



## Biennial Report 2008-2009





# INSTITUTE OF ADVANCED CHEMISTRY OF CATALONIA

## Institut de Química Avançada de Catalunya (IQAC)



## Biennial Report 2008-2009



**INSTITUTE OF ADVANCED CHEMISTRY OF CATALONIA**  
Institut de Química Avançada de Catalunya  
Consejo Superior de Investigaciones Científicas  
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# IQAC Biennial Report 2008-2009

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## DIRECTOR'S FOREWORD



The Institute of Advanced Chemistry of Catalonia (IQAC) is a research center located in Barcelona and belonging to the Consejo Superior de Investigaciones Científicas. The Institute 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 to be pursued systematically.

The present Report covers the biennium 2008-2009. It gives an account on the research carried out during our first two years of scientific activity. Analysis of the data herein reported, allows to conclude that the mission that directed the creation of our Institute has been successfully accomplished.

In addition to the information given here, we invite you to navigate our website ([www.iqac.csic.es](http://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,

A handwritten signature in black ink, appearing to read "Angel Messeguer".

Angel Messeguer  
Director of IQAC



# 1

## **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 treatment of industrial waste, 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. Among these services, it should be mentioned: Thermal Analysis and Calorimetry, Nuclear Magnetic Resonance Spectroscopy, Paramagnetic Resonance Spectroscopy, Elemental Microanalysis, Synthesis of High-Added Value Molecules, X-Ray Dispersion at Small Angle, Characterization of Colloidal Dispersions, Percutaneous Absorption and Monoclonal Antibodies Production and Characterization.

## INSTITUTE BOARD MEMBERS

|   |  |
|---|--|
| Àngel Messeguer Peypoch                       | Director   |
| Rosa Infante Martínez-Pardo                   | Deputy Director  |
| Joan Ricard Ibáñez Villar                     | Head of Administration                                     |
| Santiago Olivella Nello                       | Department of Biological Chemistry and Molecular Modelling |
| Gemma Fabriàs Domingo                         | Department of Biomedicinal Chemistry                       |
| Mª Pilar Marco Colás                          | Department of Chemical and Biomolecular Nanotechnology     |
| Ramón Pons Pons                               | Department of Chemical and Surfactants Technology          |
| Jaume Caelles Balcells                        | Personnel Representative                                   |
| Avencia Diez Ortego                           | Personnel Representative                                   |
| Meritxell Martí Gelabert                      | Personnel Representative                                   |
| Josep Carilla Auguet/<br>Pilar Domènech Duran | Invited Services Representative                            |

## ADMINISTRATION

Director:  
Deputy Director:  
Head of Administration:  
Secretaries:

Àngel Messeguer Peypoch  
Rosa Infante Martínez-Pardo  
Joan Ricard Ibáñez Villar  
Lídia Beltran Fabregat  
Josefina Estremera Solé

## «Ad honorem» MEMBERS

FRANCISCO CAMPS DIEZ  
M DOLORS DE CASTELLAR BERTRAN  
PILARERRA SERRABASA  
MIQUEL VENDRELL MELICH

## **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 Biomedicinal 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

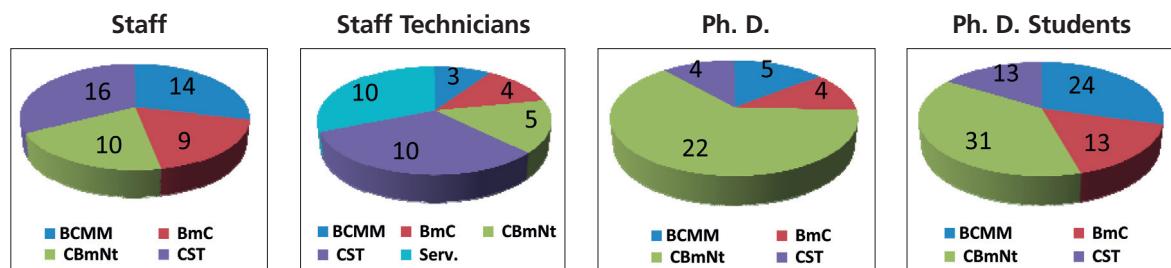
## **IQAC FACILITIES**

**Characterization of Colloidal Dispersions Service**  
**Custom Antibody Service (CAbs)**  
**Organic Microanalysis Service**  
**Biodegradation and Aquatic Toxicity Service**  
**Spectroscopy Service**  
**Skin Absorption and Skin Efficacy Services**  
**SAXS-WAXS Service**  
**Synthesis of High Added Value Molecules Service**  
**Thermal Analysis and Calorimetry Service**

## NUMERICAL SUMMARIES

| PERSONNEL | Staff           | Technicians     | Ph. D. | Ph. D. Students | Post. Graduates |
|-----------|-----------------|-----------------|--------|-----------------|-----------------|
| BCMM      | 14 <sup>a</sup> | 3               | 5      | 24              |                 |
| BmC       | 9               | 4               | 4      | 13              |                 |
| CBmNt     | 10 <sup>b</sup> | 5 <sup>c</sup>  | 22     | 31              | 4               |
| CST       | 16 <sup>b</sup> | 10 <sup>d</sup> | 4      | 13 <sup>e</sup> |                 |
| Services  |                 | 10              |        |                 |                 |
| TOTAL     | 49              | 32              | 35     | 81              | 4               |

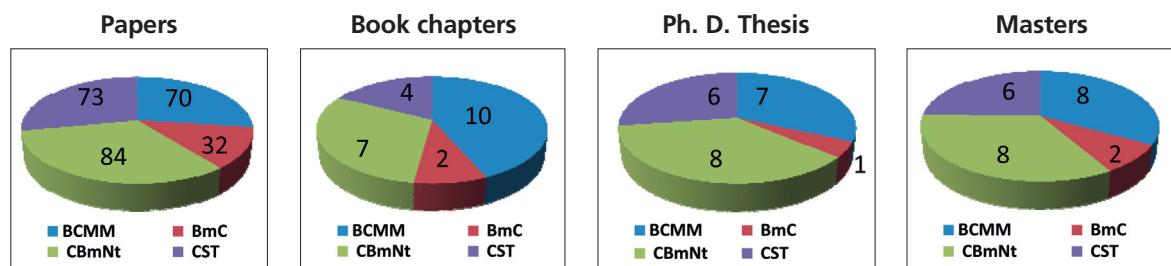
<sup>a</sup> in SC (1). <sup>b</sup> «ad honorem» (+1). <sup>c</sup> shared by service (2). <sup>d</sup> shared by service (4). <sup>e</sup> shared by service (3)



| SCIENTIFIC OUTPUT<br>(2009+2008) | ISI Journals  | No-ISI int | No-ISI nat            | Book chapters        |
|----------------------------------|---------------|------------|-----------------------|----------------------|
| BCMM                             | 70 (40+30)    | 3 (0+3)    |                       | 10 (4+6)             |
| BmC                              | 32 (17+15)    | 2 (2+0)    |                       | 2 (1+1)              |
| CBmNt                            | 84 (45+39)    | 3 (1+2)    | 1 (0+1)               | 7 <sup>†</sup> (5+1) |
| CST                              | 73 (38+35)    |            | 3* <sup>2</sup> (3+0) | 4 <sup>†</sup> (3+0) |
| Services                         |               |            | 2* <sup>2</sup> (2+0) |                      |
| TOTAL                            | 259 (140+119) | 8 (3+5)    | 6 (5+1)               | 23 (15+8)            |
| (NON DUPLICATED)                 | 225 (110+115) | 8 (3+5)    | 4 (3+1)               | 21 (13+8)            |

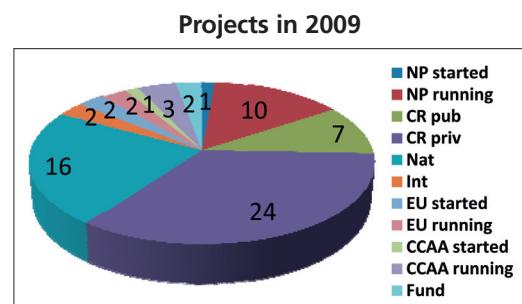
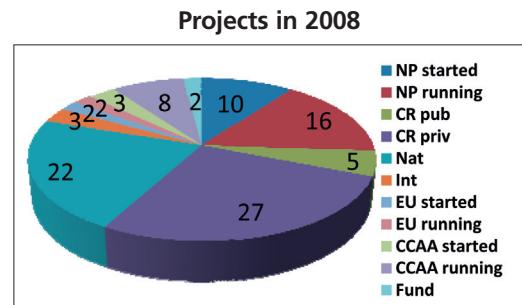
\*Duplicated (common publications in two entries). † Duplicated (common publications in one department).

| ACADEMIC OUTPUT | PhD | Thesis Masters | Courses | Conferences | Congress | Editorial |
|-----------------|-----|----------------|---------|-------------|----------|-----------|
| BCMM            | 7   | 8              | 9       | 13          | 5        | 3         |
| BmC             | 1   | 2              | 2       | 2           |          |           |
| CBmNt           | 8   | 8              |         |             |          |           |
| CST             | 6   | 6              | 2       | 17          | 8        | 1         |

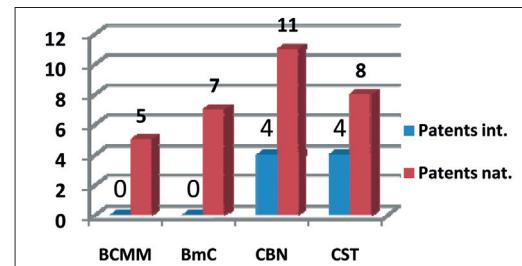


| PROJECTS      | 2008       | budget        | 2009  | budget    |               |
|---------------|------------|---------------|-------|-----------|---------------|
| NP started    | 10         | 779,2         | 1346  | 1         | 49,4          |
| NP running    | 16         | 566,8         |       |           | 335,3         |
| CR pub        | 5          | 107,4         | 833   | 7         | 141,9         |
| CR priv       | 27         | 725,6         |       |           | 739,5         |
| National      | 22         | 222,2         |       | 16        | 112,3         |
| International | 3          | 96,6          |       | 2         | 82,7          |
| EU started    | 2          | 58,8          | 127,4 | 2         | 262,1         |
| EU running    | 2          | 68,6          |       |           | 358,4         |
| CCAA started  | 3          | 80,6          | 158,1 | 1         | 44,3          |
| CCAA running  | 8          | 77,5          |       |           | 143           |
| Funds (other) | 2          | 5,8           |       | 2         | 9,6           |
| <b>TOTAL</b>  | <b>100</b> | <b>2789,1</b> |       | <b>70</b> | <b>1780,8</b> |

NP: National Project; CR: Contracted Research; CCAA: Autonomous Community



| TECHNOLOGICAL OUTPUT | Patents int | Patents nat |
|----------------------|-------------|-------------|
| BCMM                 |             | 5           |
| BmC                  |             | 7           |
| CBN                  | 4           | 11          |
| CST                  | 4           | 8           |



## 2008-2009 JOURNAL PUBLICATIONS SUMMARY

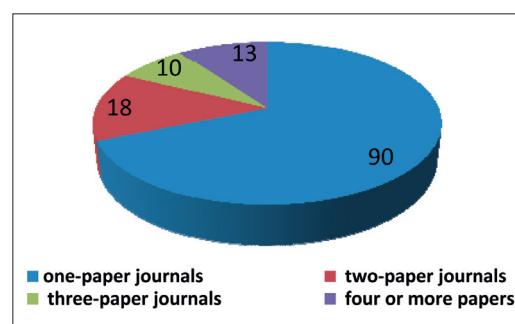
Total number of journals: 131

Number of Journals with one single paper: 90 (68.70 %)

Number of Journals with more than one paper: 41 (31.30 %)

Number of Journals with two or three papers: 10 (3); 18 (2)

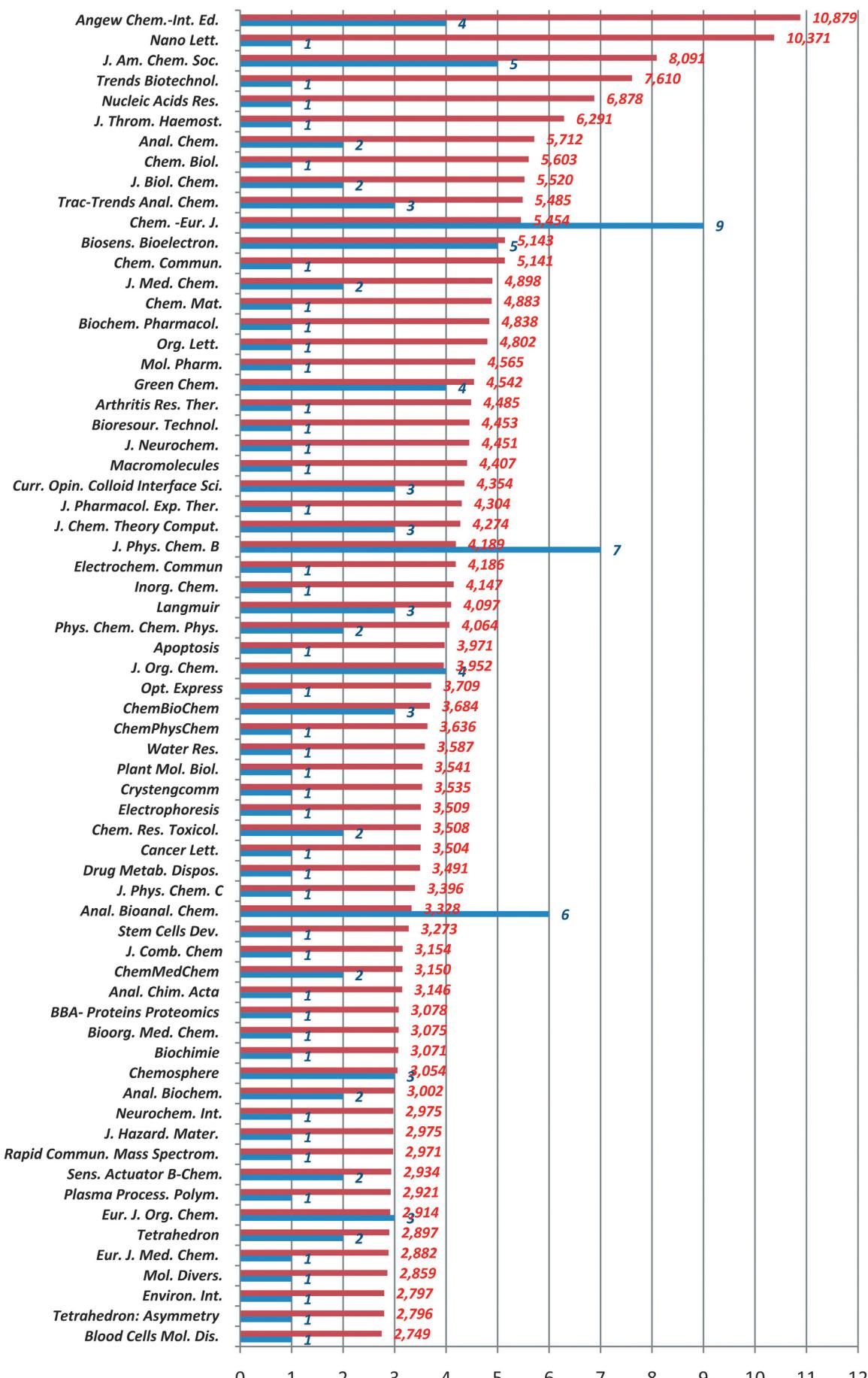
Number of Journals with more than three papers: 2 (9); 1 (7); 1 (6); 3 (5); 6 (4)

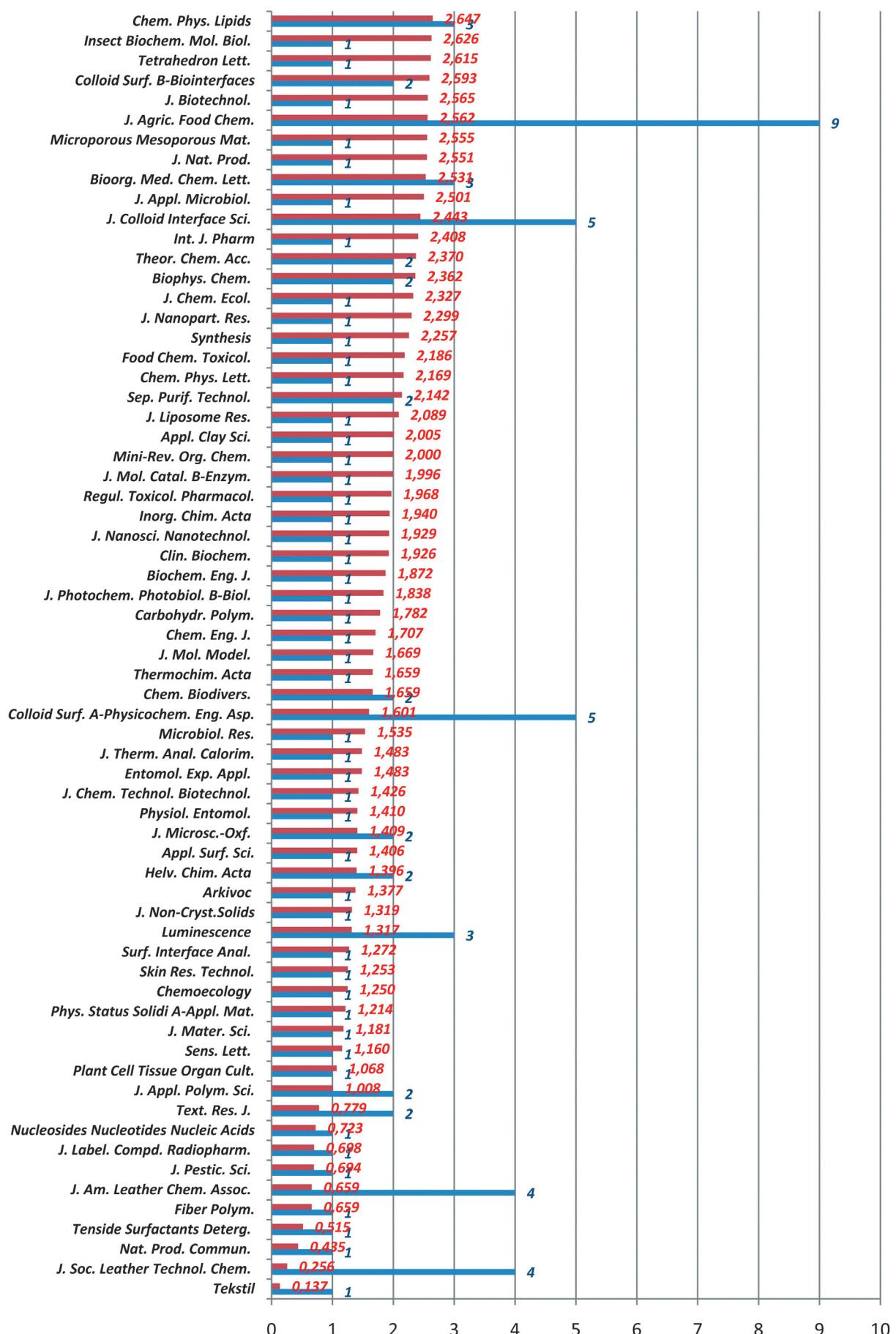


Journals listed by decreasing impact factor (next pages):

Impact factor (2009 selected value if papers in both years)

total number of papers





## SPECIAL EVENTS

### **14th Fèlix Serratosa Conference (19/01/2009)**

J. Veciana Miró

*Institut de Ciència de Materials de Barcelona.*

Nanostructuring functional molecules. From basic science to applications

H. Waldmann

*Institut Max Planck de Fisiología Molecular (Dortmund)*

Biology oriented synthesis (small molecules for biology, cheminformatics, bioinformatics)

### **Prof. Juan José García Domínguez Memorial (30/06/2009)**

E. Julià

*Instituto Químico de Sarriá, Barcelona*

El fomento de la innovación en universidades y organismos públicos de investigación

### **I Workshop CBN'09 (19/10/2009)**

Michael Gradzielski

*Technische Universität (Berlin)*

Mesodynamics: Observing self-aggregating systems in motion by means of SAXS and SANS experiments

## AWARDS AND NOMINATIONS

**A. Meseguer**

Advisory Council Member, Chemistry Faculty, Universitat de Barcelona

# 2

**DEPARTMENT OF BIOLOGICAL CHEMISTRY  
AND MOLECULAR MODELLING**



## DEPARTMENT OF BIOLOGICAL CHEMISTRY AND MOLECULAR MODELLING



**Head:** Santiago Olivella Nello (up to 30/09/2009), Jesús Joglar Tamargo (after 30/09/2009)

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 byproducts 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.

Biorational control of plagues. Characterization of insect proteins by means of proteomic and molecular biology techniques.

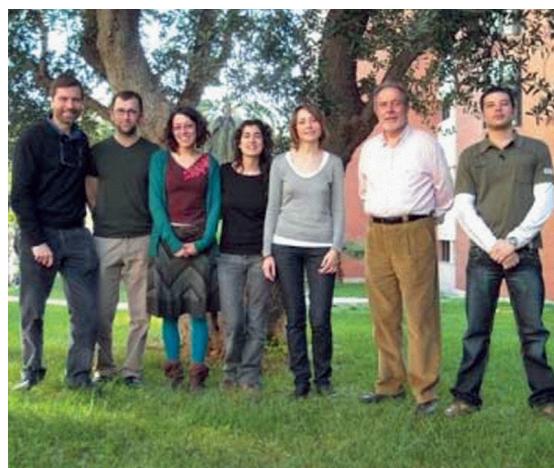
Persistent organic free radicals as biochemical sensors.

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



## STAFF

JOSEP LLUÍS TORRES SIMON, GROUP LEADER  
LUIS JULIÁ BARGÉS

## TECHNICIAN

JORDI PERACAULA PUJADAS

## Ph. D.

ELISABET FUGUET

## Publications (articles)

### All organic discotic radical with spin carrying rigid-core showing intracolumnar interactions and multifunctional properties

Castellanos, S., López-Calahorra, F., Brillas, E., Juliá, L., Velasco, D.  
*Angew. Chem.-Int. Ed.* **2009**, 48, 6516-6519

### A novel approach to enhancing cellular glutathione levels

Maher, P., Leverenz, J., Lozano, C., Torres, J.L.  
*J. Neurochem.* **2008**, 107, 690-700

### Oxidant activity of tris(2,4,6-trichloro-3,5-dinitrophenyl)methyl (HNTTM) radical with catechol and pyrogallol. Mechanistic considerations.

Carreras, A., Esparbé, I., Brillas, E., Rius, J., Torres, J.L., Juliá, L.  
*J. Org. Chem.* **2009**, 74, 2368-2373

### Taking advantage of the radical character of tris(2,4,6-trichlorophenyl)methyl to synthesize new paramagnetic glassy molecular materials

Castellanos, S., Velasco, D., López-Calahorra, F., Brillas, E., Juliá, L.  
*J. Org. Chem.* **2008**, 73, 3759-3767

### The maize ZmMYB42 represses the phenylpropanoid pathway and affects the cell wall structure, composition and degradability in *Arabidopsis thaliana*

Sonbol, F.M., Fornalé, S., Capellades, M., Encina, A., Touriño, S., Torres, J.L., Rovira, P., Ruel, K., Puigdoménech, P., Rigau, J., Caparrós-Ruiz, D.  
*Plant Mol. Biol.* **2009**, 70, 283-296

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.

## Ph. D. STUDENTS

ANNA CARRERAS CARDONA  
SONIA CASTELLANOS ORTEGA  
MARISA MATEOS MARTÍN  
JUAN ANTONIO MESA  
EUNICE MOLINAR  
SONIA TOURIÑO EIRÍN

### Highly galloylated tannin fractions from witch hazel (*Hamamelis virginiana*) bark: electron transfer capacity, in vitro antioxidant activity and effects on skin related cells

Touriño, S., Lizárraga, D., Carreras, A., Lorenzo, S., Ugartondo, V., Mitjans, M., Vinardell, M.P., Juliá, L., Cascante, M., Torres, J.L.  
*Chem. Res. Toxicol.* **2008**, 21, 696-704

### LC-ESI-MS/MS combined with high resolution LC-ESI-TOF for the identification of phenolics from grape antioxidant dietary fiber

Touriño, S., Fuguet, E., Jauregui, O., Saura-Calixto, F., Cascante, M., Torres, J.L.  
*Rapid. Commun. Mass Spectrom.* **2008**, 22, 3489-3500

### Light-emitting persistent radicals for efficient sensor devices of solvent polarity

López, M., Velasco, D., López-Calahorra, F., Juliá, L.  
*Tetrahedron Lett.* **2008**, 49, 5196-5199

### Biobased epicatechin conjugates protect erythrocytes and non tumoral cell lines from H<sub>2</sub>O<sub>2</sub>- induced oxidative stress

Ugartondo, V., Mitjans, M., Torres, J.L., Vinardell, P.  
*J. Agric. Food Chem.* **2009**, 57, 4459-4465

### Galloylated polyphenols efficiently reduce α-tocopherol radicals in a phospholipid model system composed of sodium dodecyl sulfate (SDS) micelles

Pazos, M., Torres, J.L., Andersen, M.L., Skibsted, L.H., Medina, I.  
*J. Agric. Food Chem.* **2009**, 57, 5042-5048

### **Phenolic metabolites of grape antioxidant dietary fiber in rat urine**

Touriño, S., Fuguet, E., Vinardell, P., Cascante, M., Torres, J.L.

