanoparticles.
Mihailović, D., Šaponjić, Z., Radojičić, M., Molina, R., Radetić, I., Iovančić, P., Nedeljković, J., Radetić, M.

Modifying the heat transfer and capillary pressure of loop heat pipe wicks with carbon nanotubes.
Terrado, E., Molina, R., Natividad, E., Castro, M., Erra, P., Mishkinis, D., Torres, A., Martinez, M.T.

Stability of oil-in-water paraffin emulsions prepared in a mixed ionic/nonionic surfactant system.
Vilasau, J., Solans, C., Gómez, M.J., Dabrio, J., Mújika-Garai, R., Esquena, J.

Phase behaviour of a mixed ionic/nonionic surfactant system used to prepare stable oil-in-water paraffin emulsions.
Vilasau, J., Solans, C., Gómez, M.J., Dabrio, J., Mújika-Garai, R., Esquena, J.

Publications (books and book chapters)
Rodríguez-Abreu, C., Esquena, J.

Ghosh, G., Vílchez, A., Esquena, J., Solans, C., Rodríguez-Abreu, C.

Research highlights
Pickering emulsions as templates for the preparation of macroporous solid foams
Highly concentrated emulsions (HIPEs) are characterized by possessing a volume fraction of the disperse phase that exceeds 0.74, which corresponds to the critical value for the most compact packing of monodisperse spherical droplets. HIPEs can be used as templates for the preparation of macroporous materials via the polymerization of the external emulsion phase.

Macroporous polymer foams with a magnetic response have been prepared by taking advantage of the ability of the nanoparticles to stabilize emulsions (which are typically denoted as Pickering emulsions). In analogy with surfactants, nanoparticles can be surface active, and adsorb spontaneously at the oil-water interfaces. One of the advantages of using particle-stabilized emulsions is that any additional property coming from the nanoparticle can be directly imparted to the materials.

Solid foams with up to 95% of porosity, and high magnetization saturation values resulting from the Fe3O4 nanoparticles have been obtained. As shown in Fig.1 such nanoparticles are located at the polymer-air interface after the polymerization. These magnetic macroporous materials could act as promising adsorbents for specific molecules or be used in water decontamination process.

Fig.1. SEM (left) and TEM (right) images of a macroporous solid foam with micrometer pore sizes and Fe3O4 nanoparticles placed at the polymer-air interface. Vílchez, A., Rodríguez-Abreu, C., Esquena, J., Menner, A., Bismarck, A.
Use of plasma for advanced technologies

Plasma is generated when a gas is exposed to an electric field, generating radicals, ions, electrons and other excited species of high energy. These reactive species can interact either physically or chemically with the substrate surface to a depth of a few tenths of nanometers.

As a result of plasma treatment, the surface may be functionalized (by the generation of new chemical groups), and/or degraded as a result of the etching effect (removal of surface material), whereas the bulk properties remain intact. Attending to the type of plasma gas, these effects are used in polymer surface modification in order to improve surface properties such as adhesion, wetting (hydrophilicity/hydrophobicity), incorporate reactive groups such as carboxylic or amine groups and/or thin film deposition by plasma polymerization. The combination of both, high energy reactive species and ultraviolet radiation generated in the plasma is also used for bacteria or spore sterilization, at low temperature.

Atmospheric plasma can be applied to aqueous solutions with monomers or polymers in order to obtain hydrogels or films with specific properties. Experimental parameters such as monomer concentration and plasma power play an important role in the properties of the film obtained. In this context, thin polymeric films with stimuli response properties can be obtained. Chitosan biopolymer films obtained by means of atmospheric plasma treatment are less soluble in acid medium than conventional chitosan films suggesting that crosslinking reactions between polymer chains can occur during the plasma treatment.

On the other hand, plasma treatments have been carried out in waste-water in order to eliminate chemical compounds such as dyes or pharmaceutical products.

Textiles modified with chitosan hydrogels for medical and/or therapeutical applications

Nowadays, there is an increasing demand for textiles with advanced functionalities for medical, therapeutical and cosmetic applications. They allow the administration of active molecules in a simple and controlled manner. Most of them are based on the physical immobilization or impregnation of textile fibers by a thin layer of products containing active molecules. The release of the active molecules can be induced by the chemical degradation, via molecular diffusion processes, and/or as a response to an external stimulus such as temperature, pH and ionic strength. Hence, the use of hydrogels prepared from stimuli-responsive polymers, which display changes in solvation in response to a change in temperature, pH and ionic strength, constitute an interesting strategy to confer new properties to textiles. In this context, the biopolymer chitosan, which is a pH-sensitive polymer and responds to a pH change by protonation/deprotonation of its amino groups, has been used to obtain hydrogels crosslinked with the natural crosslinker genipin.

These hydrogels have been incorporated onto the surface of polyamide fabrics by the padding technique, and its successful incorporation was confirmed by cryoSEM (Fig. 3). The water absorption ability of the treated fabrics was studied through thermogravimetric dynamic vapour sorption (TG-DVS), which showed higher moisture content of fabrics, compared to untreated. The porous structure of the fabrics was also studied by thermoporosimetry, which allows studying pore structures of materials in the presence of water.

In a second step, active molecules have been successfully incorporated in the hydrogel matrix, and drug release studies have been performed (in collaboration with the Faculty of Pharmacy of the University of Barcelona). In the case of hydrophilic active molecules, the different release when they were directly solubilized in the hydrogel or in liposomes contained in the hydrogel, has been studied (Fig. 2). On the other hand, hydrophobic active molecules were solubilized in the lipidic bilayer of liposomes contained in the hydrogel. The chemical interactions of the active molecules with the chitosan hydrogel matrix have also been studied.
DEPARTMENT OF CHEMICAL AND SURFACTANTS TECHNOLOGY
The research in the Department focus on theoretical and applied aspects of product and chemical processes technology with special incidence in the synthesis, the physical chemistry and the biology of surfactants. This research is relevant in the lines of Sustainable Chemistry and Nanotechnology of soft matter and look for environmental and human health improvement. Among the scientific activities, with relation to the Sustainable Chemistry, we can cite: research and development of biocompatible surfactants and ionic liquids, the distribution and effect of surfactants and ionic liquids in the environment, development of non contaminant industrial processes, minimization, recycling and valorization of by-products and wastes of chemical industries. In the Nanotechnology area research is performed concerning adsorption and self-aggregation of surfactant as well as the physical chemistry and biophysics of natural lipids at interfaces and membranes (of natural origin or as physical chemistry models).

Research groups

- Minimization of Industrial Wastes: Isolation of High Added-Value Biopolymers
- Development of Non-contaminant Industrial Processes
- Statistical Modelling and Fibre Physics
- Biocompatible Surfactants
- Environmental Chemistry of Surfactants and Ionic Liquids
- Physical Chemistry of Surfactant Systems
- Biophysics of Lipids and Interphases

Head: Ramon Pons Pons
Minimization of Industrial Wastes: Isolation of High Added-Value Biopolymers

The main objective of our research main line is the design and development of medical devices for skin tissue regeneration and/or improving tissue function based on bioactive materials of natural origin. Animal waste from food: meat, fish, poultry industries (slaughterhouse) and tanning industries will be used as raw material. Furthermore, the following additional waste should be included: fish waste, such as fish skins of hake, monkfish, sole and rock sole, and eggshell membrane. Of especial interest is the possibility of extracting other high-added value products closely related to collagen, glycosaminoglycans (GAGs) (dermatan sulfate, keratan sulfate, etc.) mainly from the meat and poultry industry (rooster combs, vitreous humour, synovial fluid) with hyaluronic acid as a maximum representative given its increasing use in medicine. It is expected to develop new medical devices for the rapid healing of skin injuries (burns, ulcers, etc) that have not been resolved to date. Growing numbers of elderly people in Europe suffer from skin injuries such as bedsores and vascular ulcers and need effective medical devices that can be applied in hospitals and at home.

Publications (articles)

Tailor-made biomaterials from collagenic wastes
Catalina, M., Celma, P., Cot, J., Manich, A., Marsal, A.

Magnetically separable nanocomposites with photocatalytic activity under visible light for the selective transformation of biomass-derived platform molecules.
Balu, A., Cot, J., Baruwati, B., Serrano, E., Garcia-Martinez, J., Barma, S., Luque, R.
Green Chem. 13 2750-2758, 2011

Influence of crosslinkers and crosslinking method on the properties of gelatin films extracted from leather solid waste.
Catalina, M., Attenburrow, G.E., Cot, J., Covington, A.D., Antunes, A.P.M.

Application of gelatin extracted from chrome shavings on the glazed finishing of leather.
Catalina, M., Attenburrow, G.E., Cot, J., Covington, A.D., Antunes, A.P.M.
J. Am. Leather Chem. As. 105 138-144, 2010

Research highlights

TAYLOR-MADE BIOMATERIALS FROM COLLAGENIC WASTES: FEASIBLE LINK BETWEEN TANNING INDUSTRY AND TISSUE ENGINEERING

The environment is one of the most relevant topics nowadays, the ecological conscience and the practice of an environmentally friendly and sustainable policy is increasing day by day all over the world. The concept of “Sustainable Development” transmits the idea of the rational use of the resources, the improvement of life quality and the maintenance of the ecosystems without jeopardising future generations. The improvement of the manufacturing processes, the finding of new types of renewable energies, the application of “clean” technologies in the processing, the finding of new treatments for each type of waste; are essential steps to make compatible industrial development, environmental protection and social welfare. Waste treatments, in addition of reduce the volume of industrial waste could increase their value through the production of high added value products, entailing a great progress in both, environmental and economical terms.

In terms of waste generation, the production of leather gives rise to significant quantities of solid waste product for which tanneries are responsible for the cost of disposal and since most of this waste ends up in landfill it may be considered an environmental problem. However such waste is not without some potential value since it contains collagen which could be recycled and reused. Collagen is a very versatile and special high-added value protein and the most abundant and ubiquitous in vertebrates. This collagenic nature of the tannery solid waste permits us to think about
treatments for obtaining biopolymers of reconstituted collagen, and their use in a wide range of potential applications.

Up to now, “low cost” biomaterials have been obtained. Their main applications have been: as filler, re-tanning agents and finishing agents in the tanning industry itself; and as a binder in the paper industry, partially substituting casein (much more expensive). The objective of the present work is the extraction, characterisation, optimisation and application of new “taylor-made” smart biopolymers with high-added value, finding a new and feasible link between solid tannery waste and the rising market of tissue engineering.

Tissue engineering can be defined as an interdisciplinary field which applies, for one side, the principles of tissue engineering and, for another side, the sciences of life, with the aim of obtaining “Biological Structures” in order to regenerate and/or improve the tissue function. Although lots of synthetics biodegradable or bio-stable polymers have been employed on these “special structures”, the affinity of the grafted celllies is quite low. Biologically derived materials are advantageous in that they contain information that facilitates cell attachment and function, whereas synthetics may not interact with cells in the desired manner. The importance and special appeal of collagen as a biomaterial is based on the fact that collagen is a natural material and therefore it is assimilated by the human/animal body as a normal constituent and not as a foreign material, subjected to rejection, with a minimum of immunogenicity. A great competitiveness of reconstituted collagen fibres in the field of regenerative medicine (tissues and/or organs) has been found in literature.

Biopolymers are polymers generated from renewable resources, often biodegradable and from non-toxic production. They can be produced from biological systems or chemically synthesised from biological raw materials. They are an alternative to the petrol-based polymers. The main problems of biopolymers are bio-compatibility, mechanical properties and adaptability. Collagenic biopolymers present huge possibilities due to the possibility of manufacture, and application, in different ways, forms and shapes, with well determined characteristics. We can talk about “taylor-made” biopolymers: it is possible to produce easily said biopolymers as gel, film, fibres, tissue and/or sponges, using techniques such as freeze drying/lyophilisation, extrusion, or electro-spinning for nano-fibres formation.

In addition to the technical and scientific benefits obtained from the isolation of biopolymers from solid waste, this research could entail different economical benefits: in the first place, it presents a solution to a problem of dumping/storage of wastes, avoiding taxes for accumulating those wastes. Secondly, whole hides of low quality can be used as raw material, those hides, catalogued as a 4th-5th class, would be used to produce low quality articles of very low price on the market; however, the biopolymer extracted from this hide would have a high-added value.

Thirdly, the treatment process is simple and cheap; environmentally and economically much more plausible than other treatments such as incineration, land-filling, etc. Finally, a wide range of potential applications for the produced bio-products could be taken into consideration; with specific applications on medicine, veterinary and/or cosmetics, expanding field nowadays.

The technology to be used on the development of this research is focused on the production of macro-fibres (extrusion) and nano-fibres (electro-spinning), films, sponges (lyophilisation) and different types of scaffold material for tissue engineering.

The use of mathematical experimental designs permits to study the degree of significance of the different variables and the corresponding interaction between them in the different processes for obtaining collagenic biopolymers. This ensures that the experimentation can be rationalised and the optimum determined, being able to achieve a controlled production of “taylor-made” biopolymers for each specific application.

The versatile properties of collagen have made collagenic biomaterials one of the most useful materials for tissue engineering. Those biomaterials can be in the form of and shape of natural tissue, porous scaffolds/sponges, fibres and gels. Reconstituted collagen fibres, and fibre networks have been shown to be a competitive biomaterial for soft and hard tissue replacement due to their advantageous properties. Those fibres have been used as well as a suture material. It has been postulated that such fibres could be knitted or woven into fabrics, although the production is difficult due to the large amount of material required. The traditional process for formation of collagen fibres involved the extrusion of collagen dispersions into a fibre formation buffer and subsequent solvent dehydration, air-drying and cross-linking.

**Fig. 1** Collagenic biopolymer extruded fibre. **Fig. 2** Collagenic biopolymer extruded fibre.

Collagen sponges are generally formed by freeze-drying an aqueous collagen solution. The freeze-drying process includes freezing a collagen gel
solution at a low temperature and subsequent sublimation of the ice crystals by vacuum at low temperature. The freezing temperature and freezing rate will have some effect on the porous structure of the resulting sponge.