*J. Agric. Food Chem.* **2009**, *57*, 11418-11426

### **Witch Hazel (*Hamamelis virginiana*) fractions and the importance of gallate moieties-electron transfer capacities in their antitumoral properties**

Lizárraga, D., Touriño, S., Reyes, F., Kok, T. de, Delft, J. Van, Maas, L., Briedé, J., Centelles, J.J., Torres, J.L., Cascante, M.

*J. Agric. Food Chem.* **2008**, *56*, 11675-11682

### **Novel separation of bioactive catechin derivatives from complex plant mixtures by anion exchange chromatography**

Lozano, C., Bujons, J., Torres, J.L.

*Sep. Pur. Technol.* **2008**, *62*, 317-322

### **Publications (books and book chapters)**

Medina, I., Cascante, M., Torres, J.L., Pazos, M., 2008

#### **Natural bioactive antioxidants for the enrichment of seafood**

In: Functional Food and Health

Shibamoto, T., Kanazawa, K., Shahidi, F., Ho, C.T. (Eds.)

American Chemical Society, **993**, *17*, 192-198

### **Polymerization and galloylation: two important aspects for antiproliferative properties of procyanidin-rich natural extracts**

Lizárraga, D., Lozano, C., Touriño, S., Centelles, J.J., Torres, J.L., Cascante, M.

*Elec. J. Environ. Agric. Food Chem.* **2008**, *7*, 3334-3338

### **Antioxidant/prooxidant effects of bioactive polyphenolics**

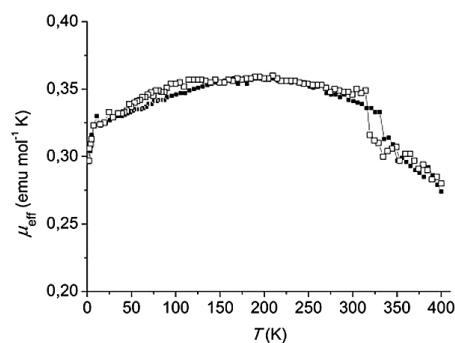
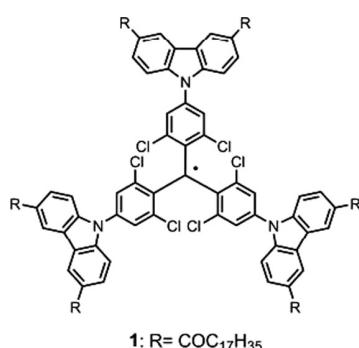
Touriño, S., Lizárraga, D., Carreras, A., Matito, C., Ugartondo, V., Mitjans, M., Centelles, J.J.,

Vinardell, M.P., Julià, L., Cascante, M., Torres, J.L.

*Elec. J. Environ. Agric. Food Chem.* **2008**, *7*, 3339-3343

### **Research highlights**

**The first paramagnetic all-organic disk-like liquid crystal that localizes the unpaired electron in the center of the aromatic core.** This compound has two enantiotropic columnar phases: a glassy rectangular columnar phase at low temperatures and an ordered hexagonal columnar mesophase above room temperature. Core-core interactions and their derived magnetic interactions during the Colho mesophase have been detected. This new radical adduct has advantageous electrochemical and photoluminescence characteristics for its application in electronic devices, such as absorption in the visible spectrum, emission in the red region of the spectrum, and ambipolar redox properties owing to the existence of the SOMO in which the single electron mainly resides.



Temperature dependence of the effective magnetic moment ( $\mu_{\text{eff}}$ ) of radical 1 at a rate of 10 K/min during the cooling (white squares) and the second heating process (black squares)

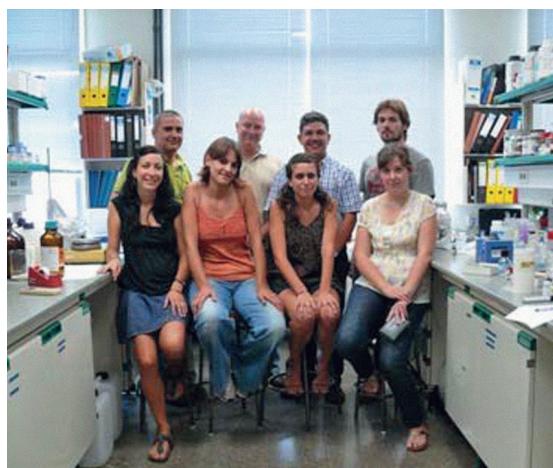
### **All organic discotic radical with spin carrying rigid-core showing intracolumnar interactions and multifunctional properties**

Castellanos, S., López-Calahorra, F., Brillas, E.,

Julià, L., Velasco, D.

*Angew. Chem.-Int. Ed.* **2009**, *48*, 6516-6519

# Biotransformation and Bioactive Molecules



## STAFF

PEDRO CLAPES SABORIT, GROUP LEADER  
JORGE BUJONS VILÀS  
GLORIA CAMINAL SAPERAS (Service Commission UAB)  
JESUS JOGLAR TAMARGO

The research is focused on the design, production and evaluation of carboligation biocatalysts and biologically active molecules. Biocatalytic carbon-carbon bond formation, in the core of a chemoenzymatic methodology, has the potential to access stereochemically complex molecules that are not easily produced by conventional organic synthesis. Hence, they are particularly appropriate for obtaining new types of structures (i.e. to generate molecular diversity) accessible for investigations in drug discovery.

## Ph. D. STUDENTS

BRUNO ALMEIDA COTRIM  
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XAVIER GARRABOU PI  
LIVIA GÓMEZ CORTÉS  
MARIANA GUTIERREZ TEJEDA  
ARISTOTELIS KOTRONOULAS  
ANNA SZEKRENYI

## Publications (articles)

### Asymmetric self- and cross-aldo reaction of glycolaldehyde catalyzed by D-fructose-6-phosphate aldolase

Garrabou, X., Castillo, J.A., Guérard-Hélaine, C., Parella, T., Joglar, J., Lemaire, M., Clapés, P. *Angew. Chem.-Int. Ed.* **2009**, 48, 5521-5525

### Protein flexibility and metal coordination changes in DHAP-dependent aldolases

Jiménez, A., Clapés, P., Crehuet, R. *Chem.-Eur. J.* **2009**, 15, 1422-1428

### D-Fructose-6-phosphate aldolase in organic synthesis: cascade chemical-enzymatic preparation of sugar-related polyhydroxylated compounds

Concia, A. L., Lozano, C., Castillo, J. A., Parella, T., Joglar, J., Clapés, P. *Chem.-Eur. J.* **2009**, 15, 3808-3816

### Dihydroxyacetone phosphate aldolase-catalyzed synthesis of structurally diverse polyhydroxylated pyrrolidine derivatives and evaluation of their glycosidase inhibitory properties

Calveras, J., Egido-Gabás, M., Gómez, L., Casas, J., Parella, T., Joglar, J., Bujons, J., Clapés, P. *Chem.-Eur. J.* **2009**, 15, 7310-7328

### Serine hydroxymethyl transferase from *Streptococcus thermophilus* and L-threonine aldolase from *Escherichia coli* as stereocomplementary biocatalysts for the synthesis of $\beta$ -hydroxy- $\alpha,\omega$ -diamino acid derivatives

Gutiérrez, M.L., Garrabou, X., Agosta, E., Servi, S., Parella, T., Joglar, J., Clapés, P. *Chem.-Eur. J.* **2008**, 14, 4647-4656

### Serotonergic neurotoxic thioether metabolites of 3,4-methylenedioxymethamphetamine (MDMA, «Ecstasy»): synthesis, isolation and characterization of diastereoisomers

Pizarro, N., Torre, R. de la, Joglar, J., Okumura, N., Perfetti, X., Lau, S.S., Monks, T.J. *Chem. Res. Toxicol.* **2008**, 21, 2271-2279

### Neurotoxic thioether adducts of MDMA identified in human urine after ecstasy ingestion

Perfetti, X., O'Mathúna, B., Pizarro, N., Cuyàs, E., Khymenets, O., Almeida, B., Pellegrini, M., Pichini, S., Lau, S. S., Monks, T. J., Farré, M., Pascual, J. A., Joglar, J., de la Torre, R. *Drug Metab. Dispos.* **2009**, 37, 1448-1455

### Ability of white-rot fungi to remove selected pharmaceuticals and identification of degradation products of ibuprofen by *Trametes versicolor*.

Marco-Urrea, E., Pérez-Trujillo, M., Vicent, T., Caminal, G. *Chemosphere* **2009**, 74, 756-772

### Metabolites from the biodegradation of triphenylmethane dyes by *Trametes versicolor* or laccase.

Casas, N., Parella, T., Vicent, T., Caminal, G., Sarrà, M. *Chemosphere* **2009**, 75, 1344-1349

### Mechanisms of trichloroethylene mineralization by the white-rot fungus *Trametes versicolor*

Marco-Urrea, E., Parella, T., Gabarrell, X., Caminal, G., Vicent, T., Reddy, C.A. *Chemosphere* **2008**, 70, 404-410

- Dechlorination of 1,2,3- and 1,2,4-trichlorobenzene by the white-rot fungus *Trametes versicolor*.**  
 Marco-Urrea, E., Pérez-Trujillo, M., Caminal G., Vicent, T.  
*J. Hazard. Mater.* **2009**, 166, 1141-1147
- Development of an antibiotic-free plasmid selection system based on glycine auxotrophy for recombinant protein overproduction in *Escherichia coli***  
 Vidal, L., Pinsach, J., Striedner, F., Caminal, G., Ferrer, P.  
*J. Biotechnol.* **2008**, 134, 127-136
- Comparative evaluation of cytotoxicity and phototoxicity of mono and diacylglycerol amino acid-based surfactants**  
 Vinardell, M.P., Benavides, T., Mitjans, M., Infante, M.R., Clapés, P., Clothier, R.  
*Food Chem. Toxicol.* **2008**, 46, 3837-3841
- Screening of plant peptidases for the synthesis of arginine-based surfactants**  
 Morcelle, S.R., Liggieri, C.S., Bruno, M.A., Priolo, N., Clapés, P.  
*J. Mol. Catal. B-Enzym.* **2009**, 57, 177-182

## Publications (books and book chapters)

Clapés, P., Sprenger, G.A., Joglar, J., 2008  
**Novel strategies in aldolase-catalyzed synthesis of iminosugars**  
 In: Modern biocatalysis: stereoselective and environmentally friendly reactions  
 Fessner, W.-D., Anthonsen, T. (Eds.)  
 Wiley-VCH, Weinheim, Germany, 19, 229-311

## Research highlights

### Small but great: *Escherichia coli* never ends to surprise us.

d-Fructose-6-phosphate aldolase (FSA) discovered in the *E. coli* genome is an amazing powerful catalyst for asymmetric C-C bond formation. The physiological role of this protein *in vivo* remains uncertain. FSA can be easily produced in the lab, it is thermostable and it catalyzes stereoselectively the synthesis of a number of natural products in efficient, clean and in environmentally friendly mild conditions. Its selective catalytic properties allow organic chemists to access easily to sugars of the ketose and aldose family and their derivatives and analogs, molecules difficult to prepare by purely chemical procedures.

### Asymmetric self- and cross-alcohol reaction of glycolaldehyde catalyzed by D-fructose-6-phosphate aldolase

Garrabou, X., Castillo, J.A., Guérard-Hélaine, C., Parella, T., Joglar, J., Lemaire, M., Clapés, P.  
*Angew. Chem.-Int. Ed.* **2009**, 48, 5521-5525

**VIP: Very Important Paper.** Highlighted in *Synfacts* **2009**, 9, 1044-1044

### Low-cost process development and scale-up of *Trametes versicolor* pellets production

Borràs, E., Blánquez, P., Sarrà, M., Caminal, G., Vicent, T.  
*Biochem. Eng. J.* **2008**, 42, 61-66

### Required equilibrium studies for designing a three-phase birreactor to degrade trichloroethylene (TCE) and tetrachloroethylene (PCE) by *Trametes versicolor*

Vilaplana, M., Marco-Urrea, E., Gabarrell, X., Sarrà, M., Caminal, G.  
*Chem. Eng. J.* **2008**, 144, 21-27

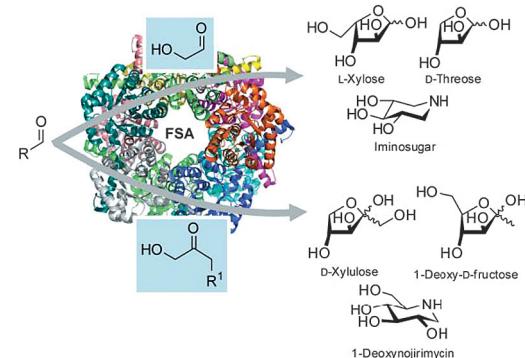
### A dynamic view of enzyme catalysis

Jiménez, A., Clapés, P., Crehuet, R.  
*J. Mol. Model.* **2008**, 14, 735-746

### Aerobic degradation by white-rot fungi of trichloroethylene (TCE) and mixtures of TCE and perchloroethylene (PCE)

Marco-Urrea, E., Gabarrell, X., Caminal, G., Vicent, T., Reddy, C.A.  
*J. Chem. Technol. Biotechnol.* **2008**, 83, 1190-1196

López-Santín, J., Álvaro, G., Clapés, P., 2008  
**Use of aldolases for asymmetric synthesis**  
 In: Enzyme biocatalysis: principles and applications  
 Illanes, A. (Ed.)  
 Springer Science, 6.5 333-335



### D-Fructose-6-phosphate aldolase in organic synthesis: cascade chemical-enzymatic preparation of sugar-related polyhydroxylated compounds

Concia, A. L., Lozano, C., Castillo, J. A., Parella, T., Joglar, J., Clapés, P.  
*Chem.-Eur. J.* **2009**, 15, 3808-3816

# 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 welldefined 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.

## STAFF

IGNACIO ALFONSO RODRIGUEZ

## Publications (articles)

### A ferromagnetic [Cu<sub>3</sub>(OH)<sub>2</sub>]<sup>4+</sup> cluster formed inside a tritopic nona-azapyridinophane. Crystal structure and solution studies.

González-Álvarez, A., Alfonso, I., Cano, J., Díaz, P., Gotor, V., Gotor-Fernández, V., García-España, E., García-Granda, S., Jiménez, H., Lloret, F. *Angew. Chem.-Int. Ed.* **2009**, 48, 6055-6058

### Supramolecular control for the modular synthesis of pseudopeptidic macrocycles through an anion-templated reaction

Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V., Rubio, J.

*J. Am. Chem. Soc.* **2008**, 130, 6137-6144

### Designed folding of pseudopeptides: the transformation of a configurationally driven preorganization into a stereoselective multicomponent macrocyclization

Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V.

*Chem.-Eur. J.* **2008**, 14, 8879-8891

### Unraveling the molecular recognition of amino acid derivatives by a pseudopeptidic macrocycle: ESI-MS, NMR, fluorescence and modeling studies

Alfonso, I., Burguete, M. I., Galindo, F., Luis, S.V., Vigara, L.

*J. Org. Chem.* **2009**, 74, 6130-6142

### A simple helical macrocyclic polyazapyridinophane as a stereoselective receptor of biologically important dicarboxylates under physiological conditions

González-Alvarez, A., Alfonso, I., Díaz, P., García-España, E., Gotor-Fernández, V., Gotor, V. *J. Org. Chem.* **2008**, 73, 374-382

### Catalyzed oxidative corrosion of porous silicon used as an optical transducer for ligand-receptor interactions

Voelcker, N.H., Alfonso, I., Ghadiri, M.R. *ChemBioChem* **2008**, 9, 1776-1786

### Crystal structures of the HCl salts of pseudopeptidic macrocycles display «knobs into holes» hydrophobic interactions between aliphatic side chains

Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V. *Crystengcomm* **2009**, 11, 735-738

### Cycloalkane-1,2-diamine derivatives as chiral solvating agents. Study of the structural variables controlling the NMR enantiodiscrimination of chiral carboxylic acids

Peña, C., González-Sabin, J., Alfonso, I., Rebollo, F., Gotor, V.

*Tetrahedron* **2008**, 64, 7709-7717

### Recent developments in chiral polynitrogenated synthetic receptors for anions

Alfonso, I.

*Mini-Rev. Org. Chem.* **2008**, 5, 33-46

## Publications (books and book chapters)

### Asymmetric organic synthesis with enzymes

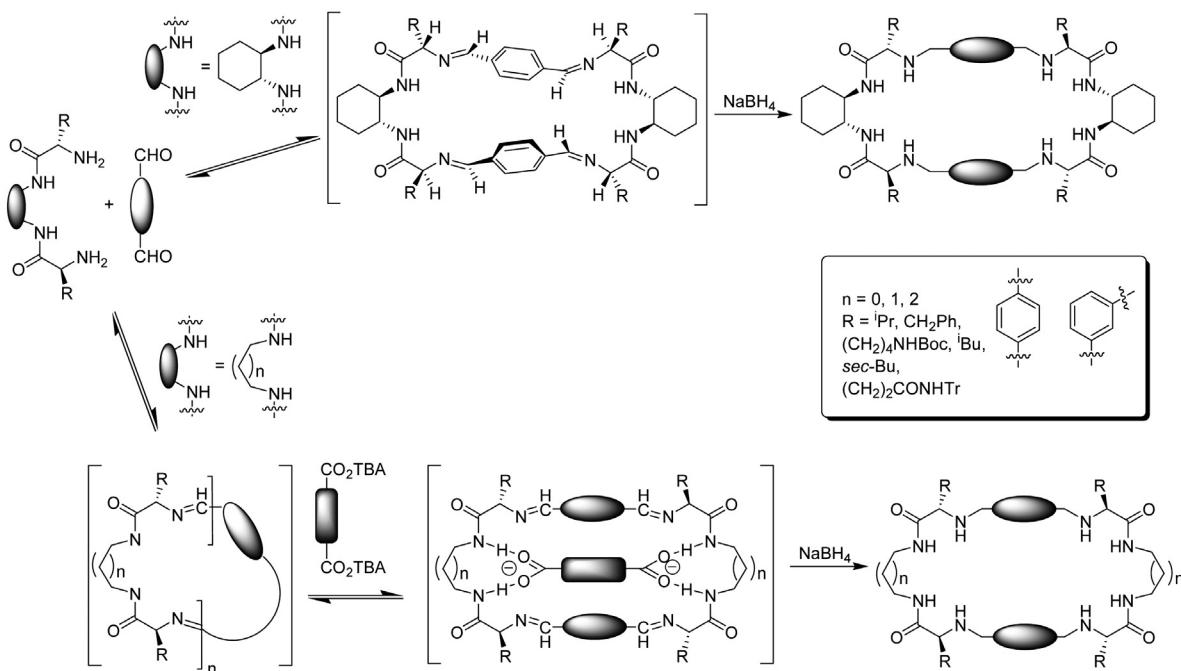
Gotor, V., Alfonso, I., García-Urdiales, E. (Eds.) 2008  
Wiley-VCH, Weinheim,  
Germany ISBN: 978-3-527-31825-4

## Research highlights

The efficient synthesis of large ring size pseudopeptidic macrocycles through a multicomponent [2+2] reductive amination reaction has been accomplished, using two conceptually different approaches.<sup>1,2</sup> The first one<sup>1</sup> is based on a configurationally driven folding of the open chain pseudopeptidic precursor bearing a rigid (*R,R*)-cyclohexane-1,2-diamine moiety. A remarkable *match/mismatch* relationship between the configurations of the chiral centers of the cyclic diamine and those of the peptidic frame was observed. The macrocyclic tetraimine intermediates have been deeply studied by NMR, CD and molecular modeling, supporting the appropriate preorganization induced by the *match* combination of the chiral centers. Structural studies showed an intrinsic lower reactivity of the *mismatch* combination, even with acyclic model systems. The second approach<sup>2</sup> took advantage of the anion-amide non-covalent interactions, by carrying out an anion templated synthesis of the corresponding

pseudopeptidic macrocycles having flexible spacers. The formation of the corresponding macrocyclic tetraimino-template supramolecular complexes was demonstrated by NMR (ROESY and PGSE) and mass spectrometry (ESI-TOF). Different variables like the aliphatic spacer between amino acidic moieties, geometry of the dialdehyde and structure of the amino acid side chains were thoroughly studied, and their effect in the formation and stability of the supramolecular complexes discussed. The conformational preorganization induced by the template has been monitored by circular dichroism (CD), reflecting the differences observed in the isolated yields, as well as by NMR spectroscopy.

Finally, X-ray analysis of the HCl salts of some of the macrocycles showed an interesting pattern. The macrocyclic rings stack in columnar aggregates stabilized by hydrogen bonding and hydrophobic non-covalent interactions.<sup>1,3</sup>



- Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V. *Chem.-Eur. J.* **2008**, *14*, 8879-8891
- Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V., Rubio, J. *J. Am. Chem. Soc.* **2008**, *130*, 6137-6144
- Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V. *CrystEngComm* **2009**, *11*, 735-738

# 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 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 in the insects antennae.

## STAFF

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## TECHNICIAN

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CARMEN QUERO LÓPEZ

## Ph. D. STUDENTS

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GERARD CAROT SANS  
BEN FURSTENAU  
RAFAEL GAGO OTERO  
JOSEP RAYÓ COMPANY  
ANNA RODRIGUEZ RIVERO

## Publications (articles)

### Improved resolution in the acidic and basic region of 2-DE of insect antennae proteins using hydroxyethyl disulfide

Acín, P., Rayó, J., Guerrero, A., Quero, C.  
*Electrophoresis* **2009**, 30, 2613-2616

### Asymmetric synthesis of (R) and (S)-4-methyl-octanoic acids. A new route to chiral fatty acids with remote stereocenters

Muñoz, L., Bosch, M.P., Rosell, G., Guerrero, A.  
*Tetrahedron: Asymmetry* **2009**, 20, 420-424

### Expression of differential antennal proteins in males and females of an important crop pest, *Sesamia nonagrioides*

Acín, P., Carrascal, M., Abián, J., Guerrero, A., Quero, C.  
*Insect Biochem. Mol. Biol.* **2009**, 39, 11-19

### Development and biological activity of a new antagonist of the pheromone of the codling moth *Cydia pomonella*

Giner, M., Sans, A., Riba, M., Bosch, D., Gago, R., Rayo, J., Rosell, G., Guerrero, A.  
*J. Agric. Food Chem.* **2009**, 57, 8514-8519

### Development of an efficient pheromone-based trapping method for the banana root borer *Cosmopolites sordidus*

Reddy, G.V.P., Cruz, Z.T., Guerrero, A.  
*J. Chem. Ecol.* **2009**, 35, 111-117

### Reduction of damage by the Mediterranean corn borer *Sesamia nonagrioides* and the European corn borer *Ostrinia nubilalis* in maize fields by a trifluoromethyl ketone pheromone analogue

Solé, J., Sans, A., Riba, M., Rosa, E., Bosch, M.P., Barrot, M., Palència, J., Castellà, J., Guerrero, A.  
*Entomol. Exp. Appl.* **2008**, 126, 28-39

### Biosynthetic pathways of the pheromone of the Egyptian armyworm, *Spodoptera littoralis*

Muñoz, L., Rosell, G., Quero, C., Guerrero, A.  
*Physiol. Entomol.* **2008**, 33, 275-290

### Differential activity of non-fluorinated and fluorinated analogues of the European corn borer pheromone

Solé, J., Sans, A., Riba, M., Rosell, G., Rosa, E., Muñoz, L., Bosch, M.P., Guerrero, A.  
*Chemoecology* **2008**, 18, 99-108

### Biorational insecticides in pest management

Rosell, G., Quero, C., Coll, J., Guerrero, A.  
*J. Pestic. Sci.* **2008**, 33, 103-121

### Penta-deuterated acid precursors in the pheromone biosynthesis of the Egyptian armyworm, *Spodoptera littoralis*

Muñoz, L., Rosell, G., Guerrero, A.  
*J. Labelled Compd. Rad.* **2009**, 52, 493-498

## Research highlights

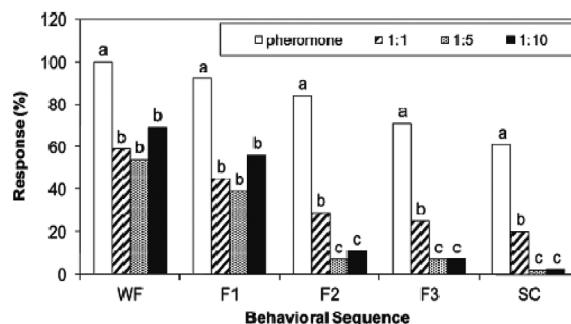
The main aim of the Chemical Ecology Group deals with studies directed to control pests by biorational, specific and environmentally-friendly methods. In this context, the main features accomplished by the Group in the period 2008-2009 are the following:

1. Discovery of a remarkable disruptant of the pheromone of the Mediterranean corn borer, *Sesamia nonagrioides*, to control the pest. Deployment of (Z)-11-hexadecenyl trifluoromethyl ketone, a close-related analogue of the pheromone, in dispensers containing 800 mg of the compound in an infested maize field caused a remarkable reduction of damage induced by larvae of *S. nonagrioides* and also of the sympatric species *Ostrinia nubilalis*. The effectiveness of the treatment was evident by the reduction in the number of larvae found per plant in the treated plot, and also by the number of plants attacked relative to the control plot. This study represents a step forward in the utilization of trifluoromethyl ketone analogues of insect pheromones in pest control (Solé et al., *Entomol. Exp. Appl.* **2008**, 126, 28-39). These compounds are considered non-toxic as proved in earlier toxicity experiments on Swiss mice.

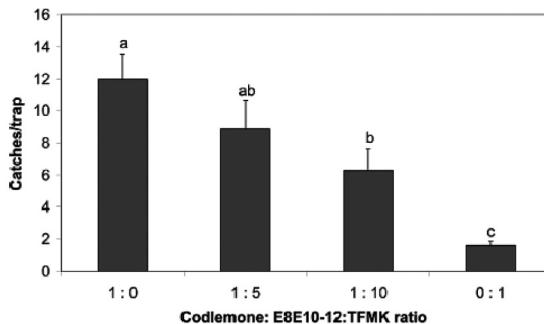
2. Development of a new antagonist of the pheromone of the codling moth *Cydia pomonella*. (E,E)-8,10-dodecadienyl trifluoromethyl ketone, a structurally related analogue of the main

component of the pheromone (codlemone), induces in a wind tunnel a remarkable disruptive effect on the behaviour of males when they are attracted to a source baited with mixtures of pheromone:antagonist in 1:1 to 1:10 ratio (Figure 1). In the field, traps baited with mixtures of pheromone:antagonist 1:10 attracted considerably lower number of males than the natural attractant (Figure 2). The antagonist might be a new interesting candidate to consider in future strategies to control the pest (Giner et al., *J. Agric. Food Chem.* **2009**, 57, 8514-8519).

3. Development of a sensitive proteomic methodology to identify antennal proteins. Characterization of the proteins implicated in the chemical communication of insects can also help to develop new methods for pest management. We have characterized some antennal proteins of *S. nonagrioides* by proteomic techniques, such as two-dimensional electrophoresis, MALDI-TOF MS and electrospray ionization tandem mass spectrometry (ESI-MS/MS). Most of the identified proteins were involved in olfaction. Pheromone binding proteins (PBP) were found in males but also in females although females did not respond electrophysiologically to their own pheromone. General odorant binding proteins (GOBP) were also identified and found to be expressed preferentially in females (Acín et al., *Insect Biochem. Mol. Biol.* **2009**, 39, 11-19).



**Figure 1.** Behavioral responses of *C. pomonella* males flying towards a source baited with mixtures of codlemone and E8,E10-12:TFMK in 1:1 (N=51), 1:5 (N=46) and 1:10 (N=45) ratio with regard to codlemone alone (N=79) in wind tunnel. Means within a specific behavior followed by the same letter are not significantly different ( $2 \times 2 \chi^2$  homogeneity test,  $P < 0.05$ ). Behavioral responses are: wing fanning (WF); flying upwind over 1/3 (F1), 2/3 (F2) or 3/3 (F3) the length of the tunnel, and source contact (SC).



**Figure 2.** Mean ( $\pm$ SD) number of catches of *C. pomonella* males per trap baited with mixtures of codlemone and (E,E)-8,10-dodecadienyl trifluoromethyl ketone in 1:0, 1:5, 1:10, and 0:1 ratios in field trials conducted in 2007 and 2008 (5 replicates per formulation each year). Bars with the same letter are not significantly different (Tukey's test,  $P < 0.05$ ).

# Theoretical and Computational Chemistry



The Theoretical and Computational Chemistry Group (QTC) studies the electronic structure and chemical 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.

## STAFF

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MIQUEL TORRENT-SUCARRAT

## Ph. D. STUDENTS

AURORA JIMÉNEZ RODRÍGUEZ  
ALEJANDRO MANSERGAS SÁNCHEZ  
ENRIQUE MARCOS BENTEO

## Publications (articles)

### Unconventional biradical character of titanium enolates

Moreira, I. de P.R., Bofill, J.M., Anglada, J.M., Solsona, J.G., Nebot, J., Romea, P., Urpí, F. *J. Am. Chem. Soc.* **2008**, 130, 3242-3243

### Theoretical and experimental studies on the mechanism of norbornadiene Pauson-Khand cycloadducts photoarrangement. Is there a pathway on the excited singlet potential energy surface?

Olivella, S., Solé, A., Lledó, A., Ji, Y., Verdaguer, X., Suau, R., Riera, A. *J. Am. Chem. Soc.* **2008**, 130, 16898-16907

### Protein flexibility and metal coordination changes in DHAP-dependent aldolases

Jiménez, A., Clapés, P., Crehuet, R. *Chem.-Eur. J.* **2009**, 15, 1422-1428

### Theoretical mechanistic study of the oxidative degradation of benzene in the troposphere: reaction of benzene-HO radical adduct with O<sub>2</sub>

Olivella, S., Solé, A., Bofill, J.M. *J. Chem. Theory Comput.* **2009**, 5, 1607-1623

### Inductive and external electric field effects in penta-coordinated phosphorus compounds

Marcos, E., Crehuet, R., Anglada, J.M. *J. Chem. Theory Comput.* **2008**, 4, 49-63

### Mechanisms for the reactions of hydroxyl radicals with acrolein: a theoretical study

Olivella, S., Solé, A. *J. Chem. Theory Comput.* **2008**, 4, 941-950

### Neutral gold(I) metallocsupramolecular compounds: synthesis and characterization, photophysical properties and density functional theory studies

Rodríguez, L., Lodeiro, C., Lima, J.C., Crehuet, R. *Inorg. Chem.* **2008**, 47, 4952-4962

### Role of vibrational anharmonicity in atmospheric radical hydrogen-bonded complexes

Torrent-Sucarrat, M., Anglada, J.M., Luis, J.M. *Phys. Chem. Chem. Phys.* **2009**, 11, 6377-6388

### Description of pentacoordinated phosphorus under an external electric field: which basis sets and semi-empirical methods are needed?

Marcos, E., Anglada, J.M., Crehuet, R. *Phys. Chem. Chem. Phys.* **2008**, 10, 2442-2450

### Different catalytic effects of a single water molecule. The gas-phase reaction of formic acid with hydroxyl radical in water vapor

Anglada, J.M., Gonzalez, J. *ChemPhysChem* **2009**, 10, 3034-3045

### Studies on the toxic oil syndrome: proposal of a mechanism for the thermal conversion of 3-N-phenylamino-1,2-propanediol esters into anilides under deodorisation conditions

Escabrós, J., Crehuet, R., Messeguer, A. *Tetrahedron* **2009**, 65, 418-426

### The 65th birthday of Professor Santiago Olivella Nello

Anglada, J.M., Bofill, J.M., Lluch, J.M. *Theor. Chem. Acc.* **2009**, 123, 1-2

**A Bohmian total potential view to quantum effects. II. Decay of temporarily trapped states**

González, M.F., Aguilar-Mogas, A., González, J., Crehuet, R., Anglada, J. M., Bofill, J.M., Giménez, X.  
*Theor. Chem. Acc.* **2009**, 123, 51-58

**Hyperconjugation in adjacent OO bonds: remarkable odd/even effects**

Martins-Costa, M., Anglada, J.M., Ruiz-López, M.F.  
*Chem. Phys. Lett.* **2009**, 481, 180-182

**A dynamic view of enzyme catalysis**

Jiménez, A., Clapés, P., Crehuet, R.  
*J. Mol. Model.* **2008**, 14, 735-746

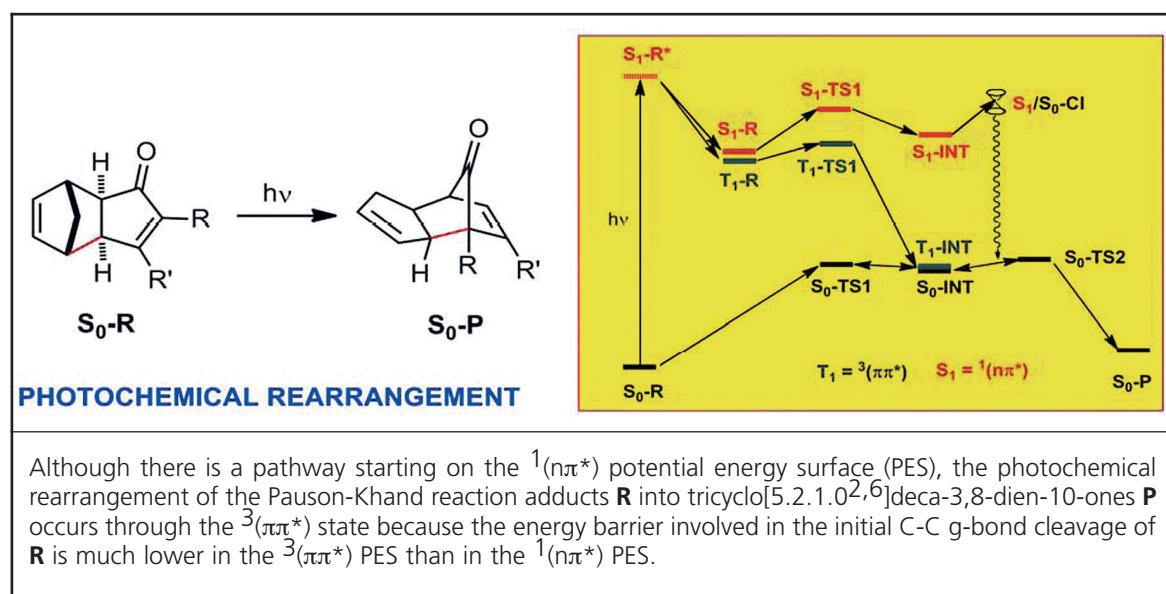
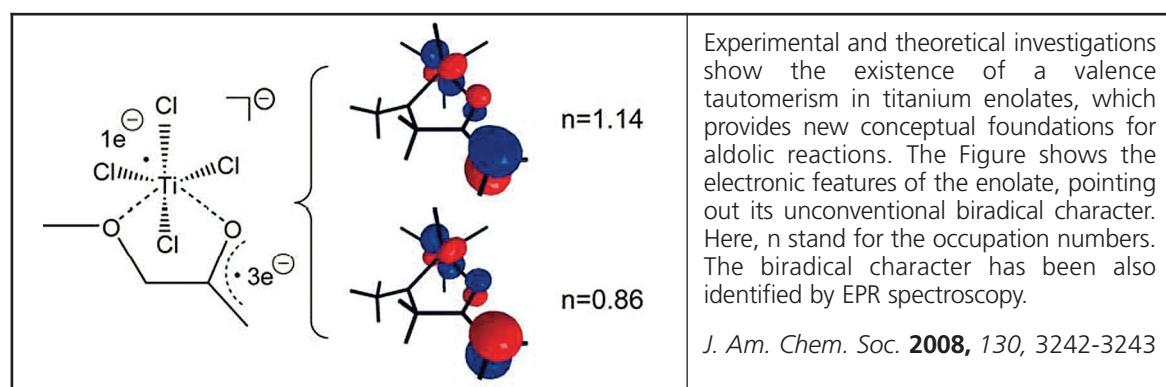
**A new flexible tripodal compound derived from indole: synthesis, complexation, spectroscopic, MALDI-TOF-MS and DFT studies**

Oliveira, F., Pedras, B., Santos, H., Rodríguez, L., Crehuet, R., Avilés, T., Capelo, J.L., Lodeiro, C.  
*Inorg. Chim. Acta* **2009**, 362, 2627-2635

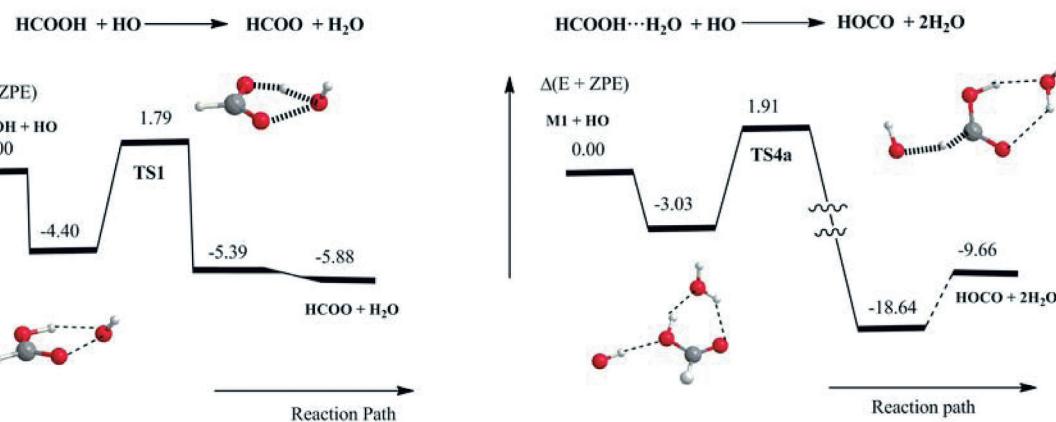
**The gas phase HO-initiated oxidation of furan: a theoretical investigation on the reaction mechanism**

Anglada, J.M.  
*Open Chem. Phys. J.* **2008**, 1, 80-93

## Research highlights

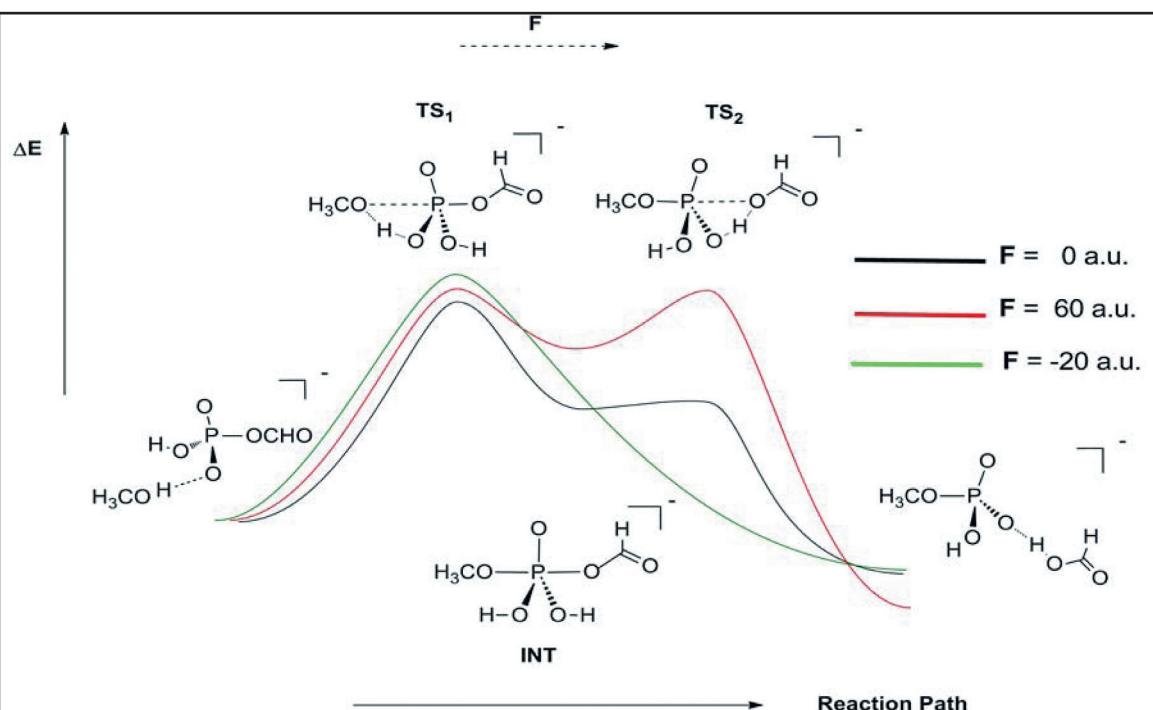


**Gas phase reaction between formic acid and hydroxyl radical with and without water**



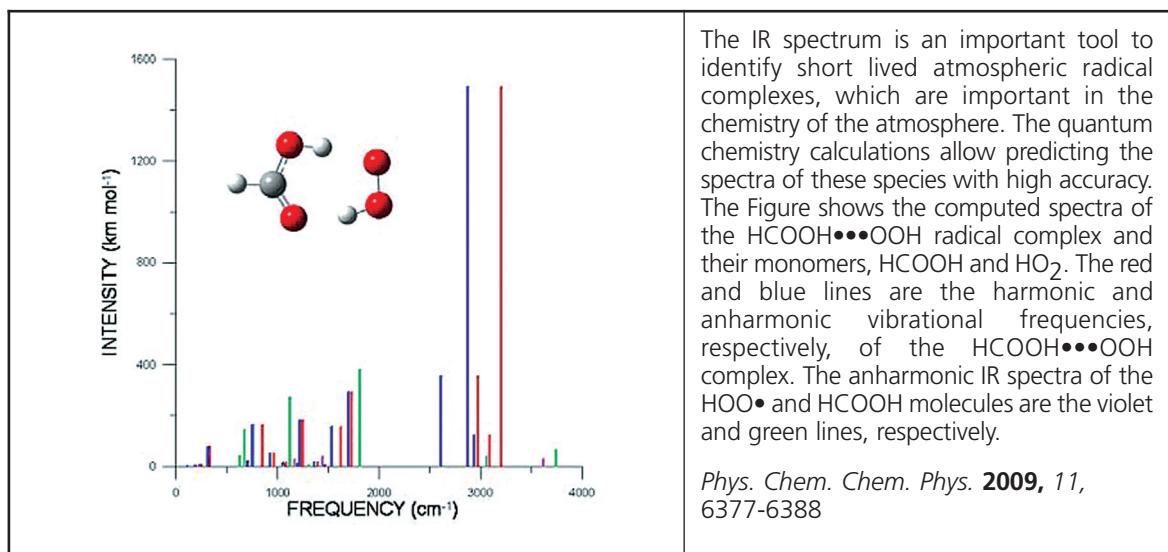
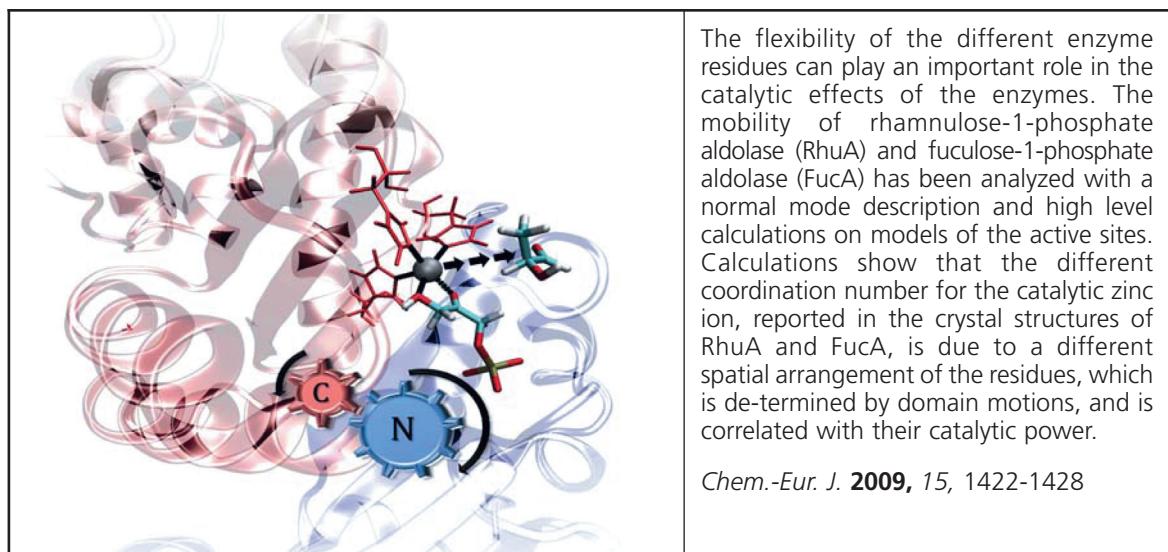
Water vapour plays an important role in the chemistry of the atmosphere. In the troposphere, formic acid can be oxidized by HO radicals. The hydroxyl radical abstracts the acidic hydrogen in a proton coupled electron transfer (*pcet*) mechanism and the reaction produces HCOO + H<sub>2</sub>O, which decompose into H + CO<sub>2</sub>. In the presence of water vapour part of the reaction changes its mechanism. The hydroxyl radical abstracts the formyl hydrogen involving a hydrogen atom transfer mechanism (*hat*) and produces HOCHO + H<sub>2</sub>O.

*ChemPhysChem* **2009**, *10*, 3034-3045

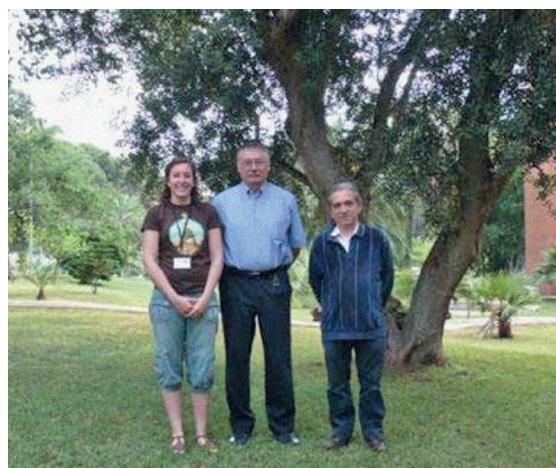


Pentacoordinate phosphorous plays an important role in a huge diversity of biochemical processes as they can be transition states or intermediates of nucleophilic substitution reactions in phosphates. Their apical bonds are highly polarisable and are influenced by external fields. The Figure shows how different external electric fields can change the reaction profile on the nucleophilic substitution in phosphates.

*J. Chem. Theory Comput.* **2008**, *4*, 49-63



# 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 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, iridoid 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 reasons of other aromatic and medicinal plants components.

## STAFF

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## TECHNICIAN

JOAN LLORIA TOLRÀ

## Ph. D. STUDENTS

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HASSNA SOUMMANE

## Publications (articles)

### Phytoecdysteroids from *Ajuga macrosperma var. breviflora* roots

Castro, A., Coll, J., Tandrón, Y.A., Pant, A.K., Mathela, Ch.S.  
*J. Nat. Prod.* **2008**, 71, 1294-1296

### Anthraquinones from *in vitro* root culture of *Morinda royoc* L.

Borroto, J., Coll, J., Rivas, M., Blanco, M., Concepción, O., Tandrón, Y.A., Hernández, M., Trujillo, R.  
*Plant Cell Tissue Organ Cult.* **2008**, 7, 25-49

### Biorational insecticides in pest management

Rosell, G., Quero, C., Coll, J., Guerrero, A.  
*J. Pestic. Sci.* **2008**, 33, 103-121

### neo-Clerodane diterpenoids from Verbenaceae: structural elucidation and biological activity

Castro, A., Coll, J.  
*Nat. Prod. Commun.* **2008**, 3, 1021-1031

## Publications (books and book chapters)

Coll, J., 2009

### Synthetic ecdysteroidal compounds

In: Ecdysone: Structures and Functions  
Smagghe, G. (Ed.)  
Springer Science Ch 4, 99-123

Coll, J., 2009

### Otros tipos estructurales de insecticidas botánicos

In: Insecticidas y repelentes de insectos de origen natural  
Burillo Alquézar, J., González Coloma, A. (Eds.)  
Centro de Investigación y Tecnología Agroalimentaria de Aragón. Cap. 11, 171-188

Coll, J., Esquivel, B., 2009

### Terpenos

In: Insecticidas y repelentes de insectos de origen natural  
Burillo Alquézar, J., González Coloma, A. (Eds.)  
Centro de Investigación y Tecnología Agroalimentaria de Aragón. Cap. 6, 71-101

Coll, J., Esquivel, B., Gutiérrez, J., González-Coloma, A., Burillo, J., 2009

### Introducción

In: Insecticidas y repelentes de insectos de origen natural

Burillo Alquézar, J., González Coloma, A. (Eds.)  
Centro de Investigación y Tecnología Agroalimentaria de Aragón. Cap. 1, 11-17

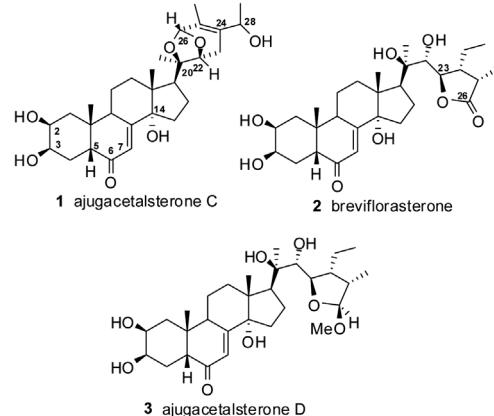
Coll, J., Tandrón, Y., 2008

### neo-Clerodane diterpenoids from *Ajuga*: structural elucidation and biological activity

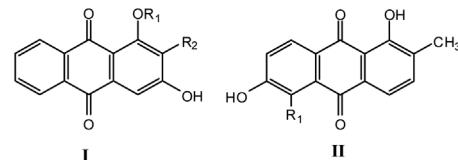
In: Perspectives on Natural Biopesticides  
Gonzalez-Coloma, A. (Ed.)  
Springer Netherlands, *Phytochemistry Rev.*, 7, 25-49

## Research highlights

Three new phytoecdysteroids, ajugacetalsterones C (**1**) and D (**3**) and breviflorasterone (**2**), were isolated from the roots of *Ajuga macrosperma* var. *breviflora* along with five known compounds, namely, 20-hydroxyecdysone, cyasterone, makisterone A, 20-hydroxyecdysone 3-acetate, and 20-hydroxyecdysone 2-acetate. The structures of **1-3** were elucidated on the basis of extensive 1D and 2D NMR spectroscopic studies. The new compounds possess acetal oxygen bridges between C-26 and C-20/C-22, or C-26/C-23, or a lactone bridge between C-23 and C-26.