- 2\textsuperscript{nd} Step _ Production of collagenic biopolymers: The biopolymer extraction, the most important part of the whole process, is carried out in a stainless steel jacketed stirred reactor (R-120). The grounded hide is submitted to a mild controlled hydrolysis reaction; then, by means of a pump (P-121) is driven to filter unit (S-125), where the suspension particles are separated from the viscous collagenic solution.

- 3\textsuperscript{rd} Step _ Ultrafiltration: The ultrafiltration is carried out by a combined sequentially connected set of three membrane-based tangential flow filtration spiral-wound modules of different cut-off ranges: 1kDa (U-141); 50kDa (U-142) and 100kDa (U-143). In each one of these subunits, the retentate fraction feeds the next subunit and the correspondent permeate fraction is kept apart. At the end of this 3\textsuperscript{rd} step, four molecular weight collagenic biopolymer fractions were isolated: 1kDa; 1–50 kDa; 50–100kDa and over 100kDa.

- 4\textsuperscript{th} Step _ Freeze-Drying: Each one of the four ultrafiltration fractions must be freeze-dried (lyophilisation) in order to keep their original structural and chemical properties. As shown on Figure 7, each unit of lyophilisation equipment was composed by the following parts: freezer (D-); condenser (E-); vacuum pump (V-) and storage tanks (T-).
The research activities of the group are focused to develop and implement cleaner technologies to attain a more environmentally friendly leather industry and to study and develop end-of-pipe approaches to eliminate the main pollutants present in tannery waste waters in an attempt to reduce the contamination produced.

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Development of Non-Contaminant Industrial Processes

The technical limitations and the considerable environmental impact of the conventional fungicide compounds (mainly TCMTB), reinforce the need to look for new fungicides to replace them. These alternatives to the fungicides conventionally used in the tanning industry should have a high efficiency towards a wide range of fungi and should be less toxic, more environmentally friendly and cost effective. With this aim, the fungicidal capacity of different selected compounds (registered in the 98/8/EC Directive) such as: diiodomethyl-p-tolylsulfone (DIMPTS), 3-iolo-2-propynyl-N-butylcarbamate (IPBC) and 2-thiazol-4-yl-1H-benzo imidazole, thiobendazole (TBZ) against different strains of fungi was studied in comparison with that of TCMTB and a mixture of phenolic compounds. It was found that low offers of two of the alternative fungicides studied (DIMPTS and IPBC) conferred satisfactory mould growth resistance to the treated wet-blue leather, resistance which was higher that that conferred by conventional compounds.

The simultaneous determination of TCMTB and seven other fungicides in hides and leather was achieved by applying easily available techniques such as HPLC with photo diode array (PDA) detection with previous extraction with acetonitrile
assisted by ultrasounds. In the last two years, there has been in Europe a rise in skin allergy and dermatitis due to goods of an Asian provenance that have been treated with dimethylfumarate (DMFU). There was a need for developing an analytical method to determine this substance in leather and footwear. Accordingly, a method has been developed that consists of two steps. In the first one, DMFU is detected in leather and footwear by applying manual headspace solid-phase micro-extraction and gas chromatography-mass spectrometry (GC-MS).

In the second step, the samples in which DMFU is detected are analysed by a solid-liquid extraction with acetone after which DMFU is quantitatively determined by GC-MS.

With the aim of developing end-of-pipe approaches to reduce the contamination load of tannery wastewaters, the recovery of solubilized proteins in the beamhouse operations for a hair-pulping process was studied. The precipitation of proteins at the isoelectric point was preferred to ultrafiltration since this suffers from several problems. The wastewaters of soaking, unhairing-liming and washings are those that offer higher prospects of the reduction of the contaminant load and the production of a valuable material. The isoelectric precipitation of solubilized proteins resulted in a major diminution of COD values and protein content.

Emulsified and suspended fats in wastewater from hide fleshings experienced co-precipitation with proteins, increasing COD diminution. Another important result was the drastic decrease in the toxicity of the wastewater due to the elimination of a bactericide added in the initial stages of the beamhouse process. This represents an important saving on the cost of wastewater treatment and associated taxes. The potential use of amino acids obtained by acid hydrolysis of the precipitated protein fraction for the production of amino acid-based surfactants as well as the application of this protein material as a retanning agent for tannery is currently being investigated.

The removal of vegetable extracts (polyphenols) which are present in aqueous solutions at the highest concentration of 2.0 g/L by tannery shavings was studied. It was found that tannery wastes such as chrome and wet white shavings were good adsorbents of polyphenols in aqueous solutions.

The adsorption capacity of wet white shavings for polyphenols was higher than that of chrome shavings. The adsorption isotherms exhibited Langmuir behaviour, indicating monolayer coverage. Thermodynamic parameters indicated that the adsorption process under study was exothermic and spontaneous. A pseudo-second order kinetic model satisfactorily described the adsorption of polyphenols onto tannery shavings.

Adsolubilization has been defined as the incorporation to solid-water interfaces of molecules that do not spontaneously adsorb to such interfaces, but can be incorporated through some type of interactions with an adsorbing surfactant molecule. The adsolubilization phenomenon may take place on fibrous collagen with different types of organic molecules. It was found that the adsorption of an anionic surfactant (sodium dodecylbenzene sulphonate, SDBS) onto hide powder collagen in an aqueous acidic medium allows the aggregation of other organic molecules that in the absence of the surfactant are not bound to the protein. The anionic surfactant is bound to the protein in the form of micelle-like aggregates termed admicelles that permit the incorporation of other molecules in a process called adsolubilization.

The adsorption of the SDBS anionic surfactant on hide powder collagen and the adsolubilization of other molecules such as 2-naphtol, two basic dyes (pararosaniline and hexamethyl-pararosaniline) and a non ionic surfactant that did not adsorb by themselves to the protein in the conditions studied. Benzyl alcohol was not significantly adsolubilized on hide powder collagen. The hydrophobicity of the molecules played a major role in the adsolubilization phenomenon.
Research work is focused on the study of structure-property relationships of natural, synthetic and sustainable fibrous materials, particularly with regard to thermal, mechanical, viscoelastic and relaxation behaviour. The influence of novel more sustainable industrial processing on the structure and properties of fibrous materials are also taken into account.

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Statistical Modelling and Fibre Physics

Adsolubilisation of organic compounds onto collagen fibres.
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Protein Biochemistry, Synthesis, Structure and Cellular Functions Series
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Research highlights
Stabilisation of Polylactide Multifilaments
Polylactides (PLA) are biodegradable, biocompatible and hydrolysable aliphatic polyesters that can be wholly obtained from renewable resources. Nature derived lactides are mostly in L-lactide form and exhibit crystalline behaviour. The microstructure of the multi-filaments is not easy to be controlled. As regards the industrial application of polylactide filaments the most important objective has been focused on the stabilisation of filaments considering the dimensional stability and the evolution of mechanical properties and dyeing behaviour.

Different post-setting treatments have been performed and the evolution of both the macromolecular orientation into the filament measured by sonic velocity SV and crystallinity measured by differential scanning calorimetry X_DSC enabled us to optimize the stabilization temperature:

<table>
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<th>T:</th>
<th>75°C</th>
<th>80°C</th>
<th>90°C</th>
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<tr>
<td>SV</td>
<td>2.0 km s⁻¹</td>
<td>2.4 km s⁻¹</td>
<td>2.5 km s⁻¹</td>
</tr>
<tr>
<td>X_DSC</td>
<td>26.7%</td>
<td>36.4%</td>
<td>39.4%</td>
</tr>
</tbody>
</table>

Sorption/desorption kinetics of cellulosic fibres
The parallel exponential kinetics model have been used to model the fast sorption and desorption processes that occurs on easily accessible sites and the slow sorption and desorption process occurring at hardly accessible sites.

![Sorption/desorption kinetics of cellulosic fibres](image)

Materials with similar sorption/desorption isotherms can be identified by the fraction of easily/hardly accessible sites.

Moisture sorption/desorption of different cellulosic fibres (Cabuya, Sisal, Jute, Kenaf, Luffa, Hemp, Flax) subjected to different treatments (retting, chemical and enzymatic scouring) have been
studied. All treatments influence the crystallinity that can be estimated through water retention.

**Drying kinetics**

Drying kinetics detect variations in fine structure of fibres, especially those induced by mechanical stresses in dry and wet thermal treatments. The decrease in mass of a completely wet sample when subjected to a drying isotherm at 97°C enables to determine the evaporation rate of covering water, and water contained in meso- and micropores. The first derivative gives the evaporation rates and when plot against humidity content yields the following characteristic plot:

The effect of cracking on polyamide 6.6 was identified by this technique that results in accordance with the SEM plots.
Biocompatible Surfactants

The activity of this research group deals with the fundamental and applied chemical investigation of novel environmentally friendly surfactants (products and processes) from natural renewable sources (proteins, polysaccharides, amino acids and natural oil derivatives), as alternatives to conventional surfactants to be applied in cosmetic, textile, dermo-pharmaceutical medical and food industrial preparations. These compounds can be classified as specialty surfactants with biodegradable, antimicrobial and low toxicity profiles, and characteristic self-aggregation properties. The objectives are focused on the preparation of safer and healthier surfactants using molecular design and the principles of toxicity and environmental mechanism of action to minimise the intrinsic toxicity/ecotoxicity of the product while maintaining its efficacy and function. This line is loosely-bound with applied surface chemistry and biological area. It is active in the following tasks: the use of renewable raw materials for the synthesis of surfactants: proteins, polysaccharides, triglycerides; Employing natural processes using biocatalyst based chemical transformations (enzymes) for efficiency and selectivity; the use of safer solvents (water systems, solvent-free processes, Ionic liquids, etc.); study of mechanism of cellular action; novel functionality: bio/nano materials; self-assembling and ecotoxicity characterization.

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Biocompatible surfactants from renewable hydrophiles.
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Chemical hydrophobic modification of inulin in aqueous media: Synthesis of \( \beta \)-hydroxyalkyl ethers of inulin.
Morros, J., Levecke, B., Infante, M.R.
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ISBN: 978-1-61761-981-6
Research highlights

For the first time, we reported a novel class of multichain lysine-based cationic amphiphilic derivatives of the type N(epsilon),N(epsilon)'-bis(n-acyloxypropyl)-l-lysine methyl ester salts (patent protected).

The research of biocompatible surfactant group relates to novel compounds having an amphiphilic character (cationic, anionic, amphoteric and non-ionic surfactants), which are intended to be used in the food, pharmaceutical and cosmetic industries as surface-active agents having a rich self-assembling, antimicrobial and low toxicity properties. Due to their interesting properties these compounds have been transferred to the industry.

At present, cationic surfactants are being tested in new biomedical applications, such as drug delivery systems in cationic vesicles.

In this field it is necessary to strike a balance between antimicrobial activities on the one hand and low toxicity and efficient biodegradability on the other. In this sense we have designed a new family of cationic surfactants from lysine, one chain/one head, one chain/two heads, and two chains/two heads with moderate antimicrobial activity and excellent non-haemolytic behaviour. The acute toxicity against Daphnia magna and biodegradability tests revealed that all three surfactants from lysine can be classified as readily biodegradable surfactants.

Surfactant/phospholipid mixtures are important in many applications, including emulsion and foam stabilization, lung surfactants and the stability of cell membranes. Acyl-glycerol amino acid conjugates constitute a class of specific lipo amino acid surfactants sharing properties with glycerides and phospholipids.

They consist of two aliphatic chains and the arginine amino acid as polar head, linked together through ester bonds in the glycerol backbone. The studies of the adsorption at the air liquid interface of diacyl glycerol derivatives and their mixtures with phospholipids helped to understand the complex mechanism of interaction with cell membranes. The results obtained with catanionic formulation acyl-glycerol amino acid surfactants/phospholipids suggests that these products are excellent candidates for developing new surfactants with tunable, well-defined properties for medical and biotechnological applications. Our results might be considered as a proof of principle of a strategy which reduces the toxicity of many surfactants, opening possibilities into clinical applications.
Environmental Chemistry of Surfactants and Ionic Liquids

The main objective is the study of the physicochemical and biological properties related to the behaviour, fate and effects of surfactants and ionic liquids in the environment for the design and selection of environmentally friendly compounds. Our research activities are mainly focused on the bioavailability, biodegradability and toxicity of surfactants and ionic liquids in the aquatic environment.

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Research highlights

Biodegradability of Ionic Liquids

Ionic liquids (ILs) are deemed greener solvent alternatives in chemical synthesis mainly because of their negligible vapor pressure, high thermal stability, low flammability and reusability in chemical applications. They are also known to have an influence on the rate and selectivity of certain chemical reactions. As research in the area of ILs continues to grow, the domain of their applications has substantially broadened. The non-volatility of ILs under operational conditions minimizes their impact on air quality during their life cycle. However, their impact on soil and water is certainly of considerable concern at the time of their disposal. Research in this area is currently vital as ILs are likely to make a transition from academic laboratories to large scale operations where disposal of any chemical is a major concern. The evaluation of the environmental impact of ILs can, in part, be gauged by parameters such as biodegradability and toxicity. Enormous structural variations are possible in the ILs by changing either the cation and/or the anion. This leads us to believe that it should be possible to manipulate their chemical architecture to achieve high biodegradability. In collaboration with Professor Peter Scammells (Monash University) research group, different structural parameters promoting biodegradation of ionic liquids commonly used as reaction media have been identified. The increase of biodegradability promotes the removal of these compounds avoiding their persistence in the environment once their function has finished. ILs with a pyridinium cation were synthesized and their biodegradability was evaluated using the CO₂ headspace test (ISO 14593). ILs bearing an ester side chain moiety were prepared from either pyridine or nicotinic acid and showed high levels of biodegradation under aerobic conditions and can be classified as ‘readily biodegradable’. This presents the possibility that substituted pyridinium rings lead to metabolites that are not refractory upon biodegradation. The study also demonstrates that the structural manipulation of the pyridinium skeleton may lead to ILs likely to possess good solvent attributes and a predisposition to biodegrade when released into an aquatic environment.