Seven AQs were isolated from *in vitro* root cultures of *M. royc* in sufficient amount to be characterized. The structures of the compounds present in the *Morinda royc* L. roots were determined on the basis of their corresponding <sup>1</sup>H-NMR spectra. For **1** and **2**, they were in accordance with the data for the structure of nordamnacanthal and damnacanthal respectively. Other AQ's, isolated as pure compounds, were lucidin (**3**), soranjidiol (**4**), rubiadin 1-methylether (**5**) morindone (**6**) and rubiadin (**7**) respectively. Rubiadin was a newly identified compound in this species, whereas nordamnacanthal was present as the major AQ in the extract.



|                        | I   | R <sub>1</sub>  | R <sub>2</sub>     |
|------------------------|-----|-----------------|--------------------|
| Nordamnacanthal        | [1] | H               | CHO                |
| Damnacanthal           | [2] | CH <sub>3</sub> | CHO                |
| Lucidin                | [3] | H               | CH <sub>2</sub> OH |
| Rubiadin 1-methylether | [5] | CH <sub>3</sub> | CH <sub>3</sub>    |
| Rubiadin               | [7] | H               | CH <sub>3</sub>    |
|                        | II  | R <sub>1</sub>  |                    |
| Soranjidiol            | [4] | H               |                    |
| Morindone              | [6] | OH              |                    |



**3**

**DEPARTMENT OF BIOMEDICINAL CHEMISTRY**



## DEPARTMENT OF BIOMEDICINAL CHEMISTRY



**Head:** Gemma Fabriàs Domingo

The Department of Biomedicinal 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

# Research Unit on BioActive Molecules



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 (sphingolipidoses) 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.

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ANA TRAPERO PUIG

## Publications (articles)

### Aggregated low density lipoprotein induces tissue factor by inhibiting sphingomyelinase activity in human vascular smooth muscle cells.

Camino-Lopez, S., Badimon, L., Gonzalez, A., Canals, D., Pena, E., Llorente-Cortes, V. *J. Thromb. Haemost.* **2009**, 7, 2137-2146

### Host cell P-glycoprotein is essential for cholesterol uptake and replication of *Toxoplasma gondii*.

Bottova, I., Hehl, A. B., Stefanic, S., Fabrias, G., Casas, J., Schraner, E., Pieters, J., Sonda, S. *J. Biol. Chem.* **2009**, 284, 17438-17448

### Dihydroxyacetone phosphate aldolase-catalyzed synthesis of structurally diverse polyhydroxylated pyrrolidine derivatives and evaluation of their glycosidase inhibitory properties

Calveras, J., Egido-Gabás, M., Gómez, L., Casas, J., Parella, T., Joglar, J., Bujons, J., Clapés, P. *Chem.-Eur. J.* **2009**, 15, 7310-7328

### cis- versus trans-Ceramides: effects of the double bond on conformation and H-bonding interactions.

Phillips, S.C., Triola, G., Fabrias, G., Goñi, F.M., DuPre, D.B., Yappert, M.C. *J. Phys. Chem. B* **2009**, 113, 15249-15255

### Synthesis of a fluorogenic analogue of sphingosine-1-phosphate and its use to determine sphingosine-1-phosphate lyase activity.

Bedia, C., Camacho, L., Casas, J., Abad, J.L., Delgado, A., Van Veldhoven, P.P., Fabrias, G. *ChemBioChem* **2009**, 10, 820-822

### Molecular basis for beta-glucosidase inhibition by ring-modified calystegine analogues

Aguilar, M., Gloster, T.M., García-Moreno, M.I., Ortiz Mellet, C., Davies, G.J., Llebaría, A., Casas, J., Egido-Gabás, M., García Fernández, J.M. *ChemBioChem* **2008**, 9, 2612-2618

### Dihydroceramide intracellular increase in response to resveratrol treatment mediates autophagy in gastric cancer cells.

Signorelli, P., Muñoz-Olaza, J. M., Gagliostro, V., Casas, J., Ghidoni, R., Fabrias, G. *Cancer Lett.* **2009**, 282, 238-243

### Sphingosine 1-phosphate regulation of extracellular signal-regulated kinase-1/2 in embryonic stem cells.

Rodgers, A., Mormeneo, D., Long, J.S., Delgado, A., Pyne, N.J., Pyne, S. *Stem Cells Dev.* **2009**, 18, 1319-1330

### **Aminocyclitol-substituted phytoceramides and their effects on iNKT cell stimulation.**

Harrak, Y., Barra, C. M., Bedia, C., Delgado, A., Castano, A. R., Llebaria, A.  
*ChemMedChem* **2009**, 4, 1608-1613

### **Synthesis and biological activity of a novel inhibitor of dihydroceramide desaturase**

Muñoz-Olaya, J.M., Matabosch, X., Bedia, C., Egido-Gabás, M., Casas, J., Llebaría, A., Delgado, A., Fabriàs, G.  
*ChemMedChem* **2008**, 3, 946-953

### **Synthesis and biological properties of Pachastrissamine (jaspine B) and diastereoisomeric jaspines**

Canals, D., Mormeneo, D., Fabrias, G., Llebaria, A., Casas, J., Delgado, A.  
*Bioorg. Med. Chem.* **2009**, 17, 235-241

### **Solid-phase synthesis of oligomers carrying several chromophore units linked by phosphodiester backbones**

Aviñó, A., Navarro, I., Farrera-Sindreu, J., Royo, M., Aymamí, J., Delgado, A., Llebaria, A., Albericio, F., Eritja, R.  
*Bioorg. Med. Chem. Lett.* **2008**, 18, 2306-2310

### **A straightforward protocol for the solution-phase parallel synthesis of ceramide analogues**

Grijalvo, S., Matabosch, X., Llebaría, A., Delgado, A.  
*Eur. J. Org. Chem.* **2008**, 150-155

### **Recent advances in the chemistry of aminocyclitols**

Delgado, A.  
*Eur. J. Org. Chem.* **2008**, 3893-3906

### **A practical access to 1,2-diaminophospholipids**

Harrak, Y., Llebaría, A., Delgado, A.  
*Eur. J. Org. Chem.* **2008**, 4647-4654

### **Promising results of the chaperone effect caused by imino sugars and aminocyclitol derivatives on mutant glucocerebrosidases causing Gaucher disease.**

Sanchez-Olle, G., Duque, J., Egido-Gabas, M., Casas, J., Lluch, M., Chabas, A., Grinberg, D., Vilageliu, L.

*Blood Cells Mol. Dis.* **2009**, 42, 159-166

### **Cytotoxicity and acid ceramidase inhibitory activity of 2-substituted aminoethanol amides**

Bedia, C., Canals, D., Matabosch, X., Harrak, Y., Casas, J., Llebaría, A., Delgado, A., Fabriàs, G.  
*Chem. Phys. Lipids* **2008**, 156, 33-40

### **Fungal growth inhibitory properties of new phytosphingolipid analogues**

Mormeneo, D., Manresa, A., Casas, J., Llebaría, A., Delgado, A.

*J. Appl. Microbiol.* **2008**, 104, 1075-1081

### **Small-scale one-pot reductive alkylation of unprotected aminocyclitols with supported reagents**

Sisa, M., Trapero, A., Llebaría, A., Delgado, A.  
*Synthesis* **2008**, 3167-3170

## **Research highlights**

### **A high throughput screening procedure**

Synthesis of a fluorogenic analogue of sphingosine-1-phosphate and its use to develop an easy procedure to measure sphingosine-1-phosphate lyase (*SGPL1*) activity. The assay was validated using both homozygous (-/-) and heterozygous (+/-) *SGPL1* knockout mouse embryonic fibroblasts and their corresponding wild type cells. The measurements can be carried out directly in microtiter plates without the need of separation of the reaction products, which represents a significant improvement of the previously reported methods. This procedure is a suitable tool for the discovery of new enzyme modulators within combinatorial libraries, as well as in research to decipher the role of *SGPL1* in disease outcome and progression.

### **Biologically active molecules**

#### Cancer

Synthesis of pachastrissamine (jaspine B) and diastereoisomeric jaspines and study of their biological activity as lethal autophagy inducers in the human lung adenocarcinoma A549 cell line. Preparation of small libraries of acid ceramidase inhibitors and investigation of their activity as proapoptotic agents in the same A549 cell line. Synthesis and biochemical characterization of a novel dihydroceramide desaturase inhibitor (XM462) and its activity to induce caspase-dependent apoptosis in the human leukemia Jurkat A3 cell line.

#### Immunology

Synthesis of nonglycosidic  $\alpha$ -galactosylceramide analogues, with a polyhydroxylated aminocyclohexane moiety as the galactose surrogate, which constitute a new class of charged NKT cell agonists. One of these compounds, HS44, promotes *in vitro* NKT cell expansion in a similar fashion to  $\alpha$ -galactosylceramide but with lower potency, and induces the release of IFNA and IL-4 in iNKT cell culture causing a biased Th2 cytokine profile response.

# 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 biological testing.

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AIMEE VASCONCELOS PACHECO

## Publications (articles)

### Antibodies against chimeric fibrin/filaggrin citrullinated synthetic peptides in rheumatoid arthritis. Diagnostic and prognostic value

Sanmartí, R., Graell, E., Pérez, M.L., Ercilla, G., Viñas, O., Gómez-Puerta, J.A., Gratacós, J., Balsa, A., Gómara, M.J., Larrosa, M., Cañete, J.D., Haro, I. *Arthritis Res. Ther.* **2009**, 11, R135 (9 pp)

### Interaction of GBV-C/HGV synthetic peptides with lipid Langmuir monolayers and large unilamellar vesicles

Pérez, S., Vila-Romeu, N., Alsina, M.A., Espina, M., Haro, I., Mestres, C. *J. Phys. Chem. B* **2009**, 113, 319-327

### Synthetic peptides of hepatitis G virus (GBV-C/HGV) in the selection of putative peptide inhibitors of the HIV-1 fusion peptide

Herrera, E., Gómara, M.J., Mazzini, S., Ragg, E., Haro, I.

*J. Phys. Chem. B* **2009**, 113, 7383-7391

### Fluorescent study of the dynamic interaction between E1(145-162) sequence of hepatitis GB virus C and liposomes

Sánchez-Martín, M.J., Amigo, J.M., Pujol, M., Haro, I., Alsina, M.A., Busquets, M.A. *Anal. Bioanal. Chem.* **2009**, 394, 1003-1010

### Behaviour of a peptide sequence from the GB virus C/hepatitis G virus E2 protein in Langmuir monolayers: its interaction with phospholipid membrane models

Pérez, S., Nieto-Suárez, M., Mestres, C., Alsina, M.A., Haro, I., Vila-Romeu, N. *Biophys. Chem.* **2009**, 141, 153-161

### Liposome destabilization induced by lipophilic derivatization of synthetic peptides belonging to NS3 and E2 proteins of GB virus C/HGV. Structural requirements for leakage

Fernández-Vidal, M., Rojo, N., Herrera, E., Gómara, M.J., Haro, I.

*Biophys. Chem.* **2008**, 132, 55-63

### Surface behaviour and peptide-lipid interactions of the E1(3-17)R and E1(3-17)G peptides from E1 capsid protein of GBV-C/HGV virus

Fontvila, O., Mestres, C., Muñoz, M., Haro, I., Alsina, M.A., Pujol, M.

*Colloid Surface A-Physicochem. Eng. Asp.* **2008**, 321, 175-180

### pH Induced destabilization of lipid model membrane by the overlapped peptides E2(26-53), E2(32-53) and E2(39-53) from the E2 glycoprotein of the capsid of hepatitis G virus

Massanés, M., Muñoz, M., Busquets, M.A., Haro, I., Alsina, M.A., Pujol, M.

*Luminescence* **2008**, 23, 247-248

**Fluorescence analysis of the interaction of the peptide sequence E1(145-162) of hepatitis GB virus C with liposomes**

Sánchez-Martin, M.J., Amigo, J.M., Pujol, M., Haro, I., Alsina, M.A., Busquets, M.A.  
*Luminescence* **2008**, 23, 263-265

**Features of antigen-antibody interaction during use of linear synthetic peptides and multipeptide antigen modeling antigenic determinants of hepatitis A virus**

Kruglov, I.V., Simonova, T.V., Pérez, J.A., Haro, I.  
*Zh. Mikrobiol. Epidemiol. Immunobiol.* **2009**, 2, 31-34

## Publications (books and book chapters)

Gómar, M.J., Haro, I., 2009

### Peptide-based diagnostic assays

In: Medicinal Protein Engineering  
Khudyakov, Y.E. (Ed.)  
CRC Press, Boca Raton, Fl, Ch 14, 333-352

## Research highlights

### Synthetic peptides of hepatitis G virus (GBV-C/HGV) in the selection of putative peptide inhibitors of the HIV-1 fusion peptide

Recent years have seen the publication of numerous works in which co-infection with GB virus C or Hepatitis G virus (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/HGV virus has a «protective effect» in patients with HIV has still not been defined. We have found a GBV-C related peptide that belong to the E2 envelop protein, with ability to interact and inhibit the activity of the HIV-1 fusion peptide in model membranes. The results were described in: **J. Phys. Chem. B, 113, 7383-7391, 2009** and show that this peptide interacts with target HIV-1 FP and modify its conformation, thus indicating that it could be able to alter the HIV-1 FP interaction with membranes. Thus, this peptide sequence could be involved in the prevention of HIV-1 entry by its binding to the HIV-1 FP that avoids the triggering of the HIV-cell fusion process.

### Antibodies against chimeric fibrin/filaggrin citrullinated synthetic peptides in rheumatoid arthritis. Diagnostic and prognostic value

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 **Arthritis Res. Ther. 11(5):R135, 2009**, highlighted a high sensitivity and specificity for RA when compared with a large series of patients with various rheumatic conditions and healthy controls, with results comparable to the commercial test. Of note that when positivity was considered as one or more positive anti-chimeric fibrin/filaggrin synthetic peptides status, sensitivity was notably higher than the commercial test while specificity remained very high. Moreover, our peptides gave better results in terms of identifying patients with poor radiographic outcome.

# 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 CC bond forming crosscoupling 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 four areas: 1) Synthesis and biological study of antinociceptive drugs. 2) Application in peptide chemistry of the iodinating reagent  $\text{IPy}_2\text{BF}_4$  (Barluenga's reagent). 3) Synthesis of transthyretin amyloidosis inhibitors. 4) Development of radiotracer probes for the imaging diagnostics of neurodegenerative diseases.

## STAFF

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## Publications (articles)

### **Synthesis, conformation, and biological characterization of a sugar derivative of morphine that is a potent, long lasting and nontolerant antinociceptive.**

Arsequell, G., Salvatella, M., Valencia, G., Fernández-Mayoralas, A., Fontanella, M., Venturi, Ch., Jiménez-Barbero, J., Marrón, E., Rodríguez, R.E.  
*J. Med. Chem.* **2009**, 52, 2656-2666

### **Arylation of phe and tyr side chains of unprotected peptides by a Suzuki-Miyaura reaction in water**

Vilaró, M., Arsequell, G., Valencia, G., Ballesteros, A., Barluenga, J.  
*Org. Lett.* **2008**, 10, 3243-3245

### **Iodination of salicylic acid improves its binding to transthyretin**

Gales, L., Almeida, M.R., Arsequell, G., Valencia, G., Saraiva, M.J., Damas, A.M.  
*BBA-Proteins Proteomics* **2008**, 1784, 512-517

### **Isatin derivatives, a novel class of transthyretin fibrillogenesis inhibitors.**

González, A., Quirante, J., Nieto, J., Almeida, M.R., Saraiva, M.J., Planas, A., Arsequell, G., Valencia, G.  
*Bioorg. Med. Chem. Lett.* **2009**, 19, 5270-5273

### **Iodine atoms: a new molecular feature for the design of potent transthyretin fibrillogenesis inhibitors.**

Mairal, T., Nieto, J., Pinto, M., Almeida, R., Gales, L., Ballesteros, A., Barluenga, J., Pérez, J.J., Vázquez, J.T., Centeno, N., Saraiva, J.M., Damas, A., Planas, A., Arsequell, G., Valencia, G.  
*PLoS ONE* **2009**, 4, e4124 (13 pp).

## Publications (books and book chapters)

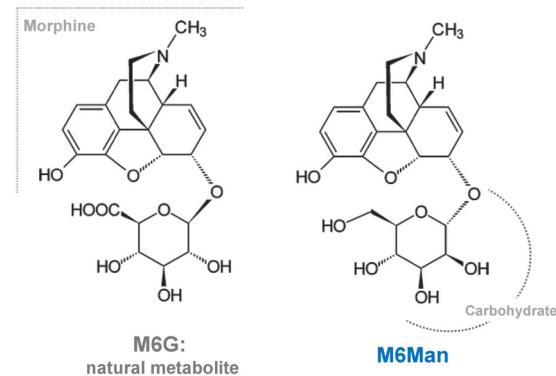
Vilaró, M., Arsequell, G., Valencia, G., Ballesteros, A., Barluenga, J., Nieto, J., Planas, A., Almeida, R., Saraiva, M.J., 2008

### **Reengineering TTR amyloid inhibition properties of diflunisal**

In: XIth International Symposium on Amyloidosis  
Skinner, M., Beck, J.L., Connors, L.H., Seldin, D.C. (Eds.)  
CRC Press, Boca Raton, FL, 205-207

## Research highlights

As part of a drug discovery project for a group of rare diseases associated with the transthyretin (TTR)-related amyloidosis, started in 2000 with a grant from the Fundació La Caixa and that continues with funding from the Fundació La Marató de TV3, it has been prepared and studied a new family of aggregation inhibitors of this protein that could be candidates for drugs. These results have been published in PLoS ONE (4, 1, 2009, e4124). Since the TTR when binding to its natural ligand, the thyroid hormones, presents a much more stable quaternary and therefore less amiloidogenic structure, the assumption that iodine atoms present in thyroid hormones could be an element of design to improve the power of other ligands has been tested. Thus, a good ligand of TTR already known, as the drug registered diflunisal and a number of their analogues were selected as starting materials. Electrophilic aromatic iodination of this family of compounds through the IPy2BF<sub>4</sub> reagent provided the corresponding iodides. Using an *in vitro* high throughput aggregation screening test, the capacity of the TTR aggregation inhibition of these molecules has been assessed. The relative binding ability of these analogues to TTR in an *ex vivo* model of patient plasma and the binding selectivity to various plasma proteins has also been evaluated. The analogues containing iodine atoms are better aggregation inhibitors than their predecessors. These results have been explained using X-ray crystallography techniques TTR and some analogues complexes, molecular modelling, and circular dicroism.



One of the recent research results from the line started in this Centre in the 1970s, directed to the study of molecules related to pain, and currently under Fundació La Marató de TV3 financing, has been the synthesis of a morphine derivative with notable biological properties (J. Med. Chem. 52, 2009, 2656-2666). It is actually morphine-6-manoside (M6Man), a new synthetic analogue of the natural metabolite morphine-6-glucuronide (M6G).

Antinociceptive activity by systemic administration in rats is 100 fold more potent and twice more durable than morphine. The product is not producing tolerance or cardiovascular effects and binds with double affinity than morphine to  $\mu$  opioid receptors. Comparative NMR studies between the natural and the synthetic compounds suggest that the difference of activity may be due to a different dynamic behavior. The work has received the «Pain Research 2009 Award» of the Grünenthal Foundation.



# 4

**DEPARTMENT OF CHEMICAL AND  
BIOMOLECULAR NANOTECHNOLOGY**



## DEPARTMENT OF CHEMICAL AND BIOMOLECULAR NANOTECHNOLOGY



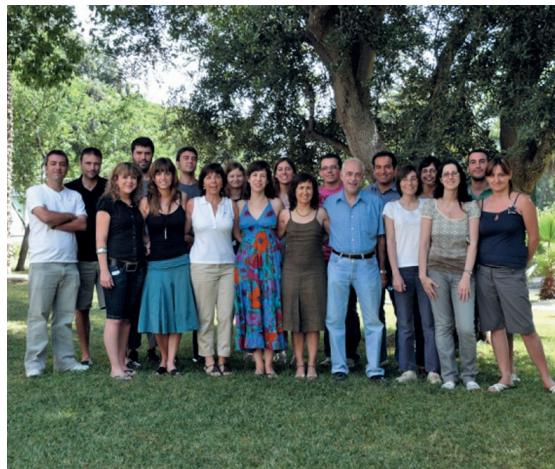
**Head:** Mª Pilar Marco Colàs

Research at the Chemical and Biomolecular Nanotechnology Department is focused on bioactive organic molecules and biomolecules, nanomaterials and devices and self-organized supramolecular or colloidal systems. Thus, the research groups of the department hold a great expertise on the chemistry of bioactive substances and their preparation using combinatorial chemistry tools, designing and screening virtual libraries. Knowledge on the chemistry of oligonucleotides allows to rationally synthesize molecules with affinity to dsDNA and G-quadruplex as well as to design new nucleic acid derivatives to control gene expression by antisense and RNA interference mechanisms. The capability to produce antibodies, natural molecules with inherent capabilities to specifically react with their counter antigen, and to direct their features according to the needs, allows designing bioreceptors for a wide range of applications. The integration of these biomolecules with certain micro(nano)materials and devices with unique physical properties allows developing novel biosensors with improved features envisaging a new generation of molecular diagnostic tools useful in the clinical and food safety fields. Finally, and regarding the preparation of new nanostructures, the expertise acquired for many years on the chemistry of the surfactants and their capability to self-aggregate to form complex supramolecular structures (micelles, liquid crystals, microemulsions, nano-emulsions, highly concentrated emulsions, etc.) has lead to investigate their use as templates for the preparation of new nanostructured materials (organic, inorganic, hybrid) with controlled size and morphology as well as new drug delivery systems.

### Research groups

- Nanobiotechnology and Molecular Diagnostics
- Nucleic Acids Chemistry
- Colloid and Interfacial Chemistry Group
- Bioorganic Chemistry
- Surface Chemistry Group

# Nanobiotechnology and Molecular Diagnostics



The **Applied Molecular Receptors Group (AMRg)** has focussed 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 raise 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 base for the construction of functional hybrid materials consisting of both organic (biomolecules) and inorganic components. Biosensors are between 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 capability to respond in a physiological manner. The unique properties of certain nanomaterials combined with the excellent features of the antibodies allow envisaging novel exquisitely sensitive chemical and biological sensors.

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## Publications (articles)

**Multifunctional nanoparticles-properties and prospects for their use in human medicine**  
Sanvicens, N., Marco, M.P.  
*Trends Biotechnol.* **2008**, 26, 425-433

**Detection of fluoroquinolone antibiotics in milk via a label-less immunoassay based upon an impedance protocol**

Sekenis, G., Garifallou, G., Davis, F., Millner, P., González, D., Sánchez, F., Marco, M.P., Gibson, T., Higson, S.  
*Anal. Chem.* **2008**, 80, 9233-9239

**Fluorescence site-encoded DNA addressable hapten-microarray for anabolic androgenic steroids**

Tort, N., Salvador, J.P., Eritja, R., Poch, M., Martínez, E., Samitier, J., Marco, M.P.  
*Trac-Trends Anal. Chem.* **2009**, 28, 718-728

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CARME PASTELLS DÍEZ  
SALVADOR PETANÁS ESTEBAN  
NÚRIA TORT ESCRIBÀ  
ESTER VILA ROCA

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Adrian, J., Pasche, S., Pinacho, D.G., Font, H., Diserens, J.-M., Sanchez-Baeza, F., Granier, B., Voirin, G., Marco, M.P.  
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*Trac-Trends Anal. Chem.* **2009**, 28, 1243-1252

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 Kreuzer, M., Quidant, R., Salvador, J.P., Marco, M.P., Badenes, G. *Anal. Bioanal. Chem.* **2008**, 391, 1618-2642
- Simultaneous immunochemical detection of stanozolol and the main human metabolite, 3'-hydroxy-stanozolol in urine and serum samples**  
 Salvador, J.P., Sánchez, F., Marco, M.P. *Anal. Biochem.* **2008**, 376, 221-228
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 Font, H., Adrián, J., Galve, R., Estévez, M.C., Castellari, M., Gratacós, M., Sánchez, F.J., Marco, M.P. *J. Agric. Food Chem.* **2008**, 56, 736-743

### **Non-specific adsorption of streptavidin on single walled carbon nanotubes**

Gonzalez, M., Tort, N., Benito, A.M., Maser, W., Marco, M.P., Martinez, M.T.  
*J. Nanosci. Nanotechnol.* **2009**, 9, 6149-6156

### **Electrogeneration of polymer films functionalized by fluoroquinolone models for the development of antibiotic immunoassays**

González, D., Gorgy, K., Cosnier, S., Marco, M.P., Sánchez, F.

*Innovation et Technologie en Biologie et Médecine* **2008**, 29, 181-186

## **Publications (books and book chapters)**

Adrián, J., Fernández, F., Muriano, A., Obregon, R., Ramon-Azcon, J., Tort, N., Marco, M.P., 2009

### **Biosensors for pharmaceuticals and emerging contaminants based on novel micro and nanotechnology approaches**

In: Biosensors for the Environmental Monitoring of Aquatic Systems. Bioanalytical and Chemical Methods for Endocrine Disruptors.

Barceló, D., Hansen, P. (Eds.)

Handbook of environmental chemistry series  
Springer Berlin / Heidelberg, 5J, 47-68

Adrián, J., Fernández, F., Muriano, A., Obregon, R., Ramon-Azcon, J., Tort, N., Marco, M.P., 2009

### **Applications of immunochemical techniques to the analysis of aquatic environments**

In: Applications of immunoanalytics

Namiesnik, J., Szefer, P. (Eds.)

Taylor and Francis Group Ltd. - 139-187

## **Research highlights**

In the last two years, AMRg has been involved in the study of novel micro and nano(bio)technological approaches to improve the efficiency of the diagnostic tools, particularly in the food safety and clinical fields. The research objectives of the group are focused on the combination of bioreceptors and micro(nano)materials to develop new generations of analytical devices in which an optical or electrical signal can be recorded as a consequence of a specific biorecognition event. In this context, AMRg has obtained different results according to the different projects that the group has been involved. Particularly, and following the main line of the group, AMRg has published relevant results involved in the development of immunochemical techniques (ELISA) for the broad detection of antibiotics such as sulfonamides and fluoroquinolones, pesticides such as triazines, bromophenols and bromopropylate, androgenic hormones such as stanozolol, boldenone, methylboldenone and THG (tetrahydrogestrinone), as well as a multianalyte immunoassay 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), food sample extracts, milk, human and cattle urine, blood and hair. This last matrix is very useful for the study of the traceability of a pollutant.

AMRg has been specialized on the production of selective antibodies and, specifically, on the synthesis and characterization of the immunoreagents. Thanks to the knowledge acquired during the last 10 years, the group has established a new generic synthesis of bioconjugates using stable symmetric dimers through disulfide bonds, which can be reduced immediately before conjugation of the biomolecules for the preparation of the bioconjugates.

Another research highlight of the group has been the development of a new transducer for biosensor applications based on a three-dimensional interdigitated electrode array (IDEA) with electrode

digits separated by an insulating barrier. This novel impedimetric immunoassay has been developed in collaboration with Dr. Bratov from CNM-CSIC and the idea has been protected by an international patent.

AMRg has also developed other electrochemical immunoassays for the detection of different environmental pollutants and some antibiotics. In this context, a novel conductimetric immunoassay mainly based on antibodies labelled to gold nanoparticles for atrazine detection has been designed and developed.

AMRg has also developed optical immunoassays for the detection of sulfonamide antibiotics in milk. The immunoassay was implemented onto a microsystem platform, the wavelength interrogated optical sensing device, which uses the evanescent field to probe changes at the interface of a waveguiding layer, and thus allows sensitive detection of biomolecule adsorption. The immunoreagents were immobilized onto the surface of the waveguide chip, and a fluidic cell allowed flowing analyte and detection solutions above the surface. Another optical immunodevice has been developed based on the use of two photon fluorescence principle as detection method of affinity binding reactions. The sensor uses a resonant grating waveguide structure as platform enhancement for detecting the interaction between fluorescent labeled androgenic hormones and a specific antibody.

Finally, AMRg has been working in a new strategy for immunochemical screening of small organic molecules based on the use of a hapten microarray. Using DNA-directed immobilization strategies, we have been able to convert a DNA chip into a hapten microarray by taking advantage of all the benefits of the structural and electrostatic homogeneous properties of DNA. The hapten microarray uses hapten-oligonucleotide probes instead of proteins, avoiding the limitations of preparing protein-oligonucleotide bioconjugates stoichiometrically-defined.

# 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.

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## Publications (articles)

### Label-free DNA biosensors based on functionalized carbon nanotube field effect transistors

Martínez, M.T., Tseng, Y.C., Ormategui, N., González-Domínguez, J.M., Loinaz, I., Eritja, R., Bokor, J.  
*Nano Lett.* **2009**, 9, 530-536

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Faustino, I., Aviñó, A., Marchán, I., Luque, F.J., Eritja, R., Orozco, M.  
*J. Am. Chem. Soc.* **2009**, 131, 12845-12853

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Saneyoshi, H., Mazzini, S., Aviñó, A., Portella, G., González, C., Orozco, M., Marquez, V., Eritja, R.  
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### Fluorescence site-encoded DNA addressable hapten-microarray for anabolic androgenic steroids

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*Trac-Trends Anal. Chem.* **2009**, 28, 718-728

### pH-Modulated Watson-Crick duplex-quadruplex equilibria of guanine-rich and cytosine-rich DNA sequences 140 base pairs upstream of the c-kit transcription initiation site

Bucek, P., Jaumot, J., Aviñó, A., Eritja, R., Gargallo, R.  
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Morales, J.C., Reina, J.J., Díaz, I., Aviñó, A., Nieto, P.M., Eritja, R.  
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Gros, J., Aviñó, A., López de la Osa, J., González, C., Lacroix, L., Pérez, A., Orozco, M., Eritja, R., Mergny, J.L.  
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van Bemmel, D.M., Brank, A. S., Eritja, R., Marquez, V.E., Christman, J.K.  
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- Targeting the G-quadruplex forming region near the P1 promoter in the human BCL-2 gene with the cationic porphyrin TMPyP4 and with the complementary C-rich strand**  
Del Toro, M., Bucek, P., Aviñó, A., Jaumot, J., González, C., Eritja, R., Gargallo, R.  
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- Study of the interaction between the G-quadruplex-forming thrombin-binding aptamer and the porphyrin 5,10,15,20-tetrakis(N-methyl-4-pyridyl)-21,23H-porphyrin tetratosylate**  
del Toro, M., Gargallo, R., Eritja, R., Jaumot, J.  
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Farrera-Sindreu, J., Aviñó, A., Navarro, I., Aymamí, J., Beteta, N.G., Varón, S., Pérez-Tomás, R., Castillo-Avila, W., Eritja, R., Albericio, F., Royo, M.  
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Grijalvo, S., Matabosch, X., Llebaria, A., Delgado, A.  
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Ramos, R., Manning, B., Aviñó, A., Gargallo, R., Eritja, R.  
*Helv. Chim. Acta* **2009**, 92, 613-622
- Assembly of two-dimensional DNA crystals carrying N4-[2-(tert-butylsulfanyl)ethyl]-cytosine residues**  
Garibotti, A.V., Sisquella, X., Martínez, E., Eritja R.  
*Helv. Chim. Acta* **2009**, 92, 1466-1472
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Manning, B., Pérez-Rentero, S., Garibotti, A.V., Ramos, R., Eritja, R.  
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- Incorporation of Zebularine from its 2'-deoxyribonucleoside triphosphate derivative and activity as a template-coding nucleobase**  
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*Nucleosides Nucleotides Nucleic Acids* **2008**, 27, 131-145
- Synthesis of oligonucleotide conjugates carrying violagen and fluorescent compounds**  
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## Publications (books and book chapters)

Saneyoshi, H., Mazzini, S., Aviñó, A., Portella, G., González, C., Orozco, M., Marquez, V., Eritja, R., 2009.

**The use of conformationally rigid nucleoside probes to study the role of sugar pucker and nucleobase orientation in the thrombin binding aptamer**

*Nucleic Acids Symp. Ser. (Oxford)* 53, 109-110.

## 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 this year we have completed a 3-year study on siRNA aimed to answer the following questions: 1) Is it possible to increase stability of siRNA without affecting RISC recognition? 2) Is it possible to increase cellular uptake / biodistribution without affecting RISC recognition? 3) Is it possible to modulate RISC recognition by chemical modification of the guide strand? 4) Is it possible to avoid off target effects by chemical modification of siRNA duplexes? 5) Is it possible to fabricate a simple pharmaceutical formulation to cure a disease based on siRNA? We used the luciferase and the TNF- $\alpha$  as target genes. TNF- $\alpha$  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.

**Synthesis of oligonucleotides carrying base analogues.** Aberrant DNA methylation is a common finding in cancer. Some drugs that inhibit DNA methylation are active against some malignancies. The cytosine analogues, 5-azacytidine and 5-aza-2'-deoxycytidine, are the most frequently studied inhibitors of DNA methylation. Zebularine (1-( $\beta$ -D-ribofuranosyl)-1,2-dihydropyrimidin-2-one), another pyrimidine analogue which lacks the 4-amino group of the other cytosine analogues, has been shown to

inhibit DNA methylation and may have activity against cancer. We synthesized oligonucleotides containing either 5-azacytosine or 2-(1H)-pyrimidinone in place of the cytosine to carry out a detailed comparisons of the interaction between purified DNA methyltransferases (bacterial M.Hhal and mammalian Dnmt1) and oligonucleotides. This study was performed by Dr. Christman (U. Omaha, USA) supporting the hypothesis that the efficacy of zebularine as an inhibitor of DNA methylation in vivo is dependent on its ability to be incorporated into DNA.

In addition we have studied the base-pairing properties of 2-thio- and 4-thiothymidine derivatives. Previous results in the literature suggested that the replacement of carbonyl oxygens by sulphur atoms lead to dramatic changes in tautomeric properties of these pyrimidine derivatives. In our work we showed that the presence of thiothymines induces only mild changes in DNA structure, stability and fidelity, becoming then excellent molecules to introduce the thiolated nucleosides in DNA.

### 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-streptoavidin 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. Thiols 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 marker can be prepared and deposited on mica substrates. However and most importantly we also demonstrated that these thiolated 2D DNA arrays are readily deposited on gold surfaces while unmodified 2D DNA arrays are not able to do so.

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

In the frame of the strategic action on nanotechnology we provided modified oligonucleotides to Dr. M<sup>a</sup> Teresa Martínez (CSIC, Zaragoza) to perform a study of DNA hybridization on field effect transistors-carbon nanotubes (CNTFET) at the Molecular Foundry of Lawrence Berkeley National Laboratory. Using oligonucleotides, a special polymer developed by CIDETEC by Iraida Loinaz and the facilities at the Molecular Foundry for the fabrication of CNTFET, M<sup>a</sup> Teresa Martínez was able to measure DNA hybridization with high precision using electrical means.

Furthermore in this same strategic action and in collaboration with the groups of Pilar Marco (CSIC, Barcelona) and Josep Samitier (IBEC, Barcelona) we have prepared oligonucleotide conjugates carrying steroids. These conjugates are being used for the development of analytic devices for anti-doping and food control of the illegal use of steroidal anabolic hormones.

Finally we have characterized by AFM peptide nanotubes formed by cyclic peptides prepared by the group of Dr. Granja (University of Santiago de Compostela).

#### **G-quadruplex.**

Aptamers are oligonucleotides that were originally derived from an in vitro evolution process known as SELEX (systematic evolution of ligands by exponential enrichment) which selects them on the basis of their specific and tight binding affinity to a ligand of choice from a library of sequences. Through this approach, aptamers with very high affinity have been developed for diagnostic, therapeutic and other technical applications. One of the most studied aptamers is the 15-base long thrombin binding aptamer (TBA). This oligonucleotide binds specifically to thrombin at nanomolar concentrations and for this reason it has interesting anticoagulant properties. TBA is characterized by a chair-like, antiparallel quadruplex structure consisting of two G-tetrads connected by two TT loops and a single TGT loop (Figure 2). We studied the effect of 2'-deoxyguanine (dG) residues with locked North- or South-bicyclo[3.1.0]hexane pseudosugars when inserted in TBA. Individual 2'-deoxyguanosines at four positions of the aptamer were replaced by these analogues where the North/anti and South/syn conformational states were confined. We conclude that locked bicyclo[3.1.0] hexane nucleosides appear to be excellent tools in the study of the role of conformational parameters that are critical for the formation of a stable, antiparallel G-tetrad DNA

structures. This work was performed in close collaboration with the groups of Dr. Orozco (IRB Barcelona), Dr. Márquez (NIH, USA), Dr. Mazzini (U. Milan, Italy) and Dr. González (CSIC, Madrid). Moreover, guanine rich sequences capable to form G-quadruplex structures have been found in telomeres and in transcriptional regulatory regions of important oncogenes such as c-myc, and c-kit. Ligands that selectively bind and stabilize these structures have become interesting anticancer drugs. We have initiated the study of G-quadruplex structures present at the initiation sites of oncogenes as well as the interaction with small drugs and the interaction with the complementary C-rich strand that may form also a quadruplex structure know as i-motif. This work is done in collaboration with the group of Raimundo Gargallo (U. Barcelona). A detailed analysis of the equilibrium formed by the G-quadruplex of bcl-2 and c-kit oncogenes and the corresponding complementary C-rich sequences was made in order to determine the relative amount of duplex or separate quadruplexes forms at different pH.

#### **Design of inhibitors of DNA repair mechanism in cancer chemotherapy.**

Cancer 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-mG). 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 is a new research line of the group that is supervised by Dr. Carme Fàbrega.

# Colloid and Interfacial Chemistry Group



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)

### Syntheses of mesostructured silica films containing conjugated polymers from tetrahydrofuran

Kirmayer, S., Dovgolevsky, E., Kalina, M., Lakin, E., Cadars, S., Epping, J.D., Fernández-Arteaga, A., Rodríguez-Abreu, C., Chmelka, B.F., Frey, G.L. *Chem. Mat.* **2008**, *20*, 3745-3756

### Epoxy networks with physical cross-links produced by tail-to-tail associations of alkyl chains

Puig, J., Zucchi, I. A., Hoppe, C.E., Pérez, C.J., Galante, M.J., Williams, R.J.J., Rodríguez-Abreu, C. *Macromolecules* **2009**, *42*, 9344-9350

### Emulsions with structured continuous phases

Rodríguez-Abreu, C., Lazzari, M. *Curr. Opin. Colloid Interface Sci.* **2008**, *13*, 198-205

### Nano-emulsions: new applications and optimization of their preparation

Gutiérrez, J.M., González, C., Maestro, A., Solé, I., Pey, C.M., Nolla, J. *Curr. Opin. Colloid Interface Sci.* **2008**, *13*, 245-251

### Mesoporous silica from reverse lyotropic liquid crystals: A novel approach

Rodríguez-Abreu, C., Esquena, J., Aramaki, K., López-Quintela, M.A. *Microporous Mesoporous Mater.* **2009**, *119*, 338-343

### Preparation of rectangular and 2D-hexagonal mesostructured silica at neutral conditions using poly(oxyethylene) cholestryl ethers and a water-soluble silica precursor

Takahashi, S., Ikkai, Y., Sakamoto, K., Rodriguez-Abreu, C., Aramaki, K. *J. Colloid Interface Sci.* **2009**, *335*, 70-76

### Monomeric and dimeric anionic surfactants: a comparative study of self-aggregation and mineralization

Rodríguez-Abreu, C., Rodríguez, E., Solans, C. *J. Colloid Interface Sci.* **2009**, *340*, 254-260

### Effect of alkyl chain asymmetry on catanionic mixtures of hydrogenated and fluorinated surfactants

Blanco, E., Rodríguez-Abreu, C., Schulz, P., Ruso, J.M. *J. Colloid Interface Sci.* **2009**, *341*, 261-266

### **Viscoelastic properties of polystyrene and poly(methyl methacrylate) dispersions sterically stabilized by hydrophobically modified inulin (polyfructose) polymeric surfactant**

Nestor, J., Obiols-Rabasa, M., Esquena, J., Solans, C., Levecke, B., Booten, K., Tadros, Th.F.  
*J. Colloid Interface Sci.* **2008**, 319, 152-159

### **Influence of the phase behaviour on the properties of ionic nano-emulsions prepared by the phase inversion composition method**

Maestro, A., Solé, I., González, C., Solans, C., Gutiérrez, J.M.

*J. Colloid Interface Sci.* **2008**, 327, 433-439

### **A novel approach to metal and metal oxide nanoparticle synthesis: the oil-in-water microemulsion reaction method**

Sánchez-Domínguez, M., Boutonnet, M., Solans, C.  
*J. Nanopart. Res.* **2009**, 11, 1823-1829

### **Structure and properties of self-assembled fluorocarbon-silica nanocomposites**

Rodríguez-Abreu, C., Botta, P.M., Rivas, J., Aramaki, K., López-Quintela, M.A.  
*J. Non-Cryst. Solids* **2008**, 354, 1074-1077

### **One-pot preparation of gold-elastomer nanocomposites using pdms-graft-peo copolymer micelles as nanoreactors**

Hoppe, C.E., Rodríguez-Abreu, C., Lazzari, M., López-Quintela, M.A., Solans, C.  
*Phys. Status Solidi A-Appl. Mat.* **2008**, 205, 1455-1459

### **Emulsion polymerization of styrene using mixtures of hydrophobically modified inulin polymeric surfactant and nonionic surfactants**

Nestor, J., Esquena, J., Solans, C., Levecke, B., Booten, K., Tadros, Th.

*J. Appl. Polym. Sci.* **2008**, 118, 811-815

## **Publications (books and book chapters)**

Solans, C., Solé, I., Fernández-Arteaga, A., Nolla, J., Azemar, N., Gutiérrez, J., Maestro, A., González, C., Pey, C.M., 2009

### **Nano-emulsion formation by low-energy methods and functional properties**

In: Structure and Functional Properties of Colloidal Systems. Surfactant Science Series **146**  
Hidalgo-Alvarez, R. (Ed.)  
CRC Press, Boca Raton, Fl, Ch 21, 457-482

Solans, C., Esquena, J., 2009

### **Highly concentrated (gel) emulsions as reaction media for the preparation of advanced materials**

Highlights in colloid Science,  
Dimo Platinakov and Dotchi Exerowa Edi., 291-297  
ISBN:978-3-527-32037-0

## **Research highlights**

### **Surfactant self-assembly**

This research line is the basis for the research 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. In this context, phase behaviour studies of novel surfactants as well as of conventional ones in novel systems have been undertaken.

An example of the former is the investigation on the phase behaviour of a dimeric amphiphile, 2,3-didodecyl-1,2,3,4-butanetetracarboxylic acid (GS-H), with alkanolamines and organic aminosilanes as counter ions (Rodriguez-Abreu et al, *J. Colloid Interface Sci.*, 2009). For comparison purposes, the phase behaviour of its monomeric counterpart (lauric acid, LA) was also investigated. The alkanolamine salts of GS-H show Krafft points below 0°C, micellar solutions ( $W_m$ ) are obtained in the dilute region whereas a hexagonal liquid crystal phase ( $H_1$ ) is formed at higher concentration but lower than its monomeric counterpart. Moreover, the

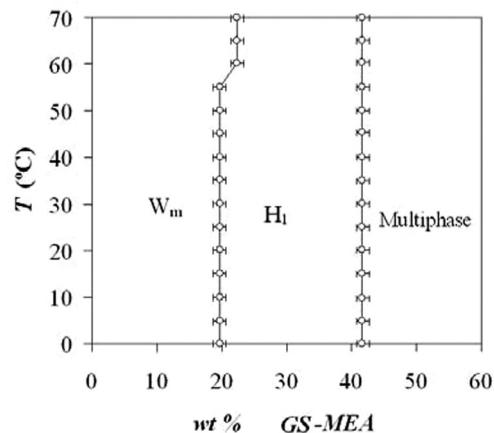
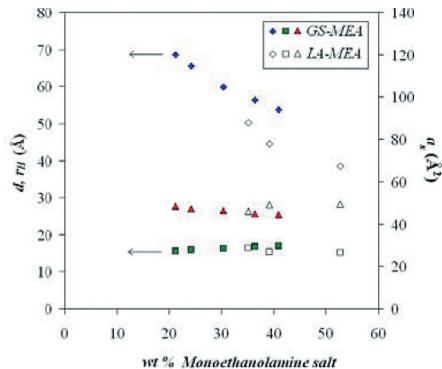


Figure 1. Phase diagram of alkanolamine dimeric surfactant GS-MEA.  $W_m$ : micellar solution;  $H_1$  = hexagonal liquid crystal.

phase boundaries are quite temperature insensitive, a behavior commonly found in ionic surfactants (Figure 1).

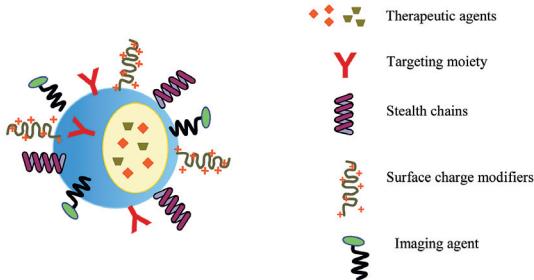
Characterization of the hexagonal liquid crystal phases by SAXS showed that the structural parameters described in Fig. 2 are similar for the dimeric (GS) and monomeric (LA) surfactants and for MEA and TEA salts.



**Figure 2.** Structural parameters derived from SAXS measurements in hexagonal liquid crystals of monoethanolamine salts at 25 °C.  $d$  = Bragg spacing (diamonds);  $rH$  = radius of lipophilic core (squares);  $a_s$  = interfacial area per surfactant molecule (triangles). Filled symbols: GS-MEA; Open symbols: LA-MEA

This gemini amphiphile with organic aminosilanes acting as reactive counterions form hexagonal and lamellar liquid crystals. Silica and alumina were prepared by a sol-gel method (mineralization) using this Gemini surfactant as structure directing agent. Silica samples showed little structuration, whereas aluminas possessed a lamellar structure, which disappears upon calcination; however, calcined solids have a high surface area ( $600 \pm 20 \text{ m}^2/\text{g}$ ) coming mainly from micropores. These results demonstrate the usefulness of this surfactant for the preparation of alumina with high surface area.

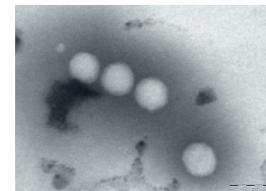
**Design of multifunctional nanocarriers, as delivery systems, by nano-emulsion templating**  
Multifunctional nanocarriers are delivery systems in the nanometric size range designed to fulfil several specific demands at a time. These multiple functions, enable the nanosystems to reach selectively the disease site at therapeutic concentrations improving efficacy and decreasing adverse effects (Fig. 3).



**Figure 3.** Schematic representation of a multifunctional nanoparticle.

We have selected polymeric nanoparticles as starting materials for the preparation of multifunctional nanocarriers. These nanoparticles have been obtained in O/W nano-emulsions by incorporating preformed hydrophobic polymers in the oily dispersed phase followed by solvent evaporation. The nano-emulsions

have been obtained by condensation or low-energy methods, making use of the phase transitions that take place during the emulsification process. The oil component consists of a biocompatible preformed polymer (hydrophobic polysaccharides or polyesters) and a non toxic volatile solvent. Polymeric nanoparticles loaded with therapeutic concentrations of a glucocorticoid drug (dexamethasone) with mean sizes around 50 nm have been obtained (Fig.4).

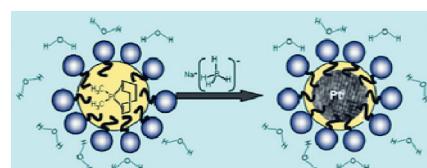


**Figure 4.** TEM micrograph of dexamethasone loaded polymeric nanoparticles obtained in O/W nano-emulsions

Surface charge modification, functionalization based on carbodiimide chemistry and fluorescent labelling rendered these nanoparticles with multifunctional properties.

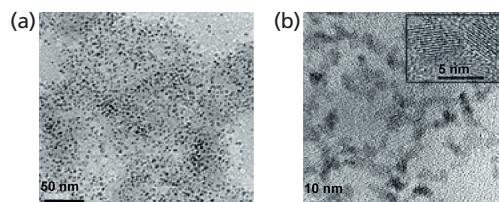
#### Development of a novel approach for the synthesis of nanoparticles: The O/W microemulsion reaction method

A novel and straightforward approach, based on O/W microemulsions, in contrast to the typically used W/O microemulsions, was developed for the synthesis of inorganic nanoparticles at ambient conditions (Sánchez-Domínguez et al, J. Nanopart. Res. 2009). It implies the use of organometallic precursors dissolved in nanometre-scale oil droplets of O/W microemulsions. Addition of reducing or oxidizing/precipitating agents results in the formation of metallic or metal oxide nanoparticles, respectively. This approach is schematically depicted in Fig.5.



**Figure 5.** Schematic representation of the synthesis of metallic nanoparticles in O/W microemulsions.

Nonionic o/w microemulsion systems were chosen for nanoparticle synthesis at 25°C. Small nanoparticles of metals (Pt, Pd and Rh) and nanocrystalline metal oxide (cerium (IV) oxide with cubic type crystalline structure of less than 7 nm can be obtained in mild conditions (Fig. 6).



**Figure 6.** Transmission Electron Microscopy (TEM) images of (a) Pt and (b)  $\text{CeO}_2$  nanoparticles synthesized by the novel O/W microemulsion reaction method.

# Bioorganic Chemistry Group



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 five patent applications in 2008-2009 and licensed two patents to pharma companies

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## Publications (articles)

### A semaphorin 3A inhibitor blocks axonal chemorepulsion and enhances axon regeneration

Montolio, M., Messeguer, J., Masip, I., Guijarro, P., Gavin, R., Del Río, J.A., Messeguer, A., Soriano, E. *Chem. Biol.* **2009**, 16, 691-701

### Inhibition of calcineurin-NFAT signaling pathway with a RCAN-derived peptide without affecting general phosphatase activity

Mulero, M.C., Aubareda, A., Orzáez, M. Messeguer, J., Serrano, E., Martínez, S., Messeguer, A., Pérez-Payá, E., Pérez-Riba, M. *J. Biol. Chem.* **2009**, 284, 9394-9401

### Modulation of cellular apoptosis with apoptotic protease-activating factor 1 (Apaf-1) inhibitors

Mondragón, L. Orzaez, M., Sanclimens, G., Moure, A., Arminan, A., Sepulveda, P., Messeguer, A., Vicent, M., Perez-Paya, E. *J. Med. Chem.* **2008**, 51, 521-529

### Participation of oxidative stress on rat middle cerebral artery changes induced by focal cerebral ischemia: beneficial effects of 3,4-dihydro-6-hydroxy-7-methoxy-2,2-dimethyl-1(2H)-benzopyran (CR-6)

Jiménez-Altayó, F., Caracuel, L., Pérez-Asensio, F.J., Martínez-Revelles, S., Messeguer, A., Planas, A.M., Vila, E. *J. Pharmacol. Exp. Ther.* **2009**, 331, 429-436

### A monolayer study on interactions of Docetaxel with model lipid membranes

Fernández-Botello, A., Comelles, F., Alsina, M.A., Cea, P., Reig, F. *J. Phys. Chem. B* **2008**, 112, 13834-13841

### A chemical inhibitor of Apaf-1 exerts mitochondrioprotective functions and interferes with the intra-S-phase DNA damage checkpoint

Mondragon, L., Galluzzi, L., Mouhamad, S., Vicencio, J.M., Vitale, I., Orzaez, M., Moure, A., Messeguer, A., Pérez-Payá, E., Kroemer, G. *Apoptosis* **2009**, 14, 182-190

### Studies on toxic oil syndrome: development of an enzyme-linked immunosorbent assay for 3-(N-phenylamino)propane-1,2-diol in human urine

Martínez-Cabot, A., Varea, B., Lloveras, M., Campos, R., Marco, M.P., Messeguer, A. *Anal. Bioanal. Chem.* **2008**, 391, 617-624

### A design, construction and validation of a library of N-alkylglycine pentamers assisted by microwave activation and validation via the identification of trypsin inhibitors

Messeguer, J., Cortés, N., García-Sanz, N., Navarro-Vendrell, G., Ferrer-Montiel, A., Messeguer, A. *J. Comb. Chem.* **2008**, 10, 974-980

**NMDA-induced neuroprotection in hippocampal neurons is mediated through the protein kinase A and CREB (cAMP-response element-binding protein) pathway**

Valera, E., Sánchez-Martín, F.J., Ferrer-Montiel, A., Messeguer, A., Merino, J.M.