Surfactant-like behaviour and antimicrobial activity of Ionic Liquids in aqueous solution

Amphiphilic imidazolium and pyridinium based ILs behave as conventional cationic surfactants in aqueous solution reducing the surface tension to 37-42 Nm/m. There is no significant difference between imidazolium and pyridinium ILs regarding surface activity and aggregation behaviour in aqueous solution which indicates a similar polarity of the methylimidazolium and pyridinium headgroups. In the homologous series of ILs investigated the tendency to micellize increases and CMC decreases regularly with the length of the alkyl tail attached to the polar headgroup. Thus, the major driving force of the micellization of these amphiphilic imidazolium and pyridinium cations seems to be the hydrophobic interaction between their alkyl tails.

The amphiphilic ILs studied displayed antimicrobial activity. The length of the alkyl side chain determines the efficiency of these ILs as antimicrobial agents. The compounds with short alkyl substituents are not active against bacteria and fungi whereas the ILs containing 10-14 C atoms in the alkyl chain show significant antimicrobial activity, the C₁₄ being the most active compounds. In addition to their unique physical properties as ionic liquids, amphiphilic imidazolium and pyridinium ILs have antimicrobial activity and surfactant-like behaviour. The improved understanding of the structural parameters affecting self-aggregation and biological activity of the long chain ILs is expected to aid in the design and selection of ionic liquids with better physicochemical and biological properties for new pharmaceutical, engineering or nanotechnology applications. These results are also significant to the environmental fate assessment of these compounds as the interfacial phenomena play a crucial role in the biodegradation processes due to changes in affinity and availability of the ionic liquids in the intercellular spaces.

Interactions between Conventional Surfactants and ILs

One of the most outstanding properties of ionic liquids (ILs) is its very low volatility that prevents environmental air pollution and consequently makes them candidates to substitute volatile organic solvents in different application fields. Accordingly with its claimed role of “green solvents”, a wide series of studies where typical ionic liquids are used as dilution media of conventional surfactants are reported. In some of these studies the surfactant is dissolved in the ionic liquid as unique solvent, whereas in others the solvent media is made of a fixed concentration of ionic liquid in water. In recent studies, we put in
evidence that even for short alkyl chain ionic liquids, a process of aggregation in aqueous solution took place. Consequently, when a surfactant is dissolved in an aqueous solution containing ionic liquid, the role of this compound as a secondary surfactant should also be considered. Then, we claimed that these systems should be treated as the typical binary surfactant systems in aqueous solution, in which case the phenomena of synergism frequently occur. One of the research lines of our group is devoted to the study of binary systems made of conventional surfactants of different families (non ionic, anionic, cationic…) and typical ionic liquids in aqueous solutions from this point of view. We planned these studies considering the total concentration of surfactant and ionic liquid, combined at different mole ratios. Then, the surfactant parameters obtained should not be attributable solely to the surfactant, but to the mixed micelles formed between the surfactant and the ionic liquid. This approach can contribute to a better understanding of the experimental results reported when only the role of solvent is considered for the ionic liquid.
The general subject of research is the physical chemistry of surfactants and surfactant based systems. Particular focus is given to dynamic transformations (emulsification and solubilisation) and to new biocompatible surfactant behaviour. The main techniques are SAXS-WAXS, light scattering, tensiometry, conductivity and selective electrode.

**STAFF**
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**TECHNICIANS**
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**Publications (articles)**

**Novel biocompatible DNA gel particles.**
Morán, M.C., Infante, M.R., Miguel, M.G., Lindman, B., Pons, R.
*Langmuir* 26 10606-10613, 2010

**Application of bicellar systems on skin: Diffusion and molecular organization effects.**
Rodríguez, G., Rubio, L., Cóceres, M., Estelrich, J., Pons, R., De La Maza, A., López, O.
*Langmuir* 26 10578-10584, 2010

**Headgroup effects on the unusual lamellar-lamellar coexistence and vesicle-to-micelle transition of salt-free catanionic amphiphiles.**
Silvas, B.F.B., Marques, E.F., Olsson, U., Pons, R.
*Langmuir* 26 3058-3066, 2010

**Dynamic properties of cationic diacyl-glycerol-arginine-based surfactant/phospholipid mixtures at the air/water interface.**
Lozano, N., Pinazo, A., Pérez, L., Pons, R.
*Langmuir* 26 2559-2566, 2010

**Structure of aggregates in diluted aqueous octyl glucoside/tetraethylene glycol monododecyl ether mixtures with different alkanols.**
Pons, R., Valiente, M., Montalvo, G.
*Langmuir* 26 2256-2262, 2010

**Biocompatible surfactants from renewable hydrophiles.**
Infante, M.R., Pérez, L., Morán, M.C., Pons, R., Mitjans, M., Vinardell, M.P., Garcia, M.T., Pinazo, A.

**Arginine diacyl-glycerolipid conjugates as multifunctional biocompatible surfactants.**
Pinazo, A., Lozano, N., Pérez, L., Morán, M.C., Infante, M.R., Pons, R.
*C.R. Chim.* 14 726-735, 2011

**Amino acids as raw material for biocompatible surfactants.**
Pinazo, A., Pons, R., Pérez, L., Infante, M.R.

**Diacyl glycerol arginine-based surfactants: Biological and physicochemical properties of catanionic formulations.**
Lozano, N., Pérez, L., Pons, R., Pinazo, A.
*Amino Acids* 40 721-729, 2011

**Isolation and partial characterization of a biosurfactant mixture produced by Sphingobacterium sp. isolated from soil.**
*J. Colloid Interface Sci.* 361 195-204, 2011
Publications (books and book chapters)

Pons, R., Moran, M. C., Infante, M. R., Pinazo, A., Pérez, L.
**Lysine-Based Surfactants.**
in *Colloids in Biotechnology* (ed. M. Fanun)
Surfactant Science Series, Vol. 152, 2010
CRC Press (Taylor and Francis).
ISBN 9781439830802

Moran, C., Pérez, L., Pons, R., Pinazo, A., Infante, M.R.
**Amino Acids, Lactic Acid and Ascorbic Acid as Raw Materials for Biocompatible Surfactant.**
in *Surfactants from Renewable Resources* (eds. M. Kjellin, I. Johansson), Ch. 5, 85-107, 2010
John Wiley & Sons, Ltd, Chichester, UK.

De Persis, F., Pons, R., Pucci, C., Tardani, F., La Mesa, C.
**Binding of Protein-Functionalized Entities onto Synthetic Vesicles.**
InTech.

Research highlights

In recent work, special effort has been devoted to the determination of structures formed by biobased surfactants obtained from the linkage of lysine or arginine with hydrophobic tails. Those studies stem from the collaboration with the Biocompatible Surfactants Group. In particular diacyl glycerol derivatives mimic the phospholipids present at membranes. Particularly relevant is the effect of small amounts of diacyl glycerolipids on the adsorption characteristics of phospholipids with a newly found boosting effect for surface tension reduction. Also natural biosurfactants obtained from bacterial growth have been studied in collaboration with the faculty of Pharmacy of the University of Barcelona.

Catanionic surfactants and mixtures show some interesting and amazing phenomena. In the phase behaviour of catanionic surfactants (1:1 catanionic mixtures without simple counterions) the coexistence of two lamellar phases was established in collaboration with the University of Porto. Catanionic vesicles have also been used as a model membrane for the study of the interaction of protein functionalised nanoparticles with bilayers. This complex subject has been undertaken within the collaboration with the University of Rome La Sapienza. Other lamellar phases of interest are constituted by nonionic surfactants of the polyethylene-glycol type which can incorporate different amounts of alcohols in the bilayers with changes in their thickness and in the extension of the bilayers. Those surfactants have been studied in collaboration with the University of Alcalá.

The interaction of cationic surfactants with anionic natural polymer (for instance DNA) form precipitates. Those precipitates can be used to form particles which can release DNA. These systems have been studied in collaboration with the University of Coimbra. Those non viral vectors are one of the DNA transfection paths that are currently explored. Our investigation has focused on the structure of the aggregates and its influence on the release kinetics. Linkage differences in the headgroup amino acid of lipoamino acids show strong influence in the packing and, consequently, on the release kinetics. Those differences have been studied by SAXS and GISAXS. In the examples below, isotropic precipitates and strongly oriented precipitates at full hydration are shown.

![Fig. 1 Oriented Sample GISAX pattern at full hydration.](image1)

![Fig. 2 Unoriented Sample GISAX pattern at full hydration.](image2)

Related to research using Small Angle X-Ray Scattering, a controlled atmosphere setup for use with the GISAXS configuration has been patented.
The main research lines of this group are: lipid assembling (liposomes, micelles, bicelles and bilayers), lipokeratinic tissues (skin, wool and human hair), percutaneous absorption and physicochemical characterization of colloids with potential industrial applications.

**Publications**

**Effect of wool keratin proteins and peptides on hair water sorption kinetics.**

**Surface-active properties of lipophilic antioxidant tyrosol and hydroxytyrosol fatty acid esters: A potential explanation for the nonlinear hypothesis of the antioxidant activity in oil-in-water emulsions.**

**Skin delivery of caffeine contained in biofunctional textiles.**

**Skin efficacy of liposomes composed of internal wool lipids rich in ceramides.**

**Water absorption/desorption of human hair and nails.**

**New anionic surface-active agent derived from wool proteins for hair treatment.**

**Influence of internal lipids on dyeing of wool fibres.**

**Bicellar systems for in vitro percutaneous absorption of diclofenac.**

**Bicosomes: Bicelles in dilute systems.**

**Application of bicellar systems on skin: Diffusion and molecular organization effects.**

**Synthesis and characterization of phenolic antioxidants with surfactant properties: Glucosyl- and glucuronosyl alkyl gallates.**

**Structural effects of flufenamic acid in DPPC/DHPC bicellar systems.**
Barrier function of intact and impaired skin: Percutaneous penetration of caffeine and salicylic acid.

Enzymatic synthesis of α-glucosides of resveratrol with surfactant activity.

Water sorption of nails treated with wool keratin proteins and peptides.

Liposome as dispersing agent into disperse dye formulation.

Synthesis and properties of ascorbyl esters catalyzed by lipzyme TL im using triglycerides as acyl donors.

Biofunctional textiles prepared with liposomes: In vivo and in vitro assessment.

Characterisation of skin states by non-crystalline diffraction.

Research highlights
Some of the main results of our group in the field of biomembranes refer to the scientific novelty related to the use of bicellar systems in cosmetic and pharmacologic skin applications. Bicelles are bilayered nano-aggregates formed by long and short chain phospholipid compounds dispersed in aqueous solution, which have proven to be interesting membrane-mimicking systems to investigate the structure of membrane proteins.

The above schematic representation shows lamellar phase bicelles:

(A) Perforated lamellae morphology of magnetically aligned dimyroryl-phosphatidylcholine/dihexanol-phosphatidyl-choline (DMPC/DHPC) bicelles consisting of both planar and high-curvature regions. DMPC and DHPC are represented by the yellow and red colours, respectively.

(B) Schematic representation of DHPC undergoing fast exchange between the planar and highly curved toroidal pore regions, as indicated by the arrows.

Structural versatility of bicellar systems and their possibilities as colloidal carriers.

Bicellar systems as modifiers of skin lipid structure.

Damaged retrieval with ceramic rich liposomes.

Publications (books and book chapters)
Barba, C., Martí, M., Roddick-Lanzilotta, A., Manich, A., Carilla, J., Parra, J.L., Coderch, L.

Martí, M., J Parra, J.L., Coderch, L.
Lipid Role in Wool Dyeing. in Natural Dyes (ed. E. Perrin Akçakoca Kumbasar) Ch. 5 80-100, 2011

Barba, C., Scott, S., Roddick-Lanzilotta, A., Parra, J.L., Coderch, L.
Keratin Proteins and Peptides from Wool, for Hair Restoration. in Advances in Medicine and Biology Vol. 5 (ed. L.V Berhardt) Ch. 13 237-242, 2011

The above schematic representation shows lamellar phase bicelles:

(A) Perforated lamellae morphology of magnetically aligned dimyroryl-phosphatidylcholine/dihexanol-phosphatidyl-choline (DMPC/DHPC) bicelles consisting of both planar and high-curvature regions. DMPC and DHPC are represented by the yellow and red colours, respectively.

(B) Schematic representation of DHPC undergoing fast exchange between the planar and highly curved toroidal pore regions, as indicated by the arrows.
According to our investigations, bicelles interact with the microstructure of the stratum corneum, affecting some of the biophysical properties of the skin. Thus, topical in vivo application of DMPC/DHPC bicelles improve skin permeation and elastic parameters and decreased skin hydration without promoting irritation and without affecting stratum corneum lipid microstructure. The increase of permeability was possibly due to changes in the stratum corneum lipids phase behaviour.

In order to deepen the interpretation of these results, we investigated the effect of these bicelles in stratum corneum in vitro using attenuated total reflectance-Fourier transform infrared spectroscopy technique. It is noteworthy that bicelles caused a phase transition from the gel or solid state to the liquid crystalline state in the lipid conformation of SC, reflecting the major order-disorder transition from hexagonally packed to disordered chains. Grazing incidence small and wide X-ray scattering (GISAXS and GIWAXS) techniques also confirmed this effect that may be probably associated to the permeabilizing effect described for these bicelles.

On the other hand, these bicelles are also able to incorporate ceramides up to 20% forming elongated or tubular structures and vesicles that grow with temperature. The four next TEM micrographs show 20%-Cer samples cryofixed using high-pressure freezing at 40 °C. In panel A, the black arrow points to a multilamellar tubule. Panel B images a cross-fracture of the tubules. Panels C and D show vesicles with sizes over 500 nm mixed with tubules with sizes varying in a large range (white arrows).

In general terms, the inclusion of ceramides in these bicelles offers the possibility of improving the current knowledge about many physiological processes associated with ceramides and give new insights for the role played by this lipid in biological cells at membrane level.

In the following two micrographs, it may be seen that bicelles formed by dipalmitoyl-phosphatidylcholine (DPPC) and DHPC are also able to penetrate the stratum corneum in vitro, to grow and to form vesicles inside the intercellular lipid spaces. This growth was also observed when bicelles were diluted with water. These changes resemble micelle-to-vesicle transitions of the lipid-surfactant systems.

The absence of surfactant in the bicellar composition and their small size gives great advantages to these structures in comparison to other systems for skin purposes. The good penetration, high skin compatibility and their ability to modulate the barrier function make bicelles a smart nano-system with promising applications as drug carriers through the skin.