*Neurochem. Int.* **2008**, 53, 148-154

**Studies on the toxic oil syndrome: proposal of a mechanism for the thermal conversion of 3-(N-phenylamino)-1,2-propanediol esters into anilides under deodorisation conditions**

Escabrós, J., Crehuet, R., Messeguer, A.

*Tetrahedron* **2009**, 65, 418-426

**Studies of patients and carriers with 2-methyl-3-hydroxybutyryl-CoA dehydrogenase (MHBD) deficiency: difficulties in the diagnosis**

García-Villoria, J., Navarro-Sastre, A., Fons, C., Pérez-Cerdà, C., Baldellou, A., Berenguer, X., Gonzalez, I., Hernández-González, A., Campistol, J., Delpiccolo, C., Cortés, N., Messeguer, A., Briones, P., Ribes, A.

*Clin. Biochem.* **2009**, 42, 27-33

**A fluorescence spectroscopy on interactions of docetaxel with model lipid membranes**

Fernández-Botello, A., Alsina, M.A., Reig, F.

*Luminescence* **2008**, 23, 199-203

## Publications (books and book chapters)

Miranda, M., Bosch-Morell, F., Muriach, M., Barcia, J., Romero, F.J., Díaz-Llopis, M., Messeguer, A., 2008.

**Are antioxidants useful in diabetic retinopathy?**

In: Free radicals in ophthalmic disorders  
Zierhut, M., Cadenas, E., Rao, N.A. (Eds.)  
Informa Healthcare USA, Inc. New York, 12,  
159-166

## Research highlights

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 (10.000 and 5.000 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 also been constructed.

Along this period of time, 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. Two more peptoids acting as potent modulators of MDR phe-

notype have been identified. 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 protected by patent, the corresponding PCT has been filed and transferred 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.

Actually, 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. 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.

Nevertheless, our group has also been interested in expanding the expertise of experimental combinatorial libraries to those designed and screened *in silico*. Thus, in the last three years we have expanded our Combichem abilities to the *in silico* design and screening of virtual combinatorial libraries. This computational approach has been applied to the elaboration and validation of a QSAR model for the inhibition of histone deacetylase (HDAC) that has been further developed in our laboratory.

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, and CR-6 has elicited a protective effect on peroxidase activity in experimental diabetes. 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. Our group has also been partner in a CENIT Project, related to the development of liposomes loaded with docetaxel and coated with peptides related to decorin leucine rich repeats (LRR). Encapsulation of docetaxel has been optimised and several LRR of different lengths have been synthesised and their biological activity determined.

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. 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 funded by private pharma or biotech companies. In both cases it is intended to discover lead compounds active in front of highly interesting pharmaceutical targets.

# Surface Chemistry Group



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.

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## Publications (articles)

### Shaping supramolecular nanofibers with complementary hydrogen bond-forming nanoparticles

Puigmartí-Luis, J., Pérez del Pino, A., Laukhina, E., Esquena, J., Laukhin, V., Rovira, C., Vidal-Gancedo, J., Kanaras, A.G., Nichols, R.J., Brust, M., Amabilino, D.B.  
*Angew. Chem.-Int. Ed.* **2008**, 47, 1861-1865

### Topographical and wettability effects of post-discharge plasma treatments on macroporous polystyrene-divinylbenzene solid foams

Canal, C., Gaboriau, F., Vílcchez, A., Erra, P., García-Celma, M.J., Esquena, J.  
*Plasma Process. Polym.* **2009**, 6, 686-692

### Mesoporous silica from reverse lyotropic liquid crystals: A novel approach

Rodríguez-Abreu, C., Esquena, J., Aramaki, K., López-Quintela, M.A.  
*Microporous Mesoporous Mater.* **2009**, 119, 338-343

### Viscoelastic properties of polystyrene and poly(methyl methacrylate) dispersions sterically stabilized by hydrophobically modified inulin (polyfructose) polymeric surfactant

Nestor, J., Obiols-Rabasa, M., Esquena, J., Solans, C., Levecke, B., Booten, K., Tadros, Th.F.  
*J. Colloid Interface Sci.* **2008**, 319, 152-159

### Chitosan contribution on wool treatments with enzyme

Vilchez, S., Manich, A.M., Jovancic, P., Erra, P.  
*Carbohyd Polym.* **2008**, 71, 515-523

### Atom-sensitive textiles as visual indicators for plasma post-discharge

Canal, C., Villegas, S., Cousty, S., Rouffet, B., Sarrette, J.P., Erra, P., Ricard, A.  
*Appl. Surf. Sci.* **2008**, 254, 5959-5966

### Wetting properties of polystyrene/divinylbenzene crosslinked porous polymers obtained using W/O highly concentrated emulsions as templates

Molina, R., Vílcchez, A., Canal, C., Esquena, J.  
*Surf. Interface Anal.* **2009**, 41, 371-377

### Antifungal efficiency of corona pretreated polyester and polyamide fabrics loaded with Ag nanoparticles

Lliç, V., Aponjić, Z., Vodnik, V., Molina, R., Dimitrijević, S., Jovanaić, P., Nedeljković, J., Radetić, M.  
*J. Mater. Sci.* **2009**, 44, 3983-3990

### Mechanism involved in the dyeing of wool with an oil-in-water microemulsion system

Paul, R., Solans, C., Erra, P.  
*J. Appl. Polym. Sci.* **2008**, 110, 156-162

**Emulsion polymerization of styrene using mixtures of hydrophobically modified inulin polymeric surfactant and nonionic surfactants**

Nestor, J., Esquena, J., Solans, C., Levecke, B., Booten, K., Tadros, Th.  
*J. Appl. Polym. Sci.* **2008**, *108*, 811-815

**Effects of low temperature plasma on wool and wool/nylon blend dyed fabrics**

Canal, C., Molina, R., Navarro, A., Bertran, E., Erra, P.  
*Fiber Polym.* **2008**, *9*, 293-300

**Publications (books and book chapters)**

Domínguez, C., Erra, P., 2009

**Wool wax removal by CO<sub>2</sub>/modifier extraction**  
In: Recent Research Developments in Applied Polymer Science  
Pandalai, S. G. (Ed.)  
Research Signpost, 497-512. ISBN: 978-81-308-0347-0.

Solans, C., Esquena, J., 2009

**Highly concentrated (gel) emulsions as reaction media for the preparation of advanced materials**  
In: Highlights in Colloid Science,  
Dimo Platinakov and Dotchi Exerowa Edi., 291-297.  
ISBN: 978-3-527-32037-0

**Chitosan hydrogels covalently crosslinked with a natural reagent**

Vílchez, S., Samitier, V., Porras, M., Esquena, J., Erra, P.  
*Tenside, Surfactants, Deterg.* **2009**, *46*, 13-17

**Study of irreversible thermochromic ink applications on textiles**

Canal, C., Villegas, S., Ricard, A., Erra, P.  
*Tekstil* **2009**, *58*, 105-111.

Vílchez, S., Erra, P., 2009.

**Scientific and technical studies on the chitosan biopolymer application on wool fibres**  
In: Recent Research Developments in Applied Polymer Science  
Pandalai, S. G. (Ed.)  
Research Signpost, 373-389. ISBN: 978-81-308-0347-0.

## Research highlights

### Preparation and characterization of novel porous materials by templating in highly concentrated emulsions

Highly concentrated emulsions are an interesting class of emulsions characterized by an internal phase volume fraction exceeding 0.74, the maximum packing of uniform spherical droplets. Consequently, their structure consists of deformed (polyhedral) and/or polydisperse droplets separated by a thin film of continuous phase, a structure resembling gas-liquid foams. Different organic and inorganic macroporous and dual meso/macroporous materials have been obtained using highly concentrated emulsions as templates. The morphology of the macropores pores is similar to that of the highly concentrated emulsion, which was used as template. Fig. 1 shows an example of a chitosan material obtained by reactions in oil-in-water highly concentrated emulsions.

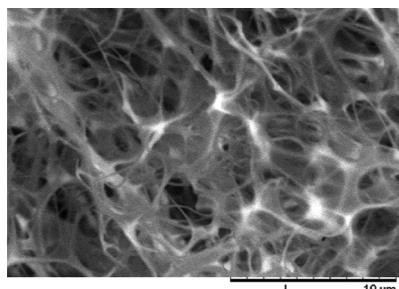


Fig. 1. SEM image of a chitosan aerogel obtained in highly concentrated emulsions. Its density is ≈ 0.1 g/mL.

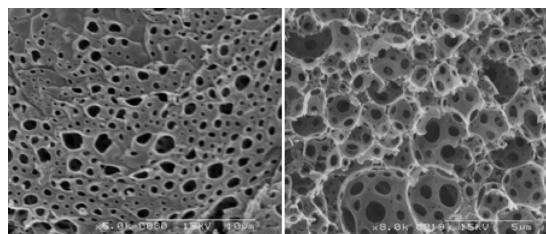
The preparation method of these chitosan materials has been patented (*Spanish patent ES2010/070198, 2009*).

Similar methodology, by templating in highly concentrated emulsions is being applied to obtain a wide variety of different porous materials, such as SiO<sub>2</sub>, TiO<sub>2</sub>, TiO<sub>2</sub>-P<sub>2</sub>O<sub>5</sub>, polystyrene, polyfurfuryl alcohol, polyvinylidene chloride, etc. Novel complex materials, such as hierarchically structured porous monoliths, are very interesting for technological applications in purification and decontamination, catalysis, fuel cells, energy storage, etc. The preparation of new structured porous materials is being studied, in the framework of the research projects CTQ2008-06892-C03-01 and PIF08-009-1.

### Formation and properties of macroporous materials with dual wettability

Porous solid foams, made of organic polymers, have found successful applications as support for catalysis, immobilization of enzymes, selective membranes or templates for the preparation of other materials. Wetting properties are of great importance due to its relationship with adhesion properties, relevant to the industrial applications. Porous polystyrene-divinylbenzene (PS-DVB) monoliths have been prepared using highly concentrated water-in-oil emulsions as templates. The polymerization of hydrophobic monomers takes place in the continuous oil phase. The materials obtained by this method exhibit structures

in the micrometer scale, resulting from the negative replica of the disperse phase (water droplets) that, after drying and purifying, results in a material with air connected channels surrounded by the hydrophobic polymer (foams). However, depending on the surface of the mold used to control the macroscopic shape of the monoliths, the materials may have a smooth skin layer with much less roughness than the interior surface (Fig. 2).



**Fig. 2.** SEM images of the external skin layer (left) and the internal highly rough surface (right). Molina, R., Vilchez, A., Canal, C., Esquena, J. *Surf. Interface Anal.* 2009, 41, 371-377.

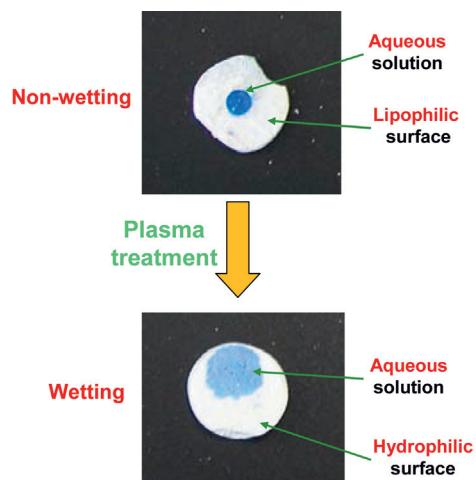
These two surfaces exhibit different wetting behaviour. Whereas the external part exhibits a Wenzel state (hydrophobic surface) using water as wetting liquid, the inner part exhibits a Cassie-Baxter state (superhydrophobic surface). These big differences cannot be explained only in terms of roughness. The analysis of the surface chemical composition by elemental microanalysis and XPS reveals that the external part of the PS-DVB monolith has a higher concentration of oxygen atoms than the inner part. This difference is attributed to a possible reaction of some non-reacted monomers with the air atmosphere. The dual wettability found between the external an inner part of the monoliths could be of relevance in absorption or desorption such us in drug delivery processes.

#### Surface modification by plasma treatment

Plasma techniques are being used in many industrial applications for surface modification of natural and synthetic polymers, because it has the advantage of being a fast and dry process, which avoids the use of water or chemicals, and therefore produces no wastewaters. Another advantage is that surface modification can be achieved at low temperature and normal pressure, with excellent control. 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 due to their high reactivity.

As a result of the 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. Very short treatments with plasma, of different gases, produce a remarkable increase in surface wettability of

porous monoliths (Fig. 3) opening new possibilities for the adsorption of hydrophilic compounds. The results show that the modification is strictly superficial, without altering neither the internal topography nor the morphology of the pores



**Fig.3.** Example of a macroporous superhydrophobic surface, which is not wetted with water. However, the surface becomes very hydrophilic after a short plasma treatment. Canal, C., Gaboriau, F., Vilchez, A., Erra, P., García-Celma, M.J., Esquena, J. *Plasma Process. Polym.* 2009, 6, 686-692

A new low temperature and low pressure plasma reactor has been developed (Spanish Patent P200803269). This plasma reactor can have applications in eliminating pollutants in aqueous systems (Spanish Patent P200900215).

#### Formation and characterization of pH-sentitive chitosan-genipin hydrogels

An increasing interest is being focused on hydrogels that are sensitive to external stimuli, for pharmaceutical applications as drug delivery systems. Chitosan is a well-known biocompatible polysaccharide, with low toxicity and antimicrobial activity. Chitosan hydrogels can be obtained by cross-linking reactions that stabilize the three-dimensional networks and its aerogels can be prepared by freeze-drying. However, many of the cross-linking agents used in industry have toxicity problems.

Chitosan hydrogels crosslinked with genipin, a non-toxic agent from renewable sources, have been studied. These hydrogels behave as solid-like elastic materials, observed by rheology. The swelling capacity is very high and it is sensitive to changes of pH (Fig. 4). At acid pH the free amino groups are protonated. Therefore, they can adsorb more water and the hydrogel swells considerably. However, at basic pH the amino groups are not protonated and the shrinkage of the hydrogel occurs. The hydrogels could be used in applications where adsorption and controlled release processes of hydrosoluble or partially hydrosoluble drugs were involved by changing the environment pH.

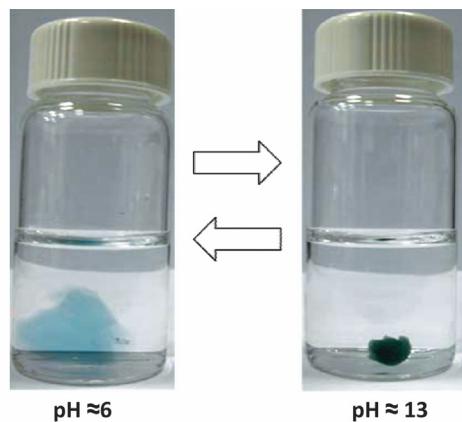


Fig.4. Reversible large swelling ability, as a function of pH.

Swelling-shrinking experiments demonstrated that the total volume can increase by a factor higher than 100. The degree of cross-linking is an important factor that influences the swelling capacity. These results have been published in: S. Vílchez, V. Samitier, M. Porras, J. Esquena and P. Erra, Tenside Surfactants Detergents, 46, (2009), 13-17. The research work also describes the preparation and characterization of low-density aerogels, which were obtained by freeze-drying the hydrogels

# 5

**DEPARTMENT OF CHEMICAL AND  
SURFACTANTS TECHNOLOGY**



## DEPARTMENT OF CHEMICAL AND SURFACTANTS TECHNOLOGY



**Head:** Ramon Pons Pons

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

# **Minimization of Industrial Wastes: Isolation of High Added-Value Biopolymers**



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ELISABET CÁRCEL CUZCO

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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 as 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) (5, 6) 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 the 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)**

### **Transformation plant for converting chromium waste into chemical products for leather industry**

Cot, J., Marsal, A., Manich, A.M., Celma, P., Fernández-Hervás, F., Cot-Gores, J.  
*J. Am. Leather Chem. Assoc.* **2008**, 103, 103-113

### **Alternative process for recovery of chrome (III)-effluents**

Cot, J., Marsal, A., Manich, A.M., Celma, P., Fernández, F., Cot-Gores, J.  
*J. Soc. Leather Technol. Chem.* **2008**, 92, 139-149

### **Whey protein isolate : A potential filler for the leather industry**

Hernandez Balaba, E., Taylor, E., Brown, E., Liu, C.K., Cot, J.  
*J. Am. Leather Chem. Assoc.* **2009**, 104, 122-130

## **Research highlights**

The tanning industry is responsible for a considerable amount of solid and liquid wastes, which poses a major problem for the environment. As regards only untanned solid wastes, potential raw materials of the medical products to be developed in this project, approximately 400 kg of untanned wastes are produced from one tonne of salted hide. Of these wastes, the use of green and limed fleshings for the recovery of collagen is not recommended because of its low collagen content. However, green and limed trimmings together with limed splits offer higher prospects of collagen recovery since 225 kg are produced per tonne of hide (i.e., ca 23 %). These wastes have found different applications to date: gelatine production; sausage casings; dog chews and composting. However, none of these applications has the high-

added value as has the medical material to be developed in this project for use in medicine. In general, biomaterials have had three applications over time. In the past, biopolymers were used mainly in the «elimination of tissues»; nowadays the main use is as «tissue substitutes» and «regeneration of tissues» is clearly the future for these materials.

Despite the existence of a wide variety of medical devices for the treatment of skin injuries, there are currently no suitable medical devices that promote the speedy regeneration of skin tissue and the healing of superficial and deep wounds, ulcers and other skin injuries. Neither are there any effective products for burns of first, second or third degree, nor any efficient products contributing to the reparation of cavities produced by dental extraction.

A great effectiveness of reconstituted collagen fibres in the field of regenerative medicine (tissues and/or organs) has been reported in the literature. During the auto-assembly stage (formation of reconstituted structures of collagen) some variables, such as temperature, ionic strength, proteoglycans presence, degree of crosslinking and/or mechanical manipulation, have significant influence. However, there is very little information in the literature about the factor that controls the biophysical characteristics prior to the reconstituted fibre formation.

Our research team has a wide experience in topics related to the treatment of industrial solid wastes. This is confirmed by the approval of several projects periodically presented at different Programs of the Spanish National Plans of Scientific Research, Development and Technological Innovation: **AMB92-1077, AM95-0079, AMB98-1014; PPQ2000-0213-P4-04; GIRD-CT-2002-0072; CTM2006-11610**, all of them related to the treatment and revalorisation of solid wastes from tannery. Likewise, the research team has participated in the European project RESTORM, where 20 institutions of 8 countries investigated the treatment of solid and liquid industrial tanning wastes.

The main objectives achieved to date are as follows:  
– Development of «cleaner» tanning and suitable treatments for industrial waste. A transformation plant for converting chromium collagenic waste into chemical products for leather industry. (*Diagram process, Figure 1*).

- Complete elimination (99% removal) of physical volume occupied by these types of chromed collagen wastes has resulted; thus a tremendous environmental problem has been solved and, consequently, a considerable reduction in the management cost of such a waste has been gained.
- Preliminary studies on extraction, modification and optimisation of biopolymer/collagen.

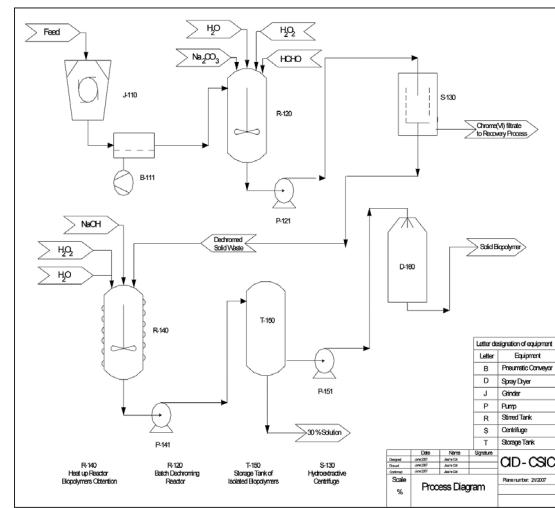
- Investigation of the potential applications for the high-value bioproducts extracted from collagen wastes, such as fertilisers, encapsulation and coating agents, surface sizing agents, printing components, binders, fillers, retanning agents, photography components, adhesives, film forming or finishing agents for the paper, wood, ink, textile and leather industries.

- Extraction of collagen from different sources, such as fish, slaughterhouse or non-tanned waste (hides, tendons, flesh...).

The experience acquired during the previous projects will help to achieve the new objectives given that a specific technology has recently been developed for the treatment of these collagen wastes. As a result, «low cost» biomaterials have been obtained. Their main applications have been: in the tanning industry itself as filler, re-tanning agents and finishing agents; and in the paper industry as a binder, partially substituting casein (much more expensive).

The use of biomaterials in medicine implies a suitable composition not only of the implanted material but also of all the particles released as a result of its debilitation or degradation. Hence, the importance of the origin and composition of the biomaterials to be obtained.

## Process Diagram – Figure 1



## BASIC STEPS OF THIS PROCESS

1<sup>st</sup> Step - Ground up chrome-tanned wastes.

Ground up collagenic chrome (III) wastes into a defibered size, fixed into a diameter of 1 to 5 mm, to obtain a more homogeneous stuff with a greater surface, therefore saving chemicals and shorten reaction time (J-110).

## 2<sup>nd</sup> Step - Dechroming process.

A stainless steel stirred reactor (oxidation reaction) and/or a modification of a conventional tannery drum, wooden-free with a suitable filter mesh (1 to 5 mm of diameter)(R-120).

### 3<sup>rd</sup> Step - Centrifuge operation.

This operation produces a filtrate (liquid effluent) and dechromed collagen fibres (solid state). The filtrate, which contains chromium (VI), is stored into a stainless steel stirred tank for further reduction to chromium (III), and adjusted to the correspondent basicity ( $33^\circ$  Sch). It can be used back in tanneries (S-130).

#### 4<sup>th</sup> Step - Isolation of collagen biopolymers.

In this step a jacketed stainless steel stirred reactor designed for viscous products is used in order to obtain different types of biopolymers (R-140).

Treated dechromed collagen wastes undergo a second process of highly controlled topochemical hydrolysis. The method of control depends on the degree of interaction of the following variables: macerators - alkaline, acid, liotropic.

activators - hydrogen peroxide, sodium percarbonate, sodium perborate, etc.

temperature : 70°C

5<sup>th</sup> Step – Storage.  
These biopolymers can be commercially available in several states; usually as a 30% solution which can be stored into a jacketed agitated tank. When temperature goes down below 14°C it is necessary to heat it up around 40°C with special equipment; thus converting it into a viscous liquid when needed (T-150). It can also be in the form of a solid powder achieved with a spray drier unit (D-160 as shown).

# Development of Non-Contaminant Industrial Processes



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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## Publications (articles)

### Biodegradability and toxicity of sulphonate-based surfactants in aerobic and anaerobic aquatic environments

García, M.T., Campos, E., Marsal, A., Ribosa, I.  
*Water Res.* **2009**, 43, 295-302

### Fate and effects of amphoteric surfactants in the aquatic environment

García, M.T., Campos, E., Marsal, A., Ribosa, I.  
*Environ. Int.* **2008**, 34, 1001-1005

### Adsorption of polyphenols in wastewater by organo-bentonites

Marsal, A., Bautista, E., Ribosa, I., Pons, P.,  
García, M.T.,  
*Appl. Clay Sci.* **2009**, 44, 151-155

### Inter-laboratory study on formaldehyde determination by HPLC

Font, J., Viera, S., Rius, T., Reyes, M., Jorba, M.,  
Verdú, E., Juárez, M.A., Cuadros, S., Marsal, A.  
*J. Am. Leather Chem. Assoc.* **2008**, 103, 53-61

### Transformation plant for converting chromium waste into chemical products for leather industry

Cot, J., Marsal, A., Manich, A.M., Celma, P.,  
Fernández-Hervás, F., Cot-Gores, J.  
*J. Am. Leather Chem. Assoc.* **2008**, 103, 103-113

### Factors that influence the physical properties of goatskins: polymeric derivatives and optimization of the process

Palop, R., Manich, A.M., Marsal, A.  
*J. Am. Leather Chem. Assoc.* **2008**, 103, 174-181

### Recovery of organic nitrogen from beamhouse wastewater in a hair recovery process

Marsal, A., Bautista, E., Cuadros, S., Reyes, M.R.,  
Rius, A., Font, A.  
*J. Soc. Leather Technol. Chem.* **2009**, 93, 176-182

### Alternative process for recovery of chrome (III)-effluents

Cot, J., Marsal, A., Manich, A.M., Celma, P.,  
Fernández, F., Cot-Gores, J.  
*J. Soc. Leather Technol. Chem.* **2008**, 92, 139-149

### Leather ageing and hexavalent chromium formation as a function of the fatliquoring agent. Part I: chrome tanned leathers

Palop, R., Parareda, J. Ballús, O., Marsal, A.  
*J. Soc. Leather Technol. Chem.* **2008**, 92, 200-204

### Leather ageing and hexavalent chromium formation as a function of the fatliquoring agent. Part II: chrome retanned leathers

Palop, R., Parareda, J. Ballús, O., Marsal, A.  
*J. Soc. Leather Technol. Chem.* **2008**, 92, 233-237

### Mecanismos de adsorción y desorción de vapor de agua en la piel

Manich, A.M., Maldonado, F., Carilla, J., Catalina,  
M., Marsal, A.  
*Lederpiel* **2009**, 78, 38-47

## Research highlights

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 recovery 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. Almost 70 % of COD and organic nitrogen in the wastewater was eliminated with this simple operation, with the consequent saving on the cost of wastewater treatment and associated taxes. The strong point of the precipitated protein fraction obtained was its high content of protein material, which by means of controlled hydrolysis could be reduced in molecular size, resulting in an increase in the proportion of peptides and free amino acids with the view to its use as a foliar fertilizer. The protein present in the precipitate did not result from the collagen decomposition of the hide but from soluble proteins such as albumin and globulin. Although the precipitates obtained meet all the requirements to be used as organic fertilizers, further studies are warranted to confirm this hypothesis. In addition, 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 vegetable extracts are normally employed in the tanning/retanning processes of leather manufacture and end up in the wastewaters. A technique for the elimination of the vegetable extracts from the wastewaters is necessary. The adsorption process with clays constitutes a simple, selective and economically acceptable approach to conventional treatments. With the objective of eliminating polyphenols (vegetable extracts) present in tannery wastewaters, organo-bentonites were prepared using commercial bentonite and cationic surfactants as hexadecyl trimethylammonium bromide (HDTMA) and benzyl triethylammonium

chloride (BTEA). Both surfactants were used at two different rates of the cation exchange capacity (50 % and 100 %) of the bentonite. SAXS measurements of the organo-bentonites revealed that the basal spacing of the HDTMA-bentonite (100 % CEC) was consistent with a bilayer arrangement of the HDTMA ions in the interlayer space. Both BTEA-bentonites and HDTMA-bentonite (50 %) intercalated surfactant monolayers. The experimental results, which were fitted to the Freundlich equation, revealed that adsorption increased with increasing amounts of surfactant adsorbed and was higher for the HDTMA-derivative. Although activated charcoal showed a higher adsorption capacity, organo-bentonites prepared from a low cost natural bentonite and cationic surfactants (HDTMA and BTEA) constitutes an efficient and attractive alternative for polyphenols removal from wastewater.

To improve the manufacturing tannery processes and hence to reduce the environmental impact, the influence of fatliquoring and retanning operations on leather ageing and hexavalent chromium formation was studied. Leather fastness to temperature and ultraviolet light was evaluated.

The temperature test gave rise to a lower ageing (yellowing) in chromium-retanned leathers than in non-retanned leathers. As for shrinkage temperature, there were no linear variations although a tendency to lower shrinkage in the retanned samples was observed. Amounts of hexavalent chromium varied as a function of the fatliquor type. It may be concluded that the oxidised chromium resulted from residual or slightly fixed chromium due to the retanning process. As regards fastness to ultraviolet light, both yellowing and shrinkage temperature diminution were lower in chromium retanned leathers. In accordance with our findings in these studies, a selection of the most suitable fatliquoring agents for different leather articles can be made: *car upholstery*: sulphited natural and synthetic oil, fatliquor polymer; *clothing, gloves and double face*: special sulphited ester, sulphited natural and synthetic oil and *footwear*: sulphated natural and fatliquor polymer.

# Statistical Modelling and Fibre Physics



Research work is focussed 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.

## STAFF

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M DOLORS DE CASTELLAR BERTRAN (ad honorem)

## TECHNICIANS

CARMEN FERRERO VIRGOS  
ROSA MATEU MATEU

## Publications (articles)

**Effect of the air-jet and the false-twist texturing processes on the thermomechanical behaviour of polyamide 6.6 yarns**  
Manich, A.M., Maíllo, J., Cayuela, D., Carilla, J., Ussman, M., Gacén, J.  
*J. Therm. Anal. Calorim.* **2008**, 93, 921-926

**Chitosan contribution on wool treatments with enzyme**

Vilchez, S., Manich, A.M., Jovancic, P., Erra, P.  
*Carbohydr Polym.* **2008**, 71, 515-523

**Ceramides extracted from wool: supercritical extraction process**

Ramírez, R., Martí, M., Garay, I., Manich, A., Parra, J.L., Coderch, L.  
*Text. Res. J.* **2009**, 79, 721-726

**Ceramides extracted from wool: pilot plant solvent extraction**

Ramírez, R., Martí, M., Manich, A., Parra, J.L., Coderch, L.  
*Text. Res. J.* **2008**, 78, 73-80

**Transformation plant for converting chromium waste into chemical products for leather industry**

Cot, J., Marsal, A., Manich, A.M., Celma, P., Fernández-Hervás, F., Cot-Gores, J.  
*J. Am. Leather Chem. Assoc.* **2008**, 103, 103-113

**Factors that influence the physical properties of goatskins: polymeric derivatives and optimization of the process**

Palop, R., Manich, A.M., Marsal, A.  
*J. Am. Leather Chem. Assoc.* **2008**, 103, 174-181

**Alternative process for recovery of chrome (III)-effluents**

Cot, J., Marsal, A., Manich, A.M., Celma, P., Fernández, F., Cot-Gores, J.  
*J. Soc. Leather Technol. Chem.* **2008**, 92, 139-149

**Mecanismos de adsorción y desorción de vapor de agua en la piel**

Manich, A.M., Maldonado, F., Carilla, J., Catalina, M., Marsal, A.  
*Lederpiel* **2009**, 78, 38-47

**Análisis térmico y solubilidad diferencial de fibras e hilos de poliéster**

Manich, A.M., Ussman, M.H., Bosch, T., Carilla, J., Maíllo, J., Gacén, J.  
*Rev. Ind. Text.* **2009**, 472-473, 51-58

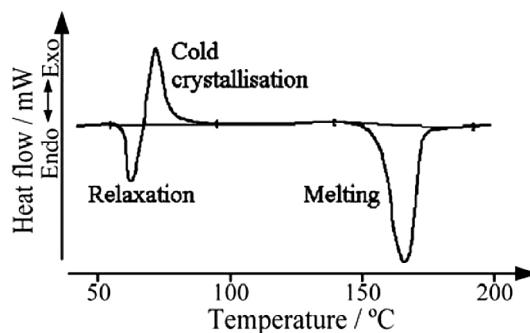
**Efecto de los procesos de acabado en tejidos cardados y peinados de lana y mezclas aplicando ensayos no destructivos**

Manich, A.M., Martí, M., Saurí, R.M., de Castellar, M.D.  
*Rev. Ind. Text.* **2009**, 467, 80-86

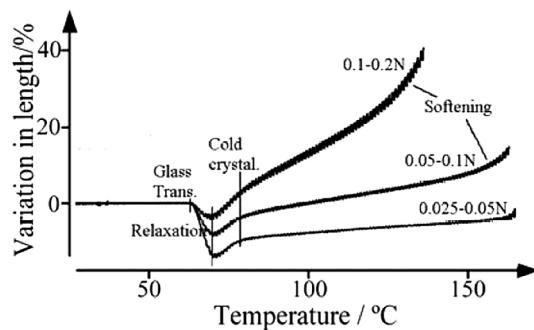
## Research highlights

### Polylactide multifilaments

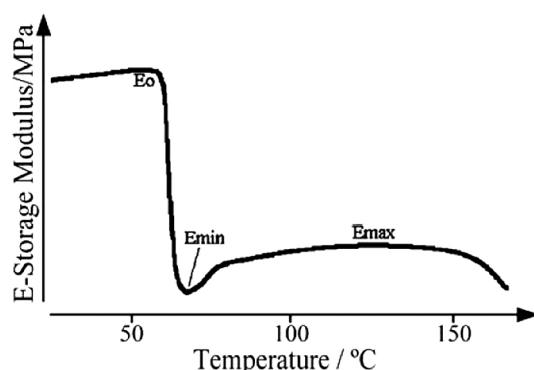
Polylactides (PLA) are biodegradable, biocompatible and hydrolysable aliphatic polyesters that can be wholly obtained from renewable resources. Nature derived lactides are mostly in L-lactide form and exhibit crystalline behavior. The microstructure of the multi-filaments is not easy to be controlled. A partially oriented melt-extruded PLA multifilament was false-twist textured to stabilize its structure. Conventional DSC analysis showed a relaxation peak at the end of the glass transition.



Simultaneous consideration of the TMA curve enabled us to evaluate both the relaxation and the cold crystallization produced during the DSC scan.

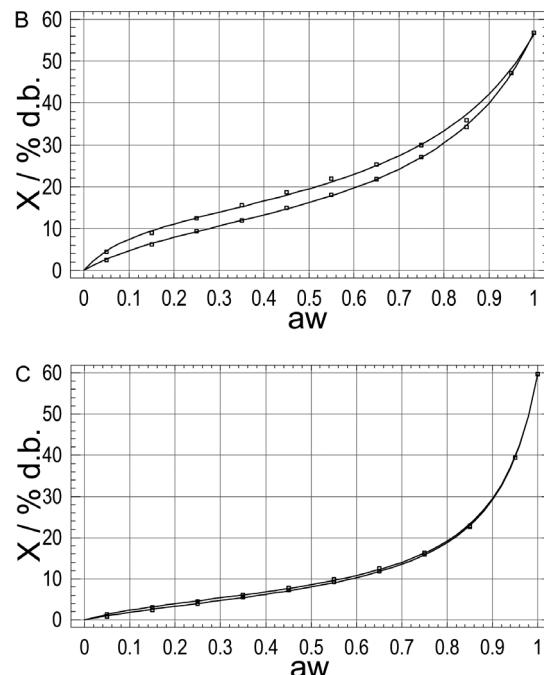


The periodic load applied during TMA experiments also enabled us to examine the evolution of Young's modulus along the glass transition, relaxation and cold crystallization phenomena. Increases in Young's modulus and in enthalpy are related because of crystallization.



### Sorption/desorption in collagen

Moisture sorption/desorption of two physical forms of collagen (hide powder and leather) was studied. Despite the fact that the testing of sorption/desorption behavior is time consuming, the application of a Dynamic Vapor Sorption analyzer enabled us to characterize the sorption/desorption behavior of materials in a relatively short time. Differences in sorption and desorption can be related to the accessibility and internal tortuousness of the materials. BET and GAB models were used to analyze variations in monolayer sorption capacity (internal sorption surface) of different forms of collagen (hide powder and leather). Variations in the energy constants related to primary and secondary sorption were also considered. Given that tests in desorption were performed, the BET and GAB models were also fitted to desorption and the differences observed in the parameters were analyzed. A model of sorption-desorption for porous materials was devised to account for the differences between sorption and desorption.



There is a very significant influence on the sorption capacity and hysteresis of collagen depending on the treatments applied.

## Biocompatible Surfactants



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### Ph. D. STUDENTS

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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, dermopharmaceutical 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

## Publications (articles)

### **A family of hydrogels based on ureido-linked aminopolyol-derived amphiphiles and bolaamphiphiles: synthesis, gelation under thermal and sonochemical stimuli and mesomorphic characterization**

Avalos, M., Babiano, R., Cintas, P., Gómez-Carretero, A., Jiménez, J.L., Lozano, M., Ortiz, A.L., Palacios, J.C., Pinazo, A.  
*Chem.-Eur. J.* **2008**, 14, 5656-5669

### **Catanionic vesicles formed with arginine-based surfactants and 1,2-dipalmitoyl-sn-glycero-3-phosphate monosodium salt**

Lozano, N., Pinazo, A., La Mesa, C., Pérez, L., Andreozzi, P., Pons, R.  
*J. Phys. Chem. B* **2009**, 4, 6321-6327

### **Aggregation properties of diacyl lysine surfactant compounds: hydrophobic chain length and counterion effect**

Pinazo, A., Pérez, L., Lozano, M., Angelet, M., Infante, M.R., Vinardell, M.P., Pons, R.  
*J. Phys. Chem. B* **2008**, 112, 8578-8585

### **Lysine-bisglycidol conjugates as novel lysine cationic surfactants**

Pinazo, A., Angelet, M., Pons, R., Lozano, M., Infante, M.R., Pérez, L.  
*Langmuir* **2009**, 25, 7803-7814

### **Gemini surfactant binding onto hydrophobically modified silica nanoparticles**

Andreozzi, P., Pons, R., Pérez, L., Infante, M.R., Mazzalupo, R., Suber, L., La Mesa, C.  
*J. Phys. Chem. C* **2008**, 112, 12142-12148

### **Cationic surfactants from lysine: synthesis, micellization and biological evaluation**

Pérez, L., Pinazo, A., García, M.T., Lozano, M., Manresa, A., Angelet, M., Vinardell, M.P., Mitjans, M., Pons, R., Infante, M.R.  
*Eur. J. Med. Chem.* **2009**, 44, 1884-1892

### **Physicochemical and toxicological properties of novel amino acid-based amphiphiles and their spontaneously formed catanionic vesicles**

Brito, R.O., Marques, E.F., Silva, S.G., do Vale, M.L., Gomes, P., Araújo, M.J., Rodriguez-Borges, J.E., Infante, M.R., Garcia, M.T., Ribosa, I., Vinardell, M.P., Mitjans, M.  
*Colloid Surf. B-Biointerfaces* **2009**, 72, 80-87

### **Surface tension and adsorption behavior of mixtures of diacyl glycerol arginine-based surfactants with DPPC and DMPC phospholipids**

Lozano, N., Pinazo, A., Pons, R., Pérez, L., Fransen, E.I.  
*Colloid Surf. B-Biointerfaces* **2009**, 74, 67-74

## **Comparative evaluation of cytotoxicity and phototoxicity of mono and diacylglycerol amino acid-based surfactants**

Vinardell, M.P., Benavides, T., Mitjans, M., Infante, M.R., Clapés, P., Clothier, R.  
*Food Chem. Toxicol.* **2008**, 46, 3837-3841

## **Human hemoglobin denaturation as an alternative to the draize test for predicting eye irritancy of surfactants**

Mitjans, M., Infante, M.R., Vinardell, P.  
*Regul. Toxicol. Pharmacol.* **2008**, 52, 89-93

## Interaction studies of diacyl glycerol arginine-based surfactants with DPPC and DMPC

**based structures with D,L-C and D,L-C monolayers, relation with antimicrobial activity**  
 Lozano, N., Pérez, L., Pons, R., Luque-Ortega, J.R., Fernández-Reyes, M., Rivas, L., Pinazo, A.  
*Colloid Surface A-Physicochem. Eng. Asp.* **2008**, 319, 196-203

## **Publications (books and book chapters)**

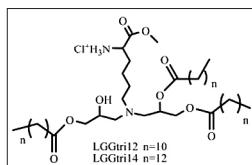
Infante, M.R., Pérez, L., Morán, C., Pons, R., Pinazo, A., 2009

## Synthesis, aggregation properties applications of biosurfactants derived from arginine

In: Biobased surfactants and detergents: synthesis, properties, and application  
Hayes, D., Dai Kitamoto, Solaimon, D., Ashby, R. (Eds.)  
AOCS Press 1, 351-387

## 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 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-aggregating capacity and number of fatty chains and the length thereof. 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) with moderate antimicrobial activity and excellent non-haemolytic behaviour. These compounds are hydrochloride salts of N(epsilon)-lauroyl lysine methyl ester, N(epsilon)-myristoyl lysine methyl ester and N(epsilon)-palmitoyllysine methyl ester. Moreover, the acute toxicity against *Daphnia*

## Aqueous self-assembly and physicochemical properties of 1,2-dilauroyl- rac-glycero-3-(N -acetyl-L-arginine)

Morán, C., Infante, M.R., Pérez, L., Pinazo, A., Coppola, L., Youssryb, M., Nicotera, I. *Colloid Surface A-Physicochem. Eng. Asp.* **2008**, 327, 111-121.

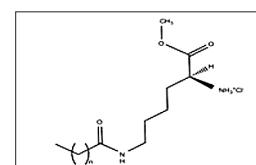
## **Antibacterial activity, structure and cmc relationships of alkanediyl alpha, omega-bis(dimethylammonium bromide) surfactants**

Laatiris, A., El Achouri, M., Infante, M.R., Bensouda, Y.

**Interaction of arginine-based cationic surfactants with membranes**

**Surfactants with membranes. An experimental and molecular simulation**  
Almeida, S., Moran, M.C., Infante, M.R., Pais, A.C.C.  
*Arkvoc* 2009, 12, 34-50

*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 reduce the toxicity of many surfactants, opening possibilities into clinical applications.

# Environmental Chemistry of Surfactants and Ionic Liquids



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## Publications (articles)

### Biodegradable, non-bactericidal oxygen-functionalised imidazolium esters: a step towards greener ionic liquids

Morrissey, S., Pegot, B., Coleman, D., Garcia, M.T., Ferguson, D., Quilty, B., Gathergood, N. *Green Chem.* **2009**, 11, 475-483

### Further investigation of the biodegradability of imidazolium ionic liquids

Harjani, J.R., Farrell, J., Garcia, M.T., Singer, R.D., Scammells, P.J. *Green Chem.* **2009**, 11, 821-829

### Phosphonium ionic liquids: design, synthesis and evaluation of biodegradability

Atefi, F., Garcia, M.T., Singer, R.D., Scammells, P.J. *Green Chem.* **2009**, 11, 1595-1604

### The design and synthesis of biodegradable pyridinium ionic liquids

Harjani, J.R., Singer, R.D., Garcia, M.T., Scammells, P.J. *Green Chem.* **2008**, 10, 42-48

### Cationic surfactants from lysine: synthesis, micellization and biological evaluation

Pérez, L., Pinazo, A., García, M.T., Lozano, M., Manresa, A., Angelet, M., Vinardell, M.P., Mitjans, M., Pons, R., Infante, M.R. *Eur. J. Med. Chem.* **2009**, 44, 1884-1892

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.

## Ph. D.

ISABEL RIBOSA FORNOVI

## Ph. D. STUDENTS

ANNA CORNELIAS PITARCH

### Physicochemical and toxicological properties of novel amino acid-based amphiphiles and their spontaneously formed catanionic vesicles

Brito, R.O., Marques, E.F., Silva, S.G., do Vale, M.L., Gomes, P., Araújo, M.J., Rodriguez-Borges, J.E., Infante, M.R., Garcia, M.T., Ribosa, I., Vinardell, M.P., Mitjans, M. *Colloid Surf. B-Biointerfaces* **2009**, 72, 80-87

### Fate and effects of amphoteric surfactants in the aquatic environments

García, M.T., Campos, E., Marsal, A., Ribosa, I. *Environ. Internat.* **2008**, 34, 1001-1005

### Biodegradability and toxicity of sulphonate-based surfactants in aerobic and anaerobic aquatic environments

García, M.T., Campos, E., Marsal, A., Ribosa, I. *Water Res.* **2009**, 43, 295-302

### A monolayer study on interactions of Docetaxel with model lipid membranes

Fernández-Botello, A., Comelles, F., Alsina, M.A., Cea, P., Reig, F. *J. Phys. Chem. B* **2008**, 112, 13834-13841

### Adsorption of polyphenols in wastewater by organo-bentonites

Marsal, A., Bautista, E., Ribosa, I., Pons, P., García, M.T., *Appl. Clay Sci.* **2009**, 44, 151-155

### Formulaciones de cristal líquido laminar con bajo contenido en tensioactivo

Comelles, F., Sánchez-Leal, J., González, J.J. *NCP (Noticias de Cosmética y Perfumería. Bol. Soc. Esp. Quim. Cosmet.)* **2008**, 299, 11-19

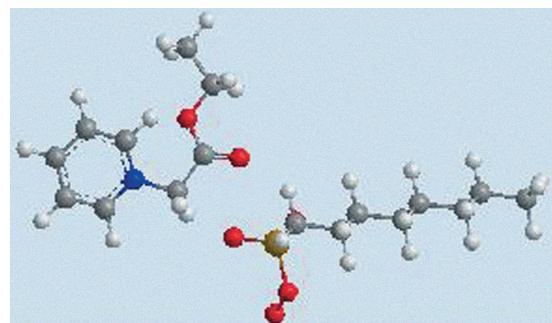
## Research highlights

### Environmental fate and effects of commonly used surfactants

Sulphonates are one of the most widely used anionic surfactant groups in the household and personal care sectors. Therefore, an understanding of their biodegradability and ecotoxicity is crucial for assessing the risk to the environment. Sulphonate-based surfactants were tested for their aerobic and anaerobic biodegradability as well as for their aquatic toxicity to assess the effect of the surfactant structure on those properties. Alkane-sulphonates,  $\alpha$ -olefin sulphonates, methyester sulphonates and sulphosuccinates are aerobically biodegraded. However, only sulphosuccinates will be partially (branched alkyl sulphosuccinates) or extensively (linear alkyl sulphosuccinates) mineralized in anaerobic digesters given that the ester linkage and its position with respect to the sulphonate group are essential for the degradation of the surfactant molecule under anaerobic conditions. On the other hand, no clear effect of the structural properties of the sulphonate-based surfactants on their toxicity to the aquatic organisms tested (*D. magna* and *P. phosphoreum*) is observed.

### 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 the research group of the Professor Peter Scammells (Monash University), 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.



Pyridinium based ionic liquid functionalized in its lateral alkyl chain and octylsulphate as counterion

A range of ionic liquids (ILs) with a pyridinium cation were synthesised and their biodegradability was evaluated using the CO<sub>2</sub> 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'. In contrast, pyridinium ILs with alkyl side chains showed significantly lower levels of biodegradability in the same test. The high biodegradation rates appear to be a characteristic of the cation and do not depend on the counter ions tested. 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 which are likely to possess good solvent attributes and a predisposition to biodegrade when released into an aquatic environment.

### Surface activity of new surfactant phosphine ligands and platinum (II) metallosurfactants

The surfactant properties of a new series of phosphines obtained by reaction between halosulphonates and sodium diphenylphosphide were determined. These phosphines were considered as ligands of the (Pt II) metallosurfactants obtained by its reaction with PtCl<sub>2</sub>. By exploring the surface properties of phosphines and their respective platinum metallosurfactants through surface tension measurements, we were able to analyze the influence of the metal coordination on the critical micelle concentration (cmc) and aggregation properties. The cmc values of platinum metallosurfactants were considerably lower than those obtained for the free phosphine. This behaviour could be understood by an analogy between the structure of these complexes and bolaform surfactants. The study of this new family of phosphines can supply information about the influence of the position of the diphenylphosphino group in surfactant properties and lead to new metallosurfactants with very attractive characteristics.

# Physical Chemistry of Surfactant Systems



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)

**Cationionic vesicles formed with arginine-based surfactants and 1,2-dipalmitoyl-sn-glycero-3-phosphate monosodium salt**  
Lozano, N., Pinazo, A., La Mesa, C., Pérez, L., Andreozzi, P., Pons, R.  
*J. Phys. Chem. B* **2009**, 113, 6321-6327

**Aggregation properties of diacyl lysine surfactant compounds: hydrophobic chain length and counterion effect**

Pinazo, A., Pérez, L., Lozano, M., Angelet, M., Infante, M.R., Vinardell, M.P., Pons, R.  
*J. Phys. Chem. B* **2008**, 112, 8578-8585

**Structure/property relationships for the thermotropic behavior of lysine-based amphiphiles: from hexagonal to smectic phases**

Brito, R.O., Marques, E.F., Gomes, P., Araujo, M.J., Pons, R.  
*J. Phys. Chem. B* **2008**, 112, 14877-14887

**Lysine-bisglycidol conjugates as novel lysine cationic surfactants**

Pinazo, A., Angelet, M., Pons, R., Lozano, M., Infante, M.R., Pérez, L.  
*Langmuir* **2009**, 25, 7803-7814

**Conformational changes in stratum corneum lipids by effect of bicellar systems**

Rodríguez, G., Barbosa-Barros, L., Rubio, L., Cócera, M., Díez, A., Estelrich, J., Pons, R., Caelles, J., de la Maza, A., López, O.  
*Langmuir* **2009**, 25, 10595-10603

**Penetration and growth of DMPC/DHPC bicelles inside the stratum corneum of the skin**

Barbosa, L., de la Maza, A., Estelrich, J., Linares, A.M., Feliz, M., Walter, P., Pons, R., López, O.  
*Langmuir* **2008**, 24, 5700-5706

## Ph. D. STUDENT

NEUS LOZANO VALDÉS

## Gemini surfactant binding onto hydrophobically modified silica nanoparticles

Andreozzi, P., Pons, R., Pérez, L., Infante, M.R., Mazzalupo, R., Suber, L., La Mesa, C.  
*J. Phys. Chem. C* **2008**, 112, 12142-12148

## Cationic surfactants from lysine: synthesis, micellization and biological evaluation

Pérez, L., Pinazo, A., García, M.T., Lozano, M., Manresa, A., Angelet, M., Vinardell, M.P., Mitjans, M., Pons, R., Infante, M.R.  
*Eur. J. Med. Chem.* **2009**, 44, 1884-1892

## Lamellar rearrangement of internal lipids from human hair

Coderch, L., Méndez, S., Barba, C., Pons, R., Martí, M., Parra, J.L.  
*Chem. Phys. Lipids* **2008**, 155, 1-6

## Surface tension and adsorption behavior of mixtures of diacyl glycerol arginine-based surfactants with DPPC and DMPC phospholipids

Lozano, N., Pinazo, A., Pons, R., Pérez, L., Franses, E.I.  
*Colloid Surf. B-Biointerfaces* **2009**, 74, 67-74

## Adsorption of polyphenols in wastewater by organo-bentonites

Marsal, A., Bautista, E., Ribosa, I., Pons, P., García, M.T.,  
*Appl. Clay Sci.* **2009**, 44, 151-155

## Interaction studies of diacyl glycerol arginine-based surfactants with DPPC and DMPC monolayers, relation with antimicrobial activity

Lozano, N., Pérez, L., Pons, R., Luque-Ortega, J.R., Fernández-Reyes, M., Rivas, L., Pinazo, A.  
*Colloid Surface A-Physicochem. Eng. Asp.* **2008**, 319, 196-203

## Publications (books and book chapters)

Infante, M.R., Pérez, L., Morán, C., Pons, R., Pinazo, A., 2009

### Synthesis, aggregation properties applications of biosurfactants derived from arginine

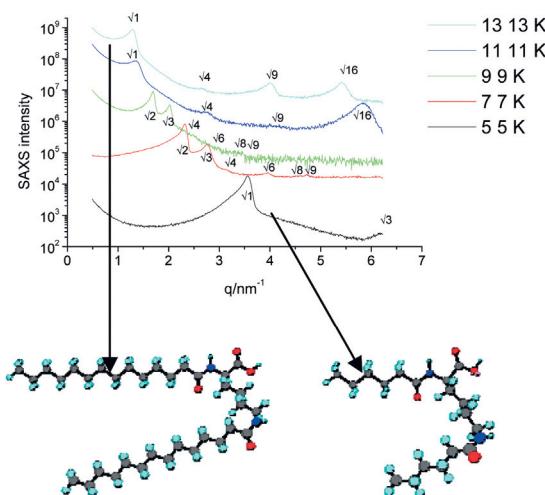
In: Biobased surfactants and detergents: synthesis, properties, and application

Hayes, D., Dai Kitamoto, Solaimon, D., Ashby, R. (Eds.)