In addition, bicelles can also incorporate other lipid species such as those present in skin (cholesterol sulfate), or drugs (flufenamic acid, diclofenac, enrofloxacin, mycostatine).

Biofunctional Textiles

In recent years, new technologies have led to the production of biofunctional textiles. These textiles are able to release therapeutic compounds or cosmetics to the skin. The biofunctional textiles contain microscopic capsules of ingredients that break as the fabric rubs the skin, releasing the actives. Absorption and desorption behaviour of active agents embedded into the different biofunctional textiles should be taken into account when determining the amount of active agents incorporated into these textiles and when following the delivery mechanism as the fabric comes in contact with the skin. This group was working into this subject, preparing biofunctional textiles in order to know what exactly happen when textiles comes in contact with human skin, and to quantify the actives.

Microcapsules or liposomes were used as vehicles. Liposomes were prepared with wool lipid (WLI) extracts enriched with ceramides. Liposomes and microcapsules containing different active principles were applied on textile fabrics. As an active principle, the ceramides present in the internal wool lipids have been used and as reference compounds caffeine and a sun filter (ethylhexyl methoxyccinnamate) have been also used as tracers. The demonstration of the active principle release by a close textile-skin contact,
using a new specific design of percutaneous absorption was carried out (see figure).

The passage of the active principle through different skin layers have been detected "in vitro". In this research textiles were applied onto volunteer forearms to prove if there were some benefits for the skin by non invasive techniques such as Tewameter and Corneometer as well as to detect the active compound in the stratum corneum by stripping method. From the results obtained, it has been demonstrated the skin effectiveness of an active compound encapsulated and applied onto a fabric when it is topically applied. IWL liposomes from the biofunctional textile increased the level of skin hydration and decreased the TEWL values. On the other hand, the sun filter has been detected in the outermost layers of the stratum corneum.

This group also does research into cosmetic field, studying changes in the properties of human keratin fibers, such as hair and nails due to water presence. Reactive cosmetic treatments of hair and nails often impair fiber structure, resulting in an adverse effect on water absorption. The moisture absorption/desorption isotherm curves for untreated hair and nails and the kinetics of these processes are studied in this research.

The effects of different chemical cosmetic treatments on hair and nail water absorption are also evaluated. The isotherms for these human keratinized tissues behaved as expected, with a characteristic hysteresis between moisture uptake and desorption. Human nails showed a lower moisture regain and a much lower diffusion coefficient with respect to human hair. Permeability, directly related to the diffusion coefficient, increased with the degradation treatment. The diffusion coefficient was important in determining the integrity of keratin fibers.
6

FACILITIES
AND
TECHNOLOGY TRANSFER
IQAC FACILITIES AND TECHNOLOGY TRANSFER

- Characterization of Colloidal Dispersions Service
- Custom Antibody Service (CAbS)
- Organic Microanalysis Service
- Biodegradation and Aquatic Toxicity Service
- Magnetic Resonance Service
- Skin Absorption and Skin Efficacy Services
- SAXS-WAXS Service
- Synthesis of High Added Value Molecules Service
- Thermal Analysis and Calorimetry Service
- Proteomics Service
- Technology transfer
Characterization of Colloidal Dispersions Service

This service deals with the characterization of nano-structured liquids (e.g. micelles, vesicles, liquid crystals, microemulsions, nanoemulsions etc.) and solid dispersions (e.g. organic inorganic or hybrid nanoparticle suspensions).

The characterization implies determination of size, morphology, phase transitions, surface, interfacial and rheological properties.

The group responsible of the service is member of TECNIO (ACC10, CIDEM/COPCA) and has been awarded with a quality certificate (similar to ISO 9001) by CIDEM (Generalitat de Catalunya).

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Relevant techniques:

- Static (SLS) and dynamic (DLS) light scattering
  Determination of particle size distribution, shape, diffusion coefficient, aggregation number, molecular weight of colloidal dispersions

Other techniques.
Laser Light Diffraction
Light back scattering
Zetameter
Differential Refractometry
Tensiometry,
Optical Microscopy

Rheology
Determination of rheological properties of fluids and soft matter in flow and deformation regimes by steady state (viscosity, shear thinning, shear thickening) and dynamic (elastic and viscous moduli, relaxation time) measurements

Electrophoretic mobility
Determination of Zeta potential of charged particles

- Electrophoretic mobility

Variation of Zeta potential as a function of pH

Variation of elastic ($G'$) and viscous ($G''$) moduli as a frequency function

Size distributions of mixed micelle and vesicle dispersions by dynamic light scattering
Custom Antibody Service

The CAbS is a joint facility established under the umbrella of the IQAC-CSIC and CIBER-BBN. The facility wants to offer a high quality service for customized monoclonal and polyclonal antibody production against many types of antigens including proteins, peptides or small organic molecules. Moreover, CAbS can offer additional services related to the preparation of immunoreagents and development of immunochemical methods and protocols.

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Detailed description of the services and features provided by CAbS

A) MONOCLONAL ANTIBODY DEVELOPMENT
The standard service includes:
1. Discussion of the project (screening system, selection criteria, etc.) and planning the work.
2. Immunization, cell fusion, screening and cloning: After their fusion with myeloma cells screening of the best hybridomas will be performed by ELISA using previously supplied antigen. Specific clones will be subcloned by limiting dilution.
3. The customer will receive two cryovials and 10 ml of culture supernatant of each positive clone.

B) POLYCLONAL ANTIBODY DEVELOPMENT
The standard service includes:
1. Discussion of the details of the project including features such as the type of immunogen, the final properties of the antibodies, and the species and number of animals used.
2. Immunization protocol: As accorded by the customer.
3. Isolation of the antiserum

4. ELISA testing: samples obtained on each boosting injection and the final antisera will be tested against the antigen following the criteria agreed upon in the previous discussion with the customer. The customer will receive 60-80 mL of the final serum from each rabbit and about 5 mL samples of the pre-immune serum, and the blood extractions made during the immunization protocol after each boosting injection.

C) ADDITIONAL SERVICES:
1. Preparation of bioconjugates: labelled antibodies, haptenized proteins and enzymes, biotynilated and fluorescent probes, gold nanoparticle conjugates, etc.
2. Antibody purification.
3. Development of immunochemical methods: ELISA, immunoaffinity columns, etc.
5. Hybridoma cryopreservation.
6. Mycoplasma testing.

Unless otherwise stated in a signed agreement, the property of immuno (bio) reagents produced or synthesized and the results obtained regarding establishment of immunochemical methods and procedures will belong to the costumer.
Organic Microanalysis Service

The Organic Microanalysis Service provides micro-determination of total carbon, hydrogen, nitrogen, sulphur, oxygen (C, H, N, S, O) and halogens present in a wide range of organic and inorganic compounds.

Since March 1999, Microanalysis Service has been accredited by ENAC, under EN45001 regulation. This was the first accredited elemental microanalysis by the CSIC and the first to be accredited in Spain.

As of November 2001, this Service has been accredited under regulation UNE-EN ISO/IEC 17025 for analysis of CHNS.

Accredited by ENAC: Certificate number 159/LE319

Biodegradation and Aquatic Toxicity Service

The Biodegradation and Aquatic Toxicity Service of the IQAC offers a full range of standardized test methods (OECD technical guidelines) for the assessment of the biodegradability and toxicity of organic compounds in the aquatic environment.

This service carries out biodegradation and aquatic toxicity tests for internal use and for external clients from industry, public administration, universities, and research organisms. Suitable technology and an expert and qualified staff guarantee the availability of results.

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Equipment
This facility has the appropriate instruments for accurate sample analysis. Primary Instruments:
1 Elemental Microanalyzer (AS) model Flash 1112, for C,H,N determination.
1 Elemental Microanalyzer for O determination.
1 Elemental Microanalyzer (A7) for C,H,N,S determination.
1 Perkin-Elmer Microscale (B2) model AD6.
2 Mettler Microscale (B3 and B4) models MT5 and MX5.
1 Metrohm Titrando model 808 for Cl,Br,I and F
The Magnetic Resonance Service is a research support facility for the IQAC, other universities and public research organisms, as well as for private companies. To two types of spectroscopy techniques are available:

**Nuclear Magnetic Resonance (NMR Unit):** The Unit provides access to the following state-of-the-art methodologies:
- Structure elucidation and quality control in synthetic chemistry by solution 1D/2D-NMR.
- NMR-based drug screening.
- NMR of cells, cell extracts, and metabolomics-by-NMR.
- Diffusion experiments and DOSY.

**Electronic Paramagnetic Resonance (EPR Unit):** The electron paramagnetic resonance spectroscopy (EPR) or electron spin resonance (ESR) studies the interaction of a paramagnetic species with the electromagnetic radiation (microwave radiation) in the presence of an external magnetic field and allows detecting and studying stable or transient paramagnetic species such as free radicals, some transition metal ions and defects in materials.

**Staff**

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**Lluís Fajari Aguado (EPR Unit Technical Manager)**

**Lluís Julià Bargés (EPR Unit Scientific Manager)**

**Technical Assistants**

**Montserrat Sindreu Grañé**

**Avencia Diez Ortego**

**Nuclear Magnetic Resonance Unit (NMR Unit)**

The NMR Unit has two Varian/Agilent Spectrometers:
- **Varian Mercury 400 MHz (9.3950 T)** is the walk-up instrument for automated heteronuclear NMR. The spectrometer has a VNMRS console with Direct Digital receiver with Performa-I Z gradients and OneNMR probe, which can be tuned automatically to any nucleus between $^{15}$N and $^{31}$p with ProTune System autotuning and is using Agilent's Chempack pulse sequences suitable for most routine measurements. This spectrometer delivers routine, rapid heteronuclear-detected spectra in automation ($^1$H, $^{19}$F, $^{31}$p, $^{13}$C, $^{11}$B, $^{15}$N, $^{29}$Si, $^{24}$Mg, $^{17}$O, $^{111}$Cd, $^{113}$Cd, $^{105}$Pd, $^{77}$Se, $^{27}$Al, $^{115}$Sn and $^{195}$Pt). An automated 100-sample changer (for standard 8" long/5 mm Ø NMR tubes) and VnmrJ3.2 software allow performing short acquisitions and quick access to spectra during the daytime hours (9 am to 7 pm), while longer experiments such as 2D HSQC or HMBC are submitted to run overnight or week-ends.
- **Varian Inova 500 MHz (11.7440 T field strength)** is used for kinetics, diffusion, drug discovery and variable temperature experiments (besides standard experiments). The spectrometer is equipped with a two-channel Inova console, Performa-II (60 G/cm) Z gradients, and an inverse detection AutoX probe. Is the instrument of choice for more demanding samples, and is frequently used for the full characterization of samples where tiny amounts of material are available. The 500 is using DOSY/Biopack pulse sequences and VnmrJ software 2.2D version.

**Electronic Paramagnetic Resonance (EPR Unit)**

Equipped with a Bruker EPR/ESR spectrometer EMX, with a microwave bridge of X-band (~9 GHz) EMX premium X, magnet of 10" ER073 with a power supply of 12 KW ER083. The following accessories are available: Standard or double cavity; different container samples (quartz tubes, quartz capillaries, cells, flat cells for tissue); liquid nitrogen dewar and variable temperature accessory: cryostat, liquid nitrogen transfer line (120 K ~ 373 K); intelligent temperature controller ITC 503S from Oxford Instruments; continuous flow cryostat system of liquid helium (4.2 K ~ 300 K); gas flow controller from Oxford Instruments; high vacuum unit HP4082 from Vacuubrand, "in situ" radiation source of UV-vis. 500 W Oriel pressure mercury lamp. Power supply Newport 69910; Bruker software acquisition, processing and simulation spectra WINEPR and SimFonia.
The Skin Absorption Service deals with the knowledge and quantitation of the skin absorption of a given compound applied topically. Using an in vitro methodology officially accepted by the OCDE (2004), the distribution of a chemical in the different skin compartments (stratum corneum, epidermis and dermis) can be detected and quantified. The studies of percutaneous absorption can be fundamentally of interest for the Pharmaceutical, Cosmetic, Veterinary and Chemical sectors.

**STAFF**

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The Skin Efficacy Service deals with the experimental design, evaluation and objective diagnostic of the skin efficacy and tolerance of cosmetic and dermatologic formulations topically applied by the use of non-invasive biophysical techniques. Evaluation and diagnosis of other keratinized tissues such as human nails and hair.

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ESTITXU FERNANDEZ
**Synthesis of High Added Value Molecules Service**

SIMchem (service of Synthesis of High added value Molecules) is a IQAC-CSIC research facility created in 2009 to give chemical and synthetic support to (R+D+i) activities in industry, university and public organizations. It is projected to fill the gap existing between custom synthesis performed by companies and the synthetic research groups in academy. The service is intended to give a synthetic support to research projects of chemistry, biology, biomedicine and drug discovery by providing both skilled personnel, instrumental and laboratory, and taking advantage of the chemical and synthetic expertise of the different groups present in the Institute.

The service will be devoted to the study of synthetic methodologies, the development of synthetic sequences and small scale synthesis of high added value organic compounds (milligram to gram). The type of compounds initially envisaged consist in broad scope bioactive molecules, including drug candidates, pharmacological tools and molecules directed to chemical, biological or biophysical tests in R+D activities.

Another goal of the service is to implement new efficient synthetic technologies in the host Institute, which could be employed by the research groups present in the IQAC, or external users. A special effort will be devoted to set up high safety methods of synthesis that could improve current laboratory practices in the Institute and reach a high level of competence and efficiency. SIMchem plans to reach the state-of-the-art in synthetic and preparative purification technologies that, in general, wouldn’t be available to individual groups in the IQAC.

**LINES OF EXPERTISE**

Medicinal chemistry

Heterocyclic and condensation chemistry, multistage synthesis.

Development and optimization of reactions and processes

Analytical support to organic synthesis

**CONTACTS**

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**SYNTHESIS**

Carousel reaction station.

Parallel synthesis station for solution phase chemistry and solid supported reagent based synthesis

Simultaneously heats/cools, stirs and reflux’s multiple samples under an inert atmosphere

Hydrogenation chamber

**INSTRUMENTAL TECHNOLOGIES**

**ANALYTICAL AND PURIFICATION TECHNIQUES**

Analytical and preparative HPLC

Automated flash and MPLC chromatography

**OTHER INSTRUMENTS and FACILITIES**

Systems for samples evaporation: Thermo Fisher SpeedVac and Stuart Sample Concentrator

Karl Fisher analysis

Hydrogenation Lab (microscale, low pressure)

Mass spectrometry
TAS was formally founded in 1999, in order to meet the growing needs in this field of existing research groups, currently in IQAC, and collaborate in the process of innovation and industrial development.

### STAFF
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JOSEP CARILLA AUGUET, CONTACTING PERSON
NURIA ÁLVAREZ MARCÓS, TECHNICIAN

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**SAXS-WAXS Service**

The SAXS-WAXS service provides measurements with a variety of set ups for the determination of structural information of ordered and semi-ordered materials. The range of distances of interest falls in the nanoscale domain (0.2-100 nm). It can allow determinations of size, space ordering, morphology, fractal dimension and total interfacial area. The materials comprise surfactant solutions, microemulsions, liquid crystals, mesoporous materials, macromolecules in solution such as proteins or DNA, nanostructured films and any conceivable material with electronic discontinuities in the above mentioned range. 1D and 2D detectors are available. GISAXS and GIXSAXS configurations are also possible.

### STAFF
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JORDI ESQUENA MORET, SUPERVISING SCIENTIST
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**Thermal Analysis Service**

The following techniques are available:
- Differential scanning calorimetry DSC
- Microdifferential scanning calorimetry
- Thermogravimetric analysis TGA
- Dynamic vapor sorption DVS
- Thermomechanical analysis TMA

TAS was formally founded in 1999, in order to meet the growing needs in this field of existing research groups, currently in IQAC, and collaborate in the process of innovation and industrial development.

### STAFF
ALBERT M. MANICH BOU, SUPERVISING SCIENTIST
JOSEP CARILLA AUGUET, CONTACTING PERSON
NURIA ÁLVAREZ MARCÓS, TECHNICIAN
The Proteomics Service has been recently created to provide support to IQAC and IDAEA researchers as well as other public and private organizations. The service is focused in the analysis of biomolecules (proteins, peptides, oligonucleotides, sugars ...) and large organic molecules (such as polymers, dendrimers, polyphenols and other macromolecules) by MALDI-TOF/TOF mass spectrometry.

The Service also offers separation, quantification, identification and characterization of peptides and proteins in biological and biomedical systems using two-dimensional electrophoresis and mass spectrometry techniques.

**STAFF**

CARME QUERO LÓPEZ, Ph.D.

---

**Proteomics Service**

The Proteomics Service has been recently created to provide support to IQAC and IDAEA researchers as well as other public and private organizations. The service is focused in the analysis of biomolecules (proteins, peptides, oligonucleotides, sugars ...) and large organic molecules (such as polymers, dendrimers, polyphenols and other macromolecules) by MALDI-TOF/TOF mass spectrometry.

**Services**

1) Molecular mass determination by MALDI-TOF mass spectrometry.
2) Identification of proteins by peptide mass fingerprint.
3) Identification of proteins by peptide mass fingerprint and peptide fragmentation by mass spectrometry (MALDI-TOF/TOF).
4) Electrophoresis Separation of proteins by one- and two-dimensional electrophoresis.
Knowledge Transfer

Knowledge Transfer encompasses the systems and processes by which technology, expertise and skilled people are transferred between the research environment (universities, centers and institutes) and the industry, commerce and public sectors to contribute to prosperity and society's benefit.

In the technology transfer process different aspects must be considered: identification of research which has potential commercial interest, adequately protection by means of patents, etc, development of strategies to transfer and final negotiation with companies who can exploit the final technology.

STAFF
ISABEL MASIP Ph.D
Deputy Vice-Presidency for Knowledge Transfer
Knowledge Transfer Manager

Technologies Available
We have available a wide range of technologies in human health, diagnostic tools, cosmetics, chemical devices, etc. and the know-how acquired by our researchers in different technological fields. Different collaborative approaches are offered, such as exclusive and non-exclusive patent licenses, and collaborative research and contract research with industry based on patent licenses or in innovative technologies.

Life Sciences

**Cancer**
IQAC_006. Aminocyclitol derivatives to regulate immune response by stimulation of natural killer T-cells.
IQAC_018. Ceramide analogues as potential anti-tumour drugs.

**Inflammatory diseases**
IQAC_009. Modified siRNAs for silencing TNF-gene expression to treat inflammatory diseases.
IQAC_012. Optimization of the therapeutic potential of siRNA by formation of complexes with plasma components.

**Rare diseases**
IQAC_008. New aminocyclitols for treatment of Gaucher disease.

**Immunology/adjuvants**
IQAC_006. Aminocyclitol derivatives to regulate immune response by stimulation of natural killer T-cells.

**Pain**
IQAC_022. Pain treatment based on TRPV1 channel blockers.

**Eating disorders**
IQAC_021. Treatment of diseases related to eating disorders.

**AIDS**
IQAC_016. Peptides derived from hepatitis G virus sequence for treatment of VIH.

**Medical diagnosis**
IQAC_002. Test for cancer diagnosis based in the quantification of acid ceramidase.
IQAC_019. Test for early diagnosis of rheumatoid arthritis based on chimeric fibrin and filaggrin peptides.
IQAC_020. Test for early diagnosis of rheumatoid arthritis based on chimeric vimentin peptides.

**Drug delivery**
IQAC_007. Bicosomes: bicelles encapsulated in liposomes and their application in diluted systems.
IQAC_010. Novel macroporous or meso/macroporous biocompatible polymers with chemical and pharmaceutical applications.

**Pharmacological tools**
IQAC_015. Galactosidase inhibitors as pharmacological tools.
Chemical Technology

Biosensors
IQAC_003. Three-dimensional biosensor for detection of analytes in a biological sample.
IQAC_004. Biosensor device for simultaneous detection of several biological samples in solution.

Food safety tests
IQAC_014. New immunochemical method for determination of bromopropylate in wine.
IQAC_017. Immunoassay to detect residual fluoroquinolone-type antibiotics in food.

Skin care
IQAC_005. Internal wool lipid extracted with supercritical fluids for application in cosmetics and dermo-pharmaceutics.

Dyes
IQAC_001. Ecological liposomic disperse dyes for textile or paper dyeing.

Characterisation Devices
IQAC_023. Kratky type X-ray scattering cameras modified to work under controlled atmosphere conditions.
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Department of Biological Chemistry and Molecular Modelling (BCMM)
Department of Biomedical Chemistry (BMC)
Department of Chemical and Biomolecular Nanotechnology (CBN)
Department of Chemical and Surfactants Technology (CST)
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## GRANTED RESEARCH PROJECTS

**MINISTERIO DE CIENCIA E INNOVACIÓN**

**SUBPROGRAMAS DE INVESTIGACIÓN FUNDAMENTAL NO ORIENTADA Y DE ACCIONES COMPLEMENTARIAS PARA PROYECTOS DE INVESTIGACIÓN FUNDAMENTAL NO ORIENTADA (…)**

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<td>Guerrero Perez, Angel</td>
<td>BCMM</td>
<td>Desarrollo de antagonistas de feromonas sexuales para un control biorracional de plagas de insectos. Actividad y estudios enzimáticos.</td>
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<td>BIO2009-07866-E</td>
<td>Caminal Saperas, Gloria</td>
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<td>Biotecnología de materiales lignocelulósicos: Retos moleculares, enzimáticos y químicos para su aplicación industrial y medioambiental.</td>
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<td>Cot Cosp, Jaume</td>
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<td>Clapes Saborit, Pere</td>
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<td>Estrategias quimo-enzimáticas para la síntesis orientada a la diversidad. Adiciones aldólicas biocatalíticas en cascada para la preparación de nuevos productos bioactivos.</td>
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<td>Marsal Monge, Agusti</td>
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<td>Haro Villar, Isabel</td>
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<td>Fabrías Domingo Gemma</td>
<td>BMC</td>
<td>E-2-Hexadecenal: Un nuevo lipido bioactivo.</td>
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<td>Control y aplicación de nanoestructuras formadas por sistemas tensioactivos catiónicos biocompatibles.</td>
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<td>CTQ2010-16964</td>
<td>Lopez, Olga</td>
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<td>CTQ2010-20517-C02-02</td>
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<td>Activación química con metales y metaloides dirigida al acoplamiento c-c/c-heteroatomo y a la modificación de biomoléculas.</td>
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<td>Eritja, Ramon</td>
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<td>Estudios estructurales de biomoléculas de interés biomédico y tecnológico.</td>
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<td>Composites de altas prestaciones de nanopartículas cerámicas en fibras de poliéster: propiedades y aplicaciones.</td>
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**SUBPROGRAMA DE PROYECTOS DE INVESTIGACIÓN FUNDAMENTAL ORIENTADA A LA TRANSMISIÓN DE CONOCIMIENTO A LA EMPRESA (TRACE)**

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<td>TRA2009-02820</td>
<td>Coderch Negra, M. Lluisa</td>
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<td>Eficacia de antioxidantes en cabello humano.</td>
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**CONVOCATORIA 2010 DEL SUBPROGRAMA INNPACTO**

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<td>IPT-300000-2010-26</td>
<td>Esquena Moret, Jordi</td>
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<td>Investigación y desarrollo de textiles de uso médico y/o terapéutico mediante procesos de funcionalización superficial.</td>
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<td>Chip architectures by joint associated labs for European diagnostics (CAJAL4EU).</td>
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### EU PROJECTS

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<td>Eritja, R./Solans, C.</td>
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<td>Multifunctional nanotechnology for selective detection and treatment of cancer.</td>
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<td>NANOITSELF 230810 Prov. Marie Curie</td>
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<td>Advanced functional nanocomposites by cooperative self assembly.</td>
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<td>NANOLOGYSE 245162</td>
<td>Solans Marsa, Concepción</td>
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<td>Nanoparticles in food: Analytical methods for detection and characterisation.</td>
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### AACC FUNDING

**GEN. CAT.- CIRIT. Ajuts a Grups de Recerca Consolidats**

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<td>2009SGR1072</td>
<td>Fabrias Domingo, Gemma</td>
<td>BMC</td>
<td>Research Unit on Biologically Active Molecules (RUBAM).</td>
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<td>2009SGR1212</td>
<td>Parra Juez, José Luis</td>
<td>CST</td>
<td>Fisicoquímica i Estructuració Vesicular de Lípids i Biopolímers Bacterians.</td>
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<td>Infante Martinéz-Pardo, Rosa</td>
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<td>Tensioactius i Química Sostenible.</td>
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<td>Marco Colas, Pilar</td>
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<td>Applied Molecular Receptors Group (AMRG).</td>
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<td>2009SGR1472</td>
<td>Olivella Nello, Santiago</td>
<td>BCMM</td>
<td>Química Teòrica i Computacional.</td>
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<td>2009SGR871</td>
<td>Guerrero Pérez, Ángel</td>
<td>BCMM</td>
<td>Unidad d’Ecologia Química (UCE).</td>
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<td>Clapés Pedro</td>
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<td>Síntesis enzimática de aminoácidos no proteínogénicos para conjugaciones bioortogonales.</td>
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<td>20100111 INNOCASH</td>
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<td>Síntesis de materiales inorgánicos nanoestructurados por el método de reacciones en microemulsiones de tipo aceite-en-agua.</td>
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RUNNING FUNDED RESEARCH PROJECTS AND CONTRACTS

(SUBPROGRAMA DE INVESTIGACIÓN FUNDAMENTAL NO ORIENTADA.
CONVOCATORIA: 2008, 2007)

Department of Biological Chemistry and Molecular Modelling

- Preparación y evaluación de inhibidores de colinaquinasa con potencial actividad antitumoral
  - MICINN (PET2008_0312)
  - Principal Investigator: J. Bujons
  - Partner: Translational Cancer Drugs Pharma S.L.
  - 2009-2011

- Reacciones de oxidación de interés en química atmosférica, en química ambiental y en procesos biológicos. Estudio teórico
  - CTO2008-06536
  - 2008-2010

- Móbius aromaticity: a new challenge for computational chemistry
  - Marie Curie Reintegration Grant
    - (PERGOS-GA-2009-249310)
  - Principal Investigator: M. Torrent Sucarrat
  - 2009-2012

Department of Biomedicinal Chemistry

- Diseño y síntesis de nuevos ciclitoles para el estudio de procesos de señalización, biosíntesis y metabolismo mediados por esfingolípidos
  - CTQ2008-01426
  - Principal Investigator: A. Llebaria
  - 2008-2010

- Dihidroceraamida desaturasa, ceramidasa lisosomal y autofagia: nuevo modo de accion de algunos agentes antitumorales
  - SAF2008-00706
  - Principal Investigator: G. Fabrias
  - 2008-2010

- Diseño racional, síntesis e caracterización de análogos d’opioides y M6G: vers un millor coneixement dels mecanismes del dolor
  - Fundació La Marató de TV3 (070430)
  - Coordinator, Principal Investigator: G. Valencia
  - 2008-2010

- Molecular bases of neuropathic pain: An integrated approach to analyze the role of Group-III metabotropic glutamate receptors.
  - Fundació La Marató de TV3 (070532)
  - Principal Investigator: A. Llebaria
  - 2008-2010
Desarrollo y demostración de nuevas tecnologías para la detección de residuos de antibióticos de uso veterinario a lo largo de la cadena de producción de alimentos de origen animal. Control y seguridad alimentaria (Detecta)

MICINN (AGL2008-05578-C05-01)
Principal Investigador: F. Sánchez-Baeza
2008-2010

Obtención por organización espontánea de nuevos nanocompuestos híbridos orgánico-inorgánicos para aplicaciones avanzadas en recubrimientos multifuncionales.

MICINN (CTQ2008-01979)
Principal Investigadores: C. Rodríguez-Abreu, C. Solans
2008-2010

Obtención y caracterización de estructuras meso/macroporosas a partir de emulsiones altamente concentradas: control de la porosidad dual y aplicaciones en medio ambiente.

MICINN (CTQ2008-06892-C03-01)
Coordinator/Principal Investigador: J. Esquena
2008-2010

Microarray de epitopos: una herramienta para el diagnóstico y la investigación de las respuestas alérgicas a antibióticos b-lactámicos (b-Array)

MICINN (SAF2008-03082)
Principal Investigador: R. Galve
2008-2010

Modulación química de rutas de señalización celular de relevancia en enfermedades degenerativas: generación de cabezas de serie

MEC/MICINN (SAF2008-00048)
Principal Investigador: A. Meseguer
2008-2010

Nanobioanlytical platforms for improved diagnosis of infections caused by pathogens (Nanomediac)

Plan Nacional de Internacionalización de la I+D (EU2008-00175)
Coordinator/Principal Investigador: J. Samitier (IBEC, Barcelona)
Principal Investigador: M. P. Marco
2009-2011

Electronic Immuno-Interfaces and Surface Nanobiotechnology: A Heterodoxical Approach
EU NMP2-CT-2003-505485 (ELISHA)
Principal Investigador: M. P. Marco
2004-2006

Multi-scale formation of functional nanocrystal-molecule assemblies and architectures (FUNMOL).
EC-STREP: Focused Research Project, NMP-2007-213382
Coordinator: A. Quinn (Tyndall NMRC, Cork, Ireland)
IQAC participant: R. Eritja
2008-2011

Design and functionality of non-linear electrochemical nanoscale devices (Dynamo).
EC-STREP, NEST-2004-ADV 028669-1
Coordinator: K. Kuntturi (Helsinki Institute of Technology, Finland).
IQAC Participant Group Leader: R. Eritja
2006-2009

Precision chemical nanoengineering: integrating top-down and bottom-up methodologies for the fabrication of 3-D adaptive nanostructured architectures (Nano-3D)
EC STREP, NMP4-CT2005-014006
Coordinator: J. Preece (U. Birmingham, UK)
IQAC Participant Group Leader: R. Eritja
2005-2008

Advances in functional organic-inorganic nanocomposites by cooperative self-assembly
FP7-PEOPLE IRSES 2008
Coordinator/Principal Investigador: J. Esquena
2009-2011

CONtaminants in Food and Feed: Inexpensive DEtection for Control of Exposure (Confidence).
EC, VII- Framework Programme. Food, Agriculture and Fisheries and Biotechnology.
Proposal No.: 211326 – CP (Collaborative Project)
Coordinator/Principal Investigador: Jacob de Jong (RIKILT, The Netherlands)
Participant Group Leader: M. P. Marco
2008-2012

Intervenció farmacològica sobre el receptor TRPV1 per atenuar el dolor crònic
Fundació Marato de TV3 (20080123)
Coordinator: A. Ferrer-Montiel (U. of Elx)
IQAC Principal Investigador: A. Meseguer
2008-2011

The Spanish Ion Channel Initiative
MICINN CSD2008-00005, Consolider Program
IQAC Participant Group Leader: A. Meseguer
2009-2013

Suport a Grups de Recerca Consolidats.
Generalitat de Catalunya (2005SGR00812)
Grup de Tensioactius
Principal Investigador: C. Solans
2006-2008
Suport a Grups de Recerca Consolidats  
Generalitat de Catalunya (2005SGR00207)  
Applied molecular receptor group  
Principal Investigator: M. P. Marco  
2006-2008  
Fundamental studies of rubber latex characterization in film formation and adhesives.  
Malaysian Rubber Board. 20100079  
Principal Investigator: J. Esquena  
2008-2011  
Diseño y síntesis de análogos químicos de inhibidores de quinásas descubiertos por Allinky  
Allinky Biopharma  
Principal Investigator: A. Messeguer  
2009-2011  
Surface coatings characterization  
20060256  
The Procter & Gamble Company  
Principal Investigator: C. Solans  
2005-2012  
Phase behavior of surfactants and polymers of fabric and hair care interest.  
20090784  
The Procter & Gamble Company  
Principal Investigator: C. Solans  
2009-2013  
Functional polyester materials for delivery of bioactives  
20091269  
Firmenich S.A.  
Principal Investigator: C. Solans  
2009-2011  
Síntesis de materiales inorgánicos nanoestructurados por el método de reacciones en microemulsiones del tipo aceite en agua  
201000111  
INNOCASH (FECYT-MICINN)  
Principal Investigator: C. Solans  
2009-2010  
Investigación en nuevos conceptos de carreteras más seguras y sostenibles.  
CDTI (CENIT2007-1014)  
Coordinator: C.Cortés (I+D+i, Serviá Cantó, Girona)  
Principal Investigator: J. Esquena  
Partner: FENIX AIE  
2007-2010  
Biodegradabilidad y toxicidad acuática de líquidos iónicos como alternativa a disolventes orgánicos convencionales  
MEC (CTQ2007-60364)  
Principal Investigator: M. T. García  
2007-2010  
Comportamiento fásico de sistemas bicelares: influencia de la composición lipídica  
MEC (CTQ2007-60409)  
Principal Investigator: O. Lopez Serrano  
2007-2010  
Caracterización, propiedades y aplicaciones de las fibras de políacido láctico  
MEC (MAT 2007-66569-C02-02)  
Coordinator: D. Cayuela (UPC)  
Subproject Principal Investigator: A. M. Manich  
2007-2010  
Contrato de licencia y explotación de la patente ES512643/ P19500027  
Principal Investigator: M. R. Infante  
2002-2015  
Biopolymer based surfactants – stabilization and functionalisation of particles and surfaces  
COST Action n. D36/0008/06  
Coordinator: M. R. Infante  
2006-2010  
Valoración objetiva de propiedades, condiciones de mantenimiento y reciclado de diversos tipos de césped artificial para optimizar sus prestaciones.  
20100088  
POLIGRAS IBÉRICA, S.A.  
Principal Investigator: A. M. Manich  
2010-2012
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<td>P201030298</td>
<td>Bicelas encapsuladas en liposomas y su aplicación en sistemas diluidos</td>
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<td>P201030533</td>
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<td>P201030611</td>
<td>Derivados lipolíicos de ácidos nucleicos</td>
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<td>Oligonucleótidos modificados como reguladores de la expresión génica</td>
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<td>P201031642</td>
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<td>P201031721</td>
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<td>Conjugado polimérico para el tratamiento de infecciones bacterianas</td>
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<td>PCT/ES2010/070732</td>
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<td>PCT/ES2010/070842</td>
<td>Derivados de aminociclitoles, procedimiento de obtención y usos</td>
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<td>PCT/ES2010/070857</td>
<td>Derivados lipófilos como surfactantes</td>
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<td>PCT/ES10/070854</td>
<td>Derivados de amida de ácidos grasos con anfetaminas para el tratamiento de desórdenes alimenticios</td>
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<td>EP09169036</td>
<td>New 3-oxopiperazinium derivatives agonists of nerve growth factor and their use as medicaments</td>
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<td>EP09169045</td>
<td>New peptoid agonists of nerve growth factor and their use as medicaments</td>
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## 2011 Spanish Priority Application

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<td>P201130537</td>
<td>Antagonistas de TRPV1 y sus usos</td>
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<td>Epoxidos y aziridinas de ciclohexano relacionados estructuralmente con la galactosa como inhibidores selectivos de galactosidasas</td>
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<td>Polipéptidos quiméricos derivados de la proteína vimentina con utilidad para el diagnóstico de la artritis reumatoide</td>
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<td>PCT/ES2011/070128</td>
<td>Bicelas encapsuladas en liposomas y su aplicación en sistemas diluidos</td>
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<td>PCT/ES2011/070800</td>
<td>Haptenos e inmunoreactivos y su uso en la obtención de anticuerpos de familia e inmunensayos para quinolonas</td>
<td>Pilar Marco, Francisco José Sánchez, Daniel González</td>
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<td>PCT/ES2011/070880</td>
<td>Éteres de hidroxirosol</td>
<td>Jesús Joglar, Pere Clapés, Rafael de La Torre, Magí Farré, Maribel Covas, Montserrat Fitó, Bruno Almeida, Fernando Rodríguez, Juan Manuel Decars, Manuel Macías, Miguel Romero</td>
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<td>P200701253</td>
<td>Impedimentric sensor and applications thereof</td>
<td>Pilar Marco, Javier Ramon Azcon, Francisco José Sánchez, Andrei Bratov, Natalia Abramova, Carlos Domínguez, Ángel Merlos</td>
<td>CSIC</td>
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<td>P200931164</td>
<td>Sistema y procedimiento multináltico basado en mediciones impedimétricas</td>
<td>Pilar Marco, Javier Ramon Azcón, Francisco José Sánchez, Andrei Bratov, Natalia Abramova, Andrey Ipatov</td>
<td>CSIC</td>
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Ph. D. THESIS

Aurora Colomer Flores.
Dpt. de Tecnología Química i de Tensioactius
Síntesis y propiedades de nuevos tensioactivos catiónicos derivados de lisina
Directores: Aurora Pinazo Gassol, Maria Lourdes Perez Muñoz
Sobresaliente "cum laude"

Carolina Denise Aubery Torres.
Dpt. de Nanotecnología Química i Biomolecular
Nonionic water-in-oil and bicontinuous microemulsions as reaction media for the synthesis of Mn-Zn ferrite nanoparticles
Directors: Concepción Solans Marsa, Margarita Sanchez Dominguez
Excel.lent "cum laude"

Mariana Gutiérrez Tejeda.
Dpt. de Química Biológica i Modelització Molecular.
Aplicaciones sintéticas de aldolrasas nativas y modificadas genéticamente dependientes de glicina y compuestos alfa-hidroxicarbonílicos.
Director: Pere Clapés Saborit.
Sobresaliente "cum laude"

Glòria Vendrell Navarro.
Dpt. de Nanotecnología Química i Biomolecular
Estudis sobre la preparació, l’anàlisi i el cribratge de quimioteques de peptidomètics
Director: Àngel Messeguer Peypoch.
Excel.lent "cum laude"

Fabio M.M. Simbari.
Dpt. de Química Biomèdica
Molecular tools for studying sphingomyelinases and dihydroceramide desaturase
Director: Josefina Casas Brugulat
Sobresaliente "cum laude"

Raquel Obregón Núñez.
Dpt. de Nanotecnología Química i Biomolecular
Nuevas metodologías racionales para el desarrollo de aplicaciones de polímeros de huella molecular para la determinación de antibióticos en alimentos.
Directores: Francisco José Sánchez Baiza, María Pilar Marco Colás.
Sobresaliente "cum laude"

Gerard Carot Sans.
Dpt. de Química Biológica i Modelització Molecular
Identificació i caracterització delsenzims implicats en la biosíntesi i degradació de feromones en lepidòpters nocturors
Directors: Angel Guerrero Perez, Gloria Rosell Pellise.
Excel.lent "cum laude"

Jordi Morros Camps.
Dpt. de Tecnología Química i de Tensioactius
Obtenció de tensioactius biopolimèrics basats en la inulina en medi aqüós
Directors: M. Rosa Infante Martinez-Pardo, Ramon Pons Pons.

Clara Barba Albanell.
Dpt. de Tecnología Química i de Tensioactius
Efectivitat cosmètica de proteïnas queratiníciques
Directores: M. Luisa Coderch Negra, José Luis Parra Juez.
Sobresaliente "cum laude"

Benjamí Fürstenau.
Dpt. de Química Biomèdica
Comunicación química interespecífica de Coroebus spp. (Coleoptera: Buprestidae) y Dociostaurus maroccanus (Orthoptera: Acrididae), dos insectos plaga de la Península Ibérica
Directores: Angel Guerrero Pérez, Glòria Rosell Pellise.
Sobresaliente "cum laude"

José M Muñoz Olaya.
Dpt. de Química Biomèdica
Dihydroceramide desaturase as therapeutic target in HIV-1 infection and cancer
Director: Gemma Fabriás Domingo
Sobresaliente "cum laude"
Lucía Díaz Bueno
Dpt. de Química Biomèdica
Applications of click chemistry and molecular modeling to the development of pharmacological chaperones for Gaucher disease
Director: Antonio Delgado Cirilo

Luz del Carmen Camacho Castillo
Dpt. de Química Biomèdica
Acid ceramidase and sphingosine-1-phosphate-lyase as biomarkers and therapeutic targets in cancer
Director: Gemma Fabriàs Domingo

Genoveva Morral Ruiz
Dpt. de Nanotecnologia Química i Biomolecular
Estudi de la formació de nanoparticules polimèriques obtingudes a part de nanoeumulsions de fase externa aquosa i associació d’antinflamatoris no esteroidals
Directors: Concepción Solans Marsa, Maria José García Celma
15/03/2011. UB. Facultat de Farmàcia. Dpt. Fisicoquímica. Sobresaliente "cum laude"

Bruno Almeida Cotrim
Dpt. de Química Biológica i Modelització Molecular
Synthesis of fatty acid derivatives of catechol compounds that exhibit negative modulation of food intake and antioxidant properties
Directors: Rafael de la Torre Fornell, Jesús Joglar Tamargo
10/01/2011. UPF. Facultad de Ciencias de la Salud y de la Vida Sobresaliente

Sandra M. Ocampo
Dpt. de Nanotecnologia Química i Biomolecular
Diseño y formulación de siRNAs para terapia anti-inflamatoria
Directors: Ramon Eritja Casadella, José Carlos Perales Losa
17/12/2010. UB. Facultat de Medicina. Dpt. Ciències Fisiològiques II. Sobresaliente "cum laude"

Ariadna Selga Pérez
Dpt. de Química Biológica i Modelització Molecular
Obtenció de tio-conjugats de flavanols a partir de subproducts agroforestals. Anàlisi, síntesi, escalat, activitat i metabolització
Directors: M. Pilar Vinardell Martínez Hidalgo, Josep Lluis Torres Simon
Cristina Alonso Merino.
**Dpt. de Tecnología Química y de Tensioactivos**
Aplicación tópica de polifenoles. Evaluación de su absorción percutánea y capacidad antioxidante mediante metodologías in vitro y ex vivo
Directors: José Luis Parra Juez, M. Luisa Coderch Negra

Meritxell Llinàs Pons.
**Dpt. Nanotecnología Química y Biomolecular**
Estudi d’emulsions altament concentrades com a sistemes d’alliberació controlada de principis actius
Directors: Gabriela Caldero Linhoff, Concepción Solans Marsa, María José García Celma
Excel.lent “cum laude”

Sonia Castellanos Ortega.
**Dpt. de Química Biológica y Modelización Molecular**
Radical and non-radical carbazole derivatives for molecular electronics
Directors: Luis Juliá Bargès, Francisco López Calahorra
20/05/2010. UB. Facultad de Química. Dpt. Química Orgánica.
Excel.lent “cum laude”

Brendan Manning.
**Dpt. de Nanotecnología Química y Biomolecular**
Photopattering of surfaces using photolabile hairpin oligonucleotides
Director: Ramon Eritja Casadella
13/05/2010. UB. Facultad de Química. Apto

Aurora Jiménez Rodríguez.
**Dpt. de Química Biológica y Modelización Molecular**
Modelització d’aldolases de classe II: paper del metall en el mecanisme catalític i en l’acoblament entre dinàmica i catàlisi
Director: Ramon Crehuet Simon
Excel.lent “cum laude”

Neus Lozano Valdés.
**Dpt. de Tecnología Química y de Tensioactivos**
Tensioactivi sintéticos biocompatibles: potencial aplicación en medicina pulmonar
Directors: Aurora Pinazo Gassol, Ramon Pons Pons
24/02/2010. UB. Facultad de Química. Excel.lent “cum laude”

Elena Herrera Carrillo.
**Dpto. Química Biomédica**
Péptidos sintéticos derivados de la proteína E2 del GB virus C como nuevos inhibidores del VIH-1
Directors: María Jose Gomara Elena, Isabel Haro Villar
Sobresaliente “cum laude”
MASTER-D.E.A.

Jonathan Miras Hernández
Aplicación de hidrogeles de Poli(N-isopropilacrilamida) en tejidos de poliamida
Directores: Jordi Esquena, Susana Vilchez
Universidad de Barcelona, Facultad de Química
02-03-2010

Gelen Rodríguez Delgado
Efecto de las bicelas sobre los lípidos del estrato corneo de la piel
Directores: Olga López
Universidad de Barcelona, Facultad de Química
30/06/2010

Manroshan Singh
Influence of hydrophobically modified polyfructose (HMP) on the stability of vulcanizad natural rubber latex
Directores: Jordi Esquena, Conxita Solans, Tharwat Tadors
Universidad de Barcelona, Facultad de Química
07/2010

Clotilde Bouaoud
Formulation of fluorescent polymeric nanoparticles from O/W nano-emulsions
Directores: Gabriela Calderó, Conxita Solans
Master Chimie et Ingénierie de la Formulation (CIF).
Ecole Nationale Supérieure de Chimie Lille (France). Sciences de la Matière
2010

Anna Cornellas Pitarch
Liquids iónics derivats d’imidazoli i piridini: sintesi, autoagregació, toxicitat aquàtica i activitat antimicrobiana
Directores: Mª Teresa Garcia, Lourdes Pérez
IQAC-CSIC
25-01-2011

Marta Escarrà Senmartí
Péptids sintètics derivats de la proteïna E2 del GB virus C com a possibles inhibidors de l’HIV-1
Directoras: Isabel Haro y María José Gomara
Master en Química Orgànica Avanzada
Facultad de Química, Universidad de Barcelona.
31-01-2011

ACADEMIC ACTIVITIES

Experimental techniques in Biophysics
M. Pilar Marco Colas
Master de Biofísica (UB) 07/12/2010

Técnicas experimentales en Biofísica
Ramon Eritja Casadella
Programa de Doctorat de Física (UB) 03/12/2010

Biocatalytic carbonation cascade reactions for asymmetric synthesis
Pedro Clapes Saborit
Master de Biotecnologia Molecular (UB) 23/11/2010

Electrónica molecular. Materiales. Procesos conductores orgánicos
Luis Julia Barges
Master de Nanomateriales y Nanotecnologia de Transferencia Electrónica (UB) 15/11/2010

Técnicas básicas
Ramon Eritja Casadella
Programa de Doctorat de Biotecnologia (UB) 11/10/2010

Terapia génica
Ramon Eritja Casadella
Programa de Doctorat de Biomedicina (UB) 31/05/2010

Applications in Biotechnology
Josep Lluís Torres Simon
Programa de Doctorat de Biotecnologia (UB) 21/04/2010

Tensoactivos y polímeros en sistemas coloidales
Jordi Esquena Moret
Master de Química Avanzada (UB) 25/02/2010

Estadística aplicada a la preformulación y formulación de medicamentos
Albert Maria Manich Bou
Licenciatura / Grado Especialista en Farmacia Industrial y Galénica (UB) 15/02/2010

Química supramolecular
Ignacio Alfonso Rodriguez
Màster en Química Sostenible. Universitat Jaume I. 11/01/2010

Introduction to small angle X-ray scattering technique and the organization of skin-collagen molecules and other examples
Olga López Serrano
Sincroton Radiation Master (UAB). 11/01/2010

Biohybrid materials and biofunctional surfaces: Recent progress towards improved diagnostics.
Pilar Marco

Python applied to computational chemistry and molecular modelling
Ramon Crehuet Simon
Xarxa de Recerca en Química Teòrica i Computacional
Xarxa de Referència de Química Teòrica i Computacional Summer School. 28/06/2010
SPECIALIZATION

Terapia genómica en Biomedicina
Ramon Eritja Casadella 24/11/2010; 28/10/2010; 22/06/2010

Formación Continuada de Profesiones Sanitarias. Consorcio Centro de Investigación Biomédica en Red. Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN)

Análisis Termogravimétrico
Albert Maria Manich Bou
Seminario. T.A. Instruments 27/05/2010

Análisis térmico de fibras termoofijadas
Albert Maria Manich Bou
Especialización en Análisis Térmico y Calorimetría. Grupo Especializado de Calorimetría y Análisis Térmico (RSEQ-RSEP) 09/02/2010

Emulsiones y micro-emulsiones: preparación, propiedades y aplicaciones industriales
María José García Celma 05/03/2010
Concepción Solans Marsa 04/05/2010
Especialización de Química/Física de Materiales. Colegio Químicos Cataluña

Prácticas de laboratorio en cosmética y dermofarmacia
Jordi Esquena Moret
Master en Cosmética y Dermofarmacía. Centro de Estudios Superiores Industria Farmaceutica 24/04/2010

INVITED CONFERENCES AND KEY LECTURES

G. Calderó
Nanoparticles for biomedical applications: Preparation in O/W nano-emulsions

G. Caminal
Sistema enzimático de Trametes versicolor implicado en la degradación de contaminantes emergentes

O. López
Nanomateriales y nuevas nanoestructuras lipídicas: Absorción percutánea

M.R. Infante
Biocompatible cationic surfactants from arginine

I. Alfonso
Constitutional dynamic chemistry with macrocyclic pseudopeptides
7th ERA-CHEMISTRY Flash Conference “Bioinspired Chemistry” (Santiago de Compostela) 26/10/2010.

A. Guerrero
Inhibition of the catabolism feromonal como nueva aproximación al control de plagas de insectos
Citefa-Conicet Control de Plagas e Insecticidas. (Buenos Aires). IC. 22/10/2010.

P. Clapés
El papel de la Academia a la hora de abrir nuevos mercados

A. Guerrero
Inhibition of the chemical communication in Insects

R. Eritja
Synthesis of modified oligonucleotide derivatives for biosensing applications

F. Fernández
Biofunctionalization of gold surfaces: Key issues and applications

P. Clapés
Enzyme catalyzed asymmetric aldol additions: Carbohydrates and iminosugars from DHAP to unphosphorylated donor analogues
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<td>M.P. Marco</td>
<td>Nuevos enfoques para el análisis de residuos en alimentos utilizando anticuerpos y</td>
<td>Kausal2010. IV Congreso Int. Autocontrol y Alimentos Inocuos para Proteger la Salud. KL.</td>
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<td>micro(nano) sistemas</td>
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<td>M.P. Marco</td>
<td>Nuevas aproximaciones micro(nano)biotecnológicas y biosensores para incrementar la</td>
<td>Seguridad Alimentaria. Azti-Tecnalia. 7/05/2010.</td>
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<td>L. Pérez, A. Pinazo, M.R. Infante</td>
<td>Biobased surfactants from renewable resources</td>
<td>102nd AOCS Annual Meeting and Expo. (Cincinnati, USA) 1-4/05/2011.</td>
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<td>Mª R. Infante</td>
<td>Bio-based surfactants from renewable resources</td>
<td>58th SEPAWA Congress. (Fulda, Alemania) 14/10/2011.</td>
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<td>J.L. Parra</td>
<td>Perfil toxicológico y niveles de exposición de los cosméticos</td>
<td>Jornada EVIC Hispania. (Barcelona), 30/06/2011.</td>
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ORAL AND POSTER CONTRIBUTIONS (ABROAD EVENTS)

Colomer, L. Pérez, A. Pinazo, M.R. Infante, A. Mezei, R. Pons
Lysine based surfactants: Relationship between chemical structure and adsorption/aggregation properties
6/9/2011. 8th Liquid Matter Conference (Viena, Austria). Poster

R. Pons, I. Carrera, J. Caelles
Nascent nanoemulsions from microemulsion dilution
6/9/2011. 8th Liquid Matter Conference (Viena, Austria). Poster

Mechanical properties, relaxation behaviour and thermal characterization of false-twist textured polylactide multfilament

J.M. Anglada
The reactivity of ozone versus the reactivity of carbonyl oxide. An analysis from a theoretical point of view.
16/7/2010. RSC 21st International Symposium on Gas Kinetics (Leuwen, Bélgica). Oral

A.M. Manich, J. Carilla, B. Baena, D. Cayuela
Thermal stability and heat setting of PLA textured filaments measured by DSC and TMA

M. Ussman, D. Lopez-Santana, J. Carilla, A.M. Manich
Cellulosic fibres and water sorption isotherms
24-27/07/2011. 10th Mediterranean Conference on Calorimetry and Thermal Analysis MEDICTA (Porto, Portugal) Poster

Cryo-tem and freeze fracture tem in the study of bicellar systems
8-10/06/2010. SCANDEM (Scandinavian Society for Electron Microscopy) (Estocolmo, Suecia). Poster

D. Cayuela, L.A. Montero and A.M. Manich
Variation of microstructure of textured and fixed polylactide fibres with the texturing conditions
3-6/10/2010. 5th International Textile, Clothing and Design Conference (Dubrovnik, Croacia). Oral

A. Moure, I. Alfonso.
Pseudopeptidic molecular cages
7/7/2011. 6th International Symposium on Macrocyclic and Supramolecular Chemistry (6-ISMSC) (Brighton, UK). Poster

S. Vílchez, A.M. Manich, J. Miras, R. Molina, P. Erra, J. Esquena
Surface modification of polyamide fabrics with chitosan hydrogels crosslinked with genipin

Preparation and characterization of highly porous materials obtained by templating in water-in-1,1-dichloroethene highly concentrated emulsions
3-6/5/2011. AMIDIQ (Academia Mexicana de Investigación y Docencia en Ingeniería Química) (Riviera Maya, Quintana Roo, México). Poster

C. Solans
Nano-emulsions prepared by low-energy methods as templates for nano-biomaterials. Oral
J. Esquena. Preparation of nanostructured porous materials using highly concentrated emulsions as templates. Oral


C. Solans Emulsions as templates for the controlled preparation nanometer-scale biomaterials. Oral

J. Esquena Porous materials with controlled texture obtained in highly concentrated emulsions. Oral

M. M. Alam Highly concentrated w/o emulsions-template for carbonaceous porous materials. Oral

23rd Conference of the European Colloid and Interface Society (5-10/09/2010; Praga, Rep. Checa)

N. Lozano, A. Pinazo, L. Pérez, C. La Mesa, R. Pons
Diacyl aminoacid/diacyl phospholipid mixtures: catanionic and cationic vesicles. Poster

A. Colomer, L. Pérez, A. Pinazo, M.R. Infante, R. Pons
Thermotropic and lyotropic phase behaviour of lysine based surfactants. Poster

Changes in skin lipid arrangement by effect of bicelles. Poster

A. Colomer, L. Perez, R. Infante, R. Pons, A. Pinazo
Lysine based surfactants: relationship between chemical structure and adsorption/aggregation properties. Poster

4th Iberian Meeting on Colloids and Interfaces (RICI4) (13-15/7/2011; Oporto, Portugal).

M. Llinás, G. Calderó, M.J. García-Celma, K. Aramaki, C. Solans
Release of actives from O/W highly concentrated emulsions: Influence of the continuous phase nanostructure. Oral

N. Vilanova, C. Rodríguez-Abreu, C. Solans
Formulation of multiple emulsions for producing silicone porous microparticles. Oral

Biocompatible polymeric nanoparticles for the encapsulation of superparamagnetic nanoparticles. Poster

NanoFormulation 2011 (26/6-1/7/2011; Singapore).

S. Viltchez, L. Pérez-Carrillo, C. Solans, J. Esquena
Highly porous carbon materials obtained by templating in oil-in-alcohol highly concentrated emulsions. Poster

N. Ahmad, R. Ramsch, M. Llinás, J. Esquena, C. Solans, R. Hashim, H. A. Tajuddin
Characterization of ternary water/oil/branched-chain glycoside systems for pharmaceutical applications. Poster

Functionalised biocompatible nanoparticle preparation from nano-emulsions. Poster


A. Vilchez, C. Rodríguez-Abreu, A. Menner, A. Bismarck, J. Esquena
Macroporous solid foams obtained in highly concentrated Pickering emulsions stabilized with magnetic nanoparticles. Oral
**New approach for the encapsulation of superparamagnetic nanoparticles in a biocompatible polymer. Poster**

R. Ramsch, N. Ahmad, M. Llinas, R. Hashim, H. A. Tajuddin, J. Esquena, C. Solans  
**Branched-chain glycolipids – versatile and biocompatible amphiphiles for new drug carrier systems. Oral**

**Synthesis of mixed and doped cerium oxides by the oil-in-water microemulsion reaction method. Oral**

K. Pemartin, H. Kusar, M. Sanchez-Dominguez, M. Boutonnet, C. Solans  
**CuO-CeO2 and CuO-ZnO nanoparticles prepared from a novel oil-in-water (O/W) microemulsion reaction method: their use as catalyst in water-gas shift reaction. Poster**

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26th Congress IFSCC (20-23/09/2010; Buenos Aires, Argentina)  
L. Coderch, C. Barba, C. Alonso, M. Martí, J.L. Parra  
**New antioxidant efficacy methods for human hair. Poster**

**Water sorption of hair and nails treated with wool keratin proteins and peptides. Poster**

L. Coderch, S. Méndez, R. Ramirez, M. Martí, A. de la Maza, O. López, and J.L. Parra  
**Skin and hair efficacy of internal wool lipid liposomes rich in ceramides. Poster**

C. Alonso, M. Martí, V. Martinez, L. Rubio, L. Coderch and J.L. Parra  
**Cosmeto-textiles: skin assessment. Poster**

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13th European Student Colloid Conference (ESCC2011) (14-17/06/2011; Falkenberg, Sweden)  
S. Leitner, G. Calderó, M. J. Garcia-Celma, C. Solans  
**Characterization of polymer in water cationic nano-emulsions and their use for nanoparticle preparation. Oral**

S. Vilchez-Maldonado, G. Calderó, R. Molina  
**Skin-care polymeric nanoparticles prepared from O/W nano-emulsions. Oral**

C. Paulme, K. Pemartin, R. Ramsch, M. Sanchez, G. Caldero, C. Solans  
**Encapsulation of magnetic nanoparticles within a biocompatible polymer. Poster**

---

N. Vilanova, C. Rodriguez-Abreu, C. Solans  
**Novel Synthesis of silicone porous microparticles by crosslinking multiple emulsions. Oral**

J. Miras, S. Vilchez, J. Esquena, C. Solans  
**Preparation and characterization of highly concentrated emulsions in the presence of chitosan. Oral**

C. Solans  
**Formation of nano-emulsions by low-energy methods and application to the preparation of functional nanoparticles. Oral**

J. Esquena  
**Macroporous foams obtained in highly concentrated Pickering emulsions stabilized solely with magnetic nanoparticles. Oral**

M.M. Alam  
**Rheology of liquids crystals: Macroscopic to microscopic scale. Oral**

12th International Conference “Perspectives in Percutaneous Penetration” (06-10/04/2010; La Grande Motte, Francia)  
L. Rubio, M. Martí, C. Alonso, V. Martinez, L. Coderch and J.L. Parra  
**Skin delivery of a sun filter contained in biofunctional textiles. Poster**

G. Rodríguez, L. Rubio, M. Cócer, J. Estelrich, R. Pons, A. de la Maza, O. López  
**Effect of dipalmitoyl-phosphatidylcholine/dihexanoyl-phosphatidylcholine (dppe/dhpc) bicelles on skin lipids molecular organization. Poster**

**Bicelles as preventive agents of thermal damage in skin collagen. Poster**

Skin Forum 12th Annual Meeting (28-29/03/2011; Frankfurt, Alemania)  
**Use of synchrotron radiation for probing skin structures and their function. Poster**

**Use two lipid nanostructures with coupled effects on skin properties. Poster**
ORAL AND POSTER CONTRIBUTIONS (EVENTS IN SPAIN)


G. Morral, C. Solans, M. L. García, M. J. García
Incorporation of ketoprofen in polyurea and
polyurethane nanoparticles obtained from
O/W nano-emulsions
2-4/2/2011. EFIG 2011 (X Congreso de la
Sociedad Española de Farmacia Industrial y
Galénica) (Madrid, España). Poster

R.M. Aparicio, A. Vílchez, J. Miras, S. Vilchez, J.
Esquena, M.J. García-Celma
Liberación de fármacos in vitro a partir de
sistemas polímericos macroporosos
2-4/2/2011. EFIG 2011 (X Congreso de la
Sociedad Española de Farmacia Industrial y
Galénica) (Madrid, España). Poster

A. Vilchez, C. Rodríguez-Abreu, C. Solans, J.
Esquena, A. Menner, A. Bismarck
Macroporous foams obtained in highly
concentrated Pickering emulsions stabilized
solely with magnetic nanoparticles

K. Pemartin, M. Sánchez-Domínguez, C. Solans
Síntesis de inorgánicos nanoparticles via a
novel O/W microemulsion reaction method
with fluorescent properties and their
dispersion

G. Calderó, S. Leitner, C. Bouaoud, M.J. García-
Celma, C. Solans
Desing of multifunctional nanocarriers for
biomedical applications

N. Sanvicens
Nanotoxicología
19/11/2010. VII Encuentro de Delegados de
Prevención de Riesgos Laborales de UGT de La
Rioja (Logroño).

G. Rodríguez, L. Rubio, M. Cócera, A. de la
Maza, O. López
Bicellar nanostructures for dermal and
pharmaceutical applications
09/05/2010. IV Jornada Aplicaciones Industriales
de la Nanotecnología (Barcelona). Poster

A.M. Manich, F. Maldonado, J. Carilla, M.
Catalina, A. Marsal
Isotermas de sorción/desorción de humedad
en el colágeno
07-09/05/2010. LIX Congreso Nacional de la
Asociación Química Española de la Industria del
Cuero (Arnedo, La Rioja). Oral

F. Maldonado, E. Bautista, A.M. Munich, A.
Marsal
Aportación experimental sobre el fenómeno
de solubilización en superficie o
adsolubilización de sustancias orgánicas
sobre fibra de colágeno
07-09/05/2010. LIX Congreso Nacional de la
Asociación Química Española de la Industria del
Cuero (Arnedo, La Rioja). Oral

A.M. Manich, J. Carilla, R.A.L. Miguel, F.G.F.
Franco, J.M. Lucas, D. Cayuela, J. Gacén,
M. Martí
Absorción y desorción de humedad: Una
característica relevante de las fibras textiles
24-25/03/2010. XXXVI Simposio de la Asociación
Española de Químicos y Coloristas Textiles
(Barcelona). Oral

D. Cayuela, A.M. Manich
Comportamiento y propiedades de las fibras
de polilactida (PLA) durante su producción y
uso
06/04/2011. XXXVII Simposio de la Asociación
Española de Químicos y Coloristas Textiles
(Barcelona). Oral

M.T. García, F. Comelles, L. Pérez, I. Ribosa
Aggregation behavior and aquatic toxicity of
long chain oxygen-functionalized ionic liquids
2011. 9th Green Chemistry Conference, (Alcala
de Henares, Madrid) Oral

M. Cócera, G. Rodríguez, L. Rubio, L. Barbosa-
Barros, A. Labrado, C. Sandt, A. de la Maza, O.
López
Skin Visualised by Synchrotron Radiation

F. Maldonado, J. Carilla, A. Marsal, A.M. Manich
Procedure for the gravimetric determination
of the relative humidity in standard-
conditioned test laboratories
27-30/09/2011. XXXI IULTCS Congress
(International Union of Leather Technologists and
Chemists Societies), (Valencia). Poster

M.E. Bautista, L. Pérez, S. Cuadros, M.T. García,
A.M Manich, A. Marsal
Surfactants obtained by acylation of the
protein fraction recovered from tannery
effluent
27-30/09/2011. XXXI IULTCS Congress
(International Union of Leather Technologists and
Chemists Societies) (Valencia). Poster

A. Marsal, F. Maldonado, A.M. Manich
Adsolubilization studies on collagen fibres
with 2-Naphtol as model substance
27-30/09/2011. XXXI IULTCS Congress
(International Union of Leather Technologists and
Chemists Societies) (Valencia). Poster
A. Patti
Molecular simulation of self-assembling colloidal systems. Oral

C. Aubéry, M. Sánchez-Dominguez, C. Solans
Nonionic water-in-oil and bicontinuous microemulsions as reaction media for the synthesis of Mn-Zn ferrite nanoparticles. Oral

S. Leitner, G. Calderó, M.J. García-Celma, C. Solans
Studies on cationic polymeric nano-emulsions and nanoparticle dispersions for biomedical applications. Poster

M. Llinàs, G. Calderó, M.J. García-Celma, A. Patti, C. Solans
Controlled drug release by pH from W/O highly concentrated emulsions. Poster

N. Vilanova, C. Rodríguez-Abreu, C. Solans
Loaded porous silicone microparticles by multiple emulsion templating. Poster

A. Vilchez, A. Menner, A. Bismarck, C. Rodríguez-Abreu, J. Esquena
Tailoring pore morphology, permeability and mechanical properties of magnetic macroporous polymers foams. Oral

Textiles modified with chitosan hydrogels for medical and/or therapeutic applications. Oral

J. Miras, S. Vilchez, C. Solans, J. Esquena
Preparation and characterization of highly concentrated emulsions in presence of chitosan. Poster

M. Martínez, C. Solans, F. Valor, J. López, E. Tomás, J. Esquena
Preparation and characterization of highly concentrated bitumen emulsion with controlled droplet size. Poster

M. Homs, M. Llinàs, C. Solans
Characterization of a polyglyceryl-derived nonionic surfactant and formation of highly concentrated emulsions. Poster

S. Leitner, G. Calderó, M. J. García-Celma, C. Solans
Preparation and characterization of polymer-in-water (P/W) cationic nano-emulsions and their use for nanoparticle preparation. Poster

C. Aubery, M. Sanchez-Dominguez, C. Solans
Synthesis of superparamagnetic mixed oxide nanoparticles in the novel oil-in-water microemulsion reaction method. Poster

M.T. García, A. Cornellas, I. Ribosa, F. Comelles, MªA. Manresa, L. Pérez
Surfactant-like behavior and antimicrobial activity of long-chain ionic liquids in aqueous solution. Oral

C. Barba, M. Martí, A. Manich, J. L. Parra and L. Coderch
Effectiveness of wool keratin proteins and peptides on hair. Poster

E. Fernández, C. Barba, C. Alonso, M. Martí, J.L. Parra and L. Coderch
Photodegradation determination of human hair. Poster

S. Leitner, G. Calderó, M.J. García-Celma, C. Solans
Cationic polymeric nanoparticles prepared from nano-emulsions, suitable for gene therapy. Oral poster

S. Fornaguera, G. Calderó, M. Llinàs, C. Solans
Design of nanoparticle dispersions for inhalatory administration. Oral poster

G. Calderó, M.J. García-Celma, C. Solans
Advanced polymeric nanoparticles from nano-emulsions. Oral poster

C. Solans, J. Esquena, M.J. García-Celma
Nanocarriers for antiapoptotic drug transport across the blood-brain-barrier (Nano-Trans-Brain). Poster
SETMANA DE LA CIÈNCIA 2010  
Conferències Divulgatives  
G. Valencia,  
Només afegiu aigua  
J. Casas  
Suïcidi cel·lular: rituals per a la supervivència  
J. L. Torres  
Darwin avui  
R. Pons  
Sabons i bombolles  
A. Messeguer  
Hi haurà química entre nosaltres?  
R. Eritja  
ADN i ordinadors

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Conferències Divulgatives  
G. Valencia,  
Foc i flames  
F. J. Sánchez Baeza  
Sensores para la detección de biomarcadores de enfermedades neurológicas y neurodegenerativas. Aplicaciones para el diagnóstico clínico de estas patologías".  
R. Eritja  
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J. Casas  
Suïcidi cel·lular: rituals per a la supervivència  
G. Fabriàs  
Fàrmacs: química que cura  
I. Alfonso  
De la materia inanimada a la vida: autoorganització i evolució molecular

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A. Messeguer  
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R. Eritja  
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Conferència del Dr. Angel Guerrero (amb motiu de l’Any Internacional de la Química)  
Museu de la Ciència i de la Tècnica de Catalunya (Terrassa)  
11/10/2011  
Utilització de feromones d’insectes en un control integrat de plagues  
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C. Solans;  
C. Rodríguez-Abreu;  
J. Esquena;  
G. Calderó  
JORNADA CIENTÍFICA. 16/06/2010
8.2. APPENDIX 2. SCIENTIFIC OUTPUT

Publications in ISI journals (journals in alphabetical order) 140
Publications in non-ISI journals (journals in alphabetical order) 151
Book Chapters 152

Highlighted:
Conference papers, Editorial, Erratum
Scopus errors
PUBLICATIONS (papers in ISI journals)

Characterization of perylene diimide dye self-assemblies and their use as templates for the synthesis of hybrid and supermicroporous nanotubes
Rodríguez Abreu, C.; Aubery, C.; Solans, C.; López-Quintela, M. A.; Tiddy, G.

Improved properties of oxygen and argon RF plasma-activated polyester fabrics loaded with TiO2 nanoparticles
Mihailovic, D., Saponjic, Z., Molina, R., Puac, N., Jovancic, P., Nedeljkovic, J., Radetic, M.
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Trapero, A., Llebaria, A.

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Martínez, M.T., Tseng, Y.-C., Salvador, J.P., Marco, M.P., Ormategui, N., Loinaz, I., Bokor, J.
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The role of counterions in the membrane-disruptive properties of pH-sensitive lysine-based surfactants
Nogueira, D.R., Miltjans, M., Infante, M.R., Vinardell, M.P.
Acta Biomater. 7 2846-2856, 2011

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Clapés, P., Garrabou, X.

Enzymatic synthesis of α-glucosides of resveratrol with surfactant activity

Redesign of the phosphate binding site of L-rhamnulose-1-phosphate aldolase towards a dihydroxyacetone dependent aldolase
Garrabou, X., Joglar, J., Parella, T., Crehuet, R., Bujons, J., Clapés, P.

A mutant D-fructose-6-phosphate aldolase (Ala129Ser) with improved affinity towards dihydroxyacetone dependent aldolase
Garrabou, X., Joglar, J., Parella, T., Crehuet, R., Bujons, J., Clapés, P.

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Gonidec, M., Luis, J.M., Costas, M.
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Jaumot, J., Eritja, R., Gargallo, R.

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Mannelli, I., Marco, M.P.

A fluorescent polarization-based assay for the identification of disruptors of the RCAN1-calcineurin A protein complex
Carme Mullero, M., Orzáez, M., Messegue, J., Messegue, A., Pérez-Payá, E., Pérez-Riba, M.

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Sánchez-Martín, M.J., Busquets, M.A., Girona, V., Haro, I., Alina, M.A., Pujol, M.

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Torrent-Sucarrat, M., Ruiz-López, M.F., Martins-Costa, M., Francisco, J.S., Anglada, J.M.

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