AOCS Press 1, 351-387

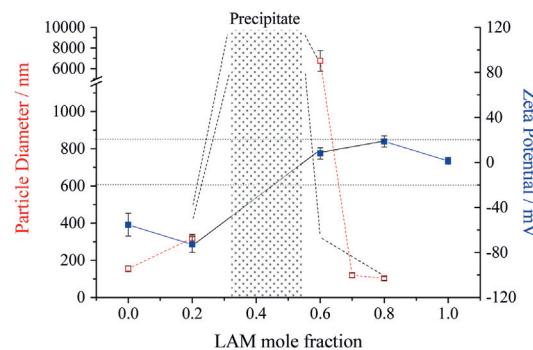
## Research highlights

Some of the main results on characterisation of surfactant nanostructures refer to the determination of the phase behaviour of diacyl lysine compounds. The thermotropic phase behaviour has been determined for several hydrophobic chain length, polarity and charge of the headgroup. An unusual direct to reverse phase trend was observed as the hydrophobic chain length decreases that was attributed to the wedge shape of the molecule that favours the formation of inverse phases. Longer acyl compounds can put the hydrophobic chains in a more overall parallel conformation to allow for the formation of lamellar phases.

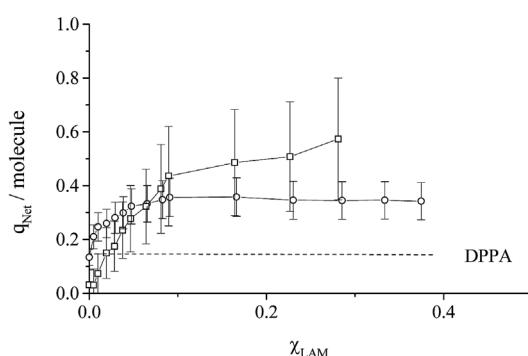


Catanionic surfactants and mixtures show some interesting and amazing phenomena. In the phase behaviour of catanionic surfactants (1:1 catanionic mixtures without simple counterions) the coexistence of two lamellar phases was established.

On the other hand, the study of catanionic vesicles of the pseudotricatenary and pseudotetracatenary type shows an increase of the absolute value of Z-potential for small values of neutralization. That is, the negative charge of the anionic phospholipid vesicles of DPPA is reinforced when small amounts of cationic diacyl gliceroarginine compounds are added. Conversely the cationic charge of the cationic vesicles is reinforced when small amounts of the anionic phospholipid are added.



This particular behaviour has been explained on the basis of strong counterion release due to hydrogen bonding charge stabilisation.



Counterion binding as a function of cationic surfactant rapidly increases and stabilises.

Related to research using Small Angle X-Ray Scattering, a humidity chamber for use with the GISAXS configuration has been built and patented. Measurements of skin samples using this chamber have been also published.

In relation with cationic lipoaminoacid surfactants, a selective electrode with sensibility down to 1 micromolar has been set up and patented.

# Biophysics of Lipids and Interphases



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.

## STAFF

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Mª LUISA CODERCH NEGRA  
ALFONS DE LA MAZA RIBERA  
OLGA LÓPEZ SERRANO

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GELEN RODRÍGUEZ DELGADO  
LAIA RUBIO TOLEDANO

## Publications (articles)

### Lipid nanostructures: self-assembly and effect on skin properties

Barbosa-Barros, L., Barba, C., Rodríguez, G., Cócera, M., Coderch, L., López-Iglesias, C., de la Maza, A., López, O.  
*Mol. Pharm.* **2009**, 6, 1237-1245

### Conformational changes in stratum corneum lipids by effect of bicellar systems

Rodríguez, G., Barbosa-Barros, L., Rubio, L., Cócera, M., Díez, A., Estelrich, J., Pons, R., Caelles, J., de la Maza, A., López, O.  
*Langmuir* **2009**, 25, 10595-10603

### Penetration and growth of DMPC/DHPC bicelles inside the stratum corneum of the skin

Barbosa, L., de la Maza, A., Estelrich, J., Linares, A.M., Feliz, M., Walter, P., Pons, R., López, O.  
*Langmuir* **2008**, 24, 5700-5706

### Lamellar rearrangement of internal lipids from human hair

Coderch, L., Méndez, S., Barba, C., Pons, R., Martí, M., Parra, J.L.  
*Chem. Phys. Lipids* **2008**, 155, 1-6

### Effect of bicellar systems on skin properties

Barbosa, L., Barba, C., Cócera, M., Coderch, L., López-Iglesias, C., de la Maza, A., López, O.  
*Int. J. Pharm.* **2008**, 352, 263-272

### Supercritical fluid extraction to obtain ceramides from wool fibres

Ramírez, R., Garay, I., Álvarez, J., Martí, J., Parra, J.L., Coderch, L.  
*Sep. Purif. Technol.* **2008**, 63, 552-557

### Liposome formation with wool lipid extracts rich in ceramides

Ramírez, R., Martí, M., Cavaco-Paulo, A., Silva, R., de la Maza, A., Parra, J.L., Coderch, L.  
*J. Liposome Res.* **2009**, 19, 77-83

### An ex vivo methodology to asses the lipid peroxidation in stratum corneum

Alonso, C., Barba, C., Rubio, L., Scott, S., Kilimnik, A., Coderch, L., Notario, J., Parra, J.L.  
*J. Photochem. Photobiol. B-Biol.* **2009**, 97, 71-76

### Water content of hair and nails

Barba, C., Méndez, S., Martí, S., Parra, J.L., Coderch, L.  
*Thermochim. Acta* **2009**, 494, 136-140

### Ceramide effects in the micelle structure

Barbosa, L., de la Maza, A., López-Iglesias, C., López, O.  
*Colloid Surface A-Physicochem. Eng. Asp.* **2008**, 317, 576-584

### Use of high pressure freeze fixation and freeze fracture electron microscopy to study the influence of the phospholipid molar ratio in the morphology and alignment of bicelles

Barbosa-Barros, L., de la Maza, O., Walter, P., Linares, A.M., Feliz, M., Estelrich, J., López, O.  
*J. Microsc.-Oxf.* **2009**, 233, 35-41

### Morphological effects of ceramide on DMPC/DHPC bicelles

Barbosa, L., López-Iglesias, M.C., de la Maza, A., López, O.  
*J. Microsc.-Oxf.* **2008**, 230, 16-26

### Cosmetic effectiveness of topically applied hydrolysed keratin peptides and lipids derived from wool

Barba, C., Méndez, S., Roddick-Lanzilotta, A., Kelly, R., Parra, J.L., Coderch, L.  
*Skin Res. Technol.* **2008**, 14, 243-248

### Application of internal wool lipids to hair

Méndez, S., Barba, C., Roddick-Lanzilotta, A., Kelly, R., Parra, J.L., Coderch, L.  
*Skin Res. Technol.* **2008**, 14, 448-453

## Publications (books and book chapters)

López, O., Cócera, M., Coderch, L., Barbosa-Barros, L., Parra, J. L., de la Maza, A., 2009

### Applications of alkyl glucosides in the solubilization of liposomes and cell membranes

In: Sugar-based surfactants: fundamentals and applications  
Carnero Ruiz, C. (Ed.)  
CRC Press, Boca Raton, Fl, 143, Ch 15, 585-626

### Ceramides extracted from wool: supercritical extraction process

Ramírez, R., Martí, M., Garay, I., Manich, A., Parra, J.L., Coderch, L.  
*Text. Res. J.* **2009**, 79, 721-726

### Ceramides extracted from wool: pilot plant solvent extraction

Ramírez, R., Martí, M., Manich, A., Parra, J.L., Coderch, L.  
*Text. Res. J.* **2008**, 78, 73-80

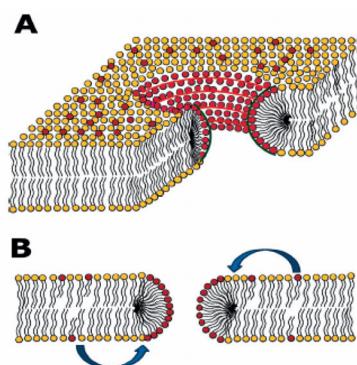
Costa, M., Bentseny-Cases, N., Cócera, M., Texeira, C., Alsina, M., Cladera, N., López, O., Fernández, M., Sabes, M., 2009

### Diagnosis applications of non-crystalline diffraction of collagen fibres: breast cancer and skin diseases

In: Applications of Synchrotron Light to Scattering and Diffraction in Materials and Life Sciences. Lect. Notes Phys. 776  
Ezquerra, T.A.; Garcia-Gutierrez, M.C.; Nogales, A.; Gomez, M. (Eds.)  
Springer Berlin / Heidelberg, Ch 13, 265–280

## 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:

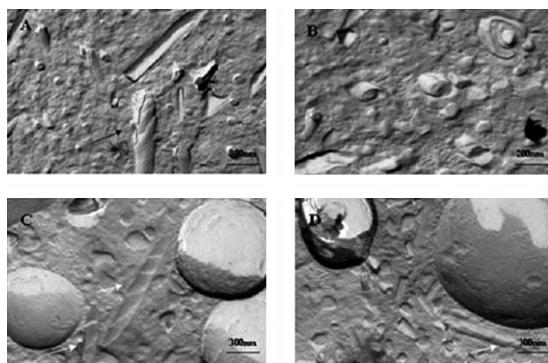
(A) Perforated lamellae morphology of magnetically aligned dimyristoyl-phosphatidylcholine/dihexanoyl-phosphatidyl-choline (DMPC/DHPC) bicelles consisting of both planar and high-curvature regions. DMPC and DHPC are represented by the yellow and red colors, respectively.

(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

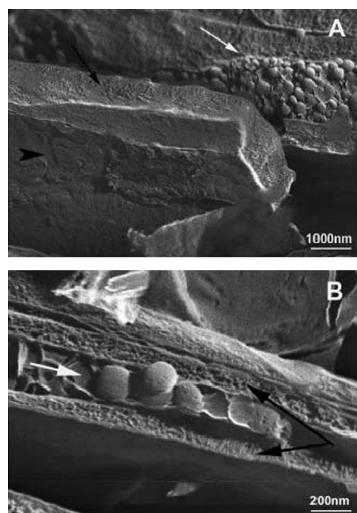
some of the biophysical properties of the skin. Thus, topical *in vivo* application of DMPC/DHPC bicelles improve skin permeation and elastic parameters and decreased skin hydration without promoting irritation and without affecting stratum corneum lipid microstructure. The increase of permeability was 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 blackarrow 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

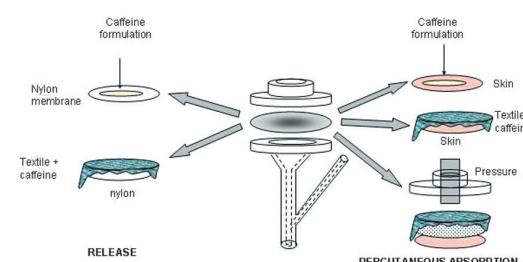
### Biofunctional textiles

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 into 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.

As vehicles, microcapsules or liposomes were used, liposomes were prepared with wool lipid (IWL) 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 methoxycinnamate) 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 fibres, such as hair and nails due to water presence. Reactive cosmetic treatments of hair and nails often impair fibre 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. Humanails 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 fibres

# 6

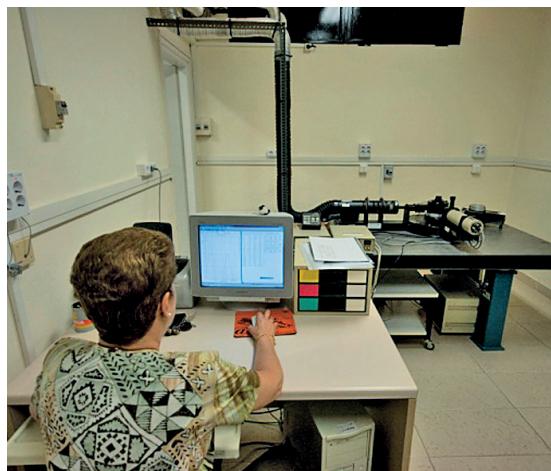
## FACILITIES



## **IQAC FACILITIES**

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

# Characterization of Colloidal Dispersions Service



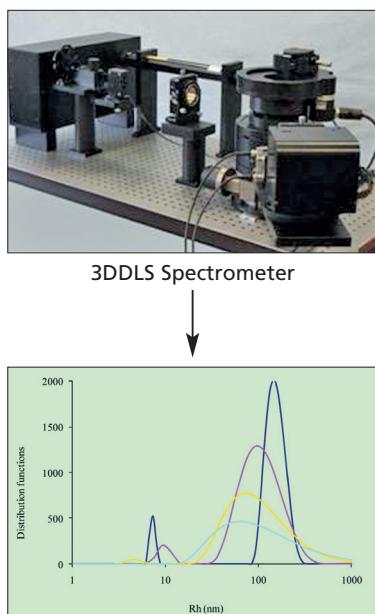
## SUPERVISING SCIENTISTS

NURIA AZEMAR SAZATORNIL  
CONXITA SOLANS MARSÀ

## Relevant techniques:

### Static (SLS) and dynamic (DLS) light scattering

Determination of particle size distribution, shape, diffusion coefficient, aggregation number, molecular weight of colloidal dispersions



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

### Other techniques.

Laser Light Diffraction  
Differential Refractometry  
Tensiometry,  
Optical Microscopy

This service deals with the characterization of nano-structured liquids (e.g. micelles, vesicles, liquid crystals, microemulsions, nano-emulsions 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 service responsible group is member of TECNIO (ACC1Ó, CIDEM/COPCA) and has been awarded with a quality certificate (similar to ISO 9001) by CIDEM (Generalitat de Catalunya).

### Rheology

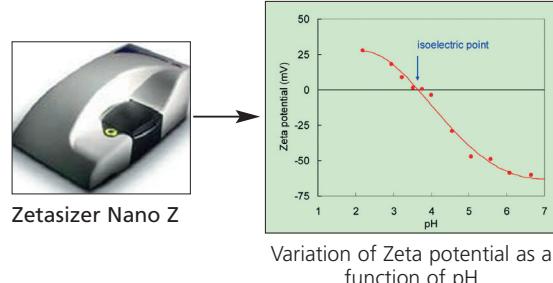
Determination of rheological properties of fluids and soft matter in flow and deformation regimes by steady state (viscosity, shear thinning, shear thickening) and dynamic (elastic and viscous moduli, relaxation time) measurements



Rheometer AR-G2  
Variation of elastic ( $G'$ ) and viscous ( $G''$ ) moduli as a function of frequency

### Electrophoretic mobility

Determination of Zeta potential of charged particles



Zetasizer Nano Z  
Variation of Zeta potential as a function of pH

## 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.

### STAFF

M<sup>a</sup> PILAR MARCO COLÁS (SUPERVISING SCIENTIST)  
NURIA PASCUAL DURAN  
MARTA RUIZ ARRIBAS

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.

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

#### 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 costumer. The costumer 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: labeled antibodies, haptenized proteins and enzymes, biotinylated and fluorescent probes, gold nanoparticle conjugates, etc.
2. Antibody purification.
3. Development of immunochemical methods: ELISA, immunoaffinity columns, etc.
4. Antibody characterization (Isotyping).
5. Hybridoma cryopreservation.
6. Mycoplasma testing

## 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

### STAFF

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MARIA TERESA VILA TERRADES

NURIA BARRERA DE PAZ

ANA DOMÈNECH DURAN

### Equipment

This facility has the appropriate instruments for accurate sample analysis. Primary Instruments:

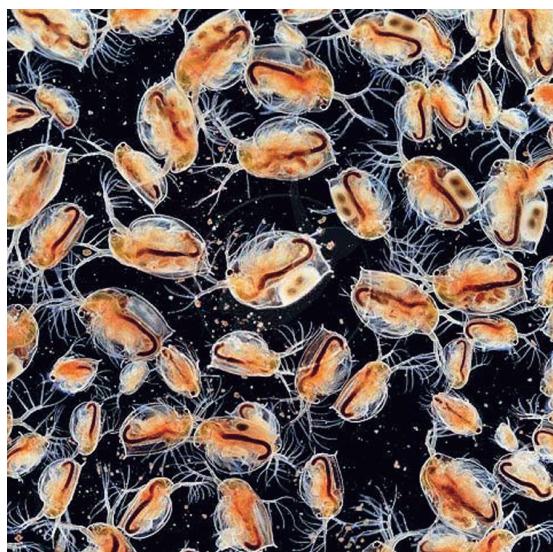
- 1 Elemental Microanalyzer (A5) model Flash 1112, for C,H,N determination.
- 1 Elemental Microanalyzer (A3) model 1500, for O determination.
- 1 Elemental Microanalyzer (A4) model 1108, for C,H,N,S determination.

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 determination.

## 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.

### STAFF

MARÍA TERESA GARCÍA RAMÓN (Contacting person)

ISABEL MUÑOZ LIRÓN

ROSA MARÍA SALVIA PEIRÓ

## Spectroscopic Service



The Spectroscopic Service is a research support unit for the Institute, Universities and other Public Research Organisms, as well as for private companies.

In this research support unit, three types of spectroscopy techniques are available:

**a) Molecular Spectroscopy:** The systems available in our laboratory allow analytical studies, both qualitative and quantitative, of organic and inorganic molecules (in solid or liquid state) in the ultraviolet, visible and infrared energy range. It is also possible the determination of rotatory optical activity of samples in solution.

**b) Nuclear Magnetic Resonance:** The available systems in this service allow carrying out 1D and 2D  $^1\text{H}$ NMR,  $^{13}\text{C}$ NMR and  $^{19}\text{F}$ NMR spectra of organic compounds in solution.

**c) Electronic Paramagnetic Resonance:** The electron paramagnetic resonance allows detection and study of transient and stable paramagnetic species such as free radicals

### STAFF

LLUÍS JULIÀ BARGES (Supervising scientist, Contacting person)

LOURDES PÉREZ MUÑOZ (Supervising scientist, Contacting person)

AVENCIA DIEZ ORTEGO

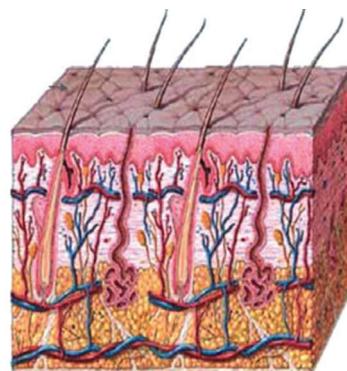
MONTSERRAT SINDREU GRAÑÉ



## Skin Absorption Service



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

JOSÉ LUIS PARRA JUEZ (Supervising scientist,  
Contacting person)  
CRISTINA ALONSO MERINO  
LAIA RUBIO TOLEDANO

## Skin Efficacy Service



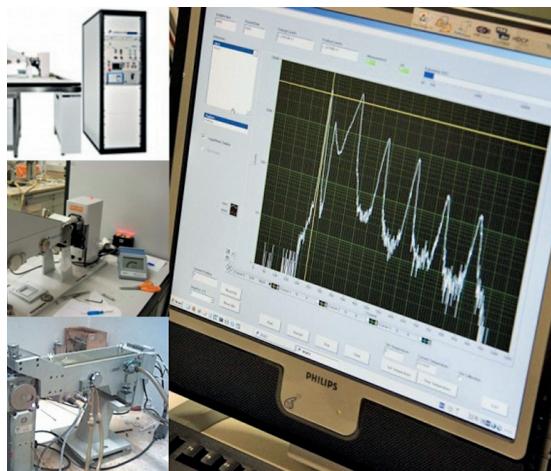
The **Skin Efficacy Service** deals with the experimental design, evaluation and objective diagnostic of the skin efficacy and tolerance of cosmetic and dermatologic formulations topically applied by the use of non-invasive biophysical techniques. Evaluation and diagnosis of other keratinized tissues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



### STAFF

LUISA CODERCH NEGRA (Supervising scientist,  
Contacting person)  
CLARA BARBA ALBANEZ  
ISABEL YUSTE HERNÁNDEZ

## 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). The materials comprise surfactant solutions and liquid crystals, mesoporous materials, microemulsions, proteins in solution, DNA in solution and any conceivable material with electronic discontinuities in the above mentioned range.

### STAFF

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JORDI ESQUENA MORET (Supervising scientist, Contacting person)  
JAUME CAELLES BALCELLS

# Synthesis of High Added Value Molecules Service

The service (SIMChem) is a new IQAC service that has been created in 2009, and it will be dedicated to the preparation of **organic compounds**.

The purpose is to carry out **research** in synthetic organic chemistry to give **support** to research groups present in IQAC, other CSIC Institutes or external organizations, both in academic or industrial environments.

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 molecular probes 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. Through this service, it is projected 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.



## STAFF

AMADEU LLEBARIA (Scientific director)  
CARME SERRA (Technical director)  
MARINA LOZANO (Specialist technician)



## Services

- Organic synthesis
- Chemical advice
- Organic pathway design
- Karl-Fischer
- Chromatographic purification
- Microwaves
- HPLC
- Low pressure hydrogenation (max. 3 atm)

## Thermal Analysis Service



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 AUGET (Contacting person)  
AMELIA LOPEZ NAVARRO  
ROCÍO VICENTE FERNÁNDEZ.

The following techniques are available:

- Differential scanning calorimetry DSC
- Microdifferential scanning calorimetry
- Thermogravimetric analysis TGA
- Dynamic vapor sorption DVS
- Thermomechanical analysis TMA



## Publications (articles)

### Mecanismos de adsorción y desorción de vapor de agua en la piel

Manich, A.M., Maldonado, F., Carilla, J., Catalina, M., Marsal, A.  
*Lederpiel* **2009**, 78, 38-47

### Análisis térmico y solubilidad diferencial de fibras e hilos de poliéster

Manich, A.M., Ussman, M.H., Bosch, T., Carilla, J., Maíllo, J., Gacén, J.  
*Rev. Ind. Text.* **2009**, 472-473, 51-58



# 7

## APPENDIXES



## **APPENDIX 1. OTHER RESULTS**

### **General activities**

Invited Conferences  
I Workshop CBN'09  
Science Week  
Expoquimia 2008  
Visita IE Ernest Lluch

### **Department of Biological Chemistry and Molecular Modelling**

Research Projects  
Patents  
Ph. D. Thesis  
Masters-D.E.A.  
Academic activities  
Congress Organization  
Invited Conferences  
Editorial Activity in Journals

### **Department of Biomedicinal Chemistry**

Research Projects  
Patents  
Ph. D. Thesis  
Masters-D.E.A.  
Invited Conferences  
Editorial Activity in Journals

### **Department of Chemical and Biomolecular Nanotechnology**

Research Projects  
Patents  
Ph. D. Thesis  
Masters-D.E.A.  
Academic activities  
Congress Organization  
Invited Conferences  
Editorial Activity in Journals

### **Department of Chemical and Surfactants Technology**

Research Projects  
Patents  
Ph. D. Thesis  
Masters-D.E.A.  
Academic activities  
Congress Organization  
Invited Conferences  
Editorial Activity in Journals

## **APPENDIX 2. 2008-2009 PUBLICATIONS**

1. List of ISI journals in alphabetical order (and impact factor)
2. Publications listed by decreasing impact factor  
(2009 listed first if papers in both years)
3. Publications in non-ISI journals (journals in alphabetical order)
4. Book chapters
5. Conference Proceedings

The contents of appendixes 1 and 2 are to be found in  
the CD version



## **APPENDIX 1: OTHER RESULTS**

|  |            |
|--|------------|
| General activities   | <b>100</b> |
| Department of biological chemistry and molecular modelling | <b>102</b> |
| Department of biomedical chemistry                         | <b>108</b> |
| Department of chemical and biomolecular nanotechnology     | <b>111</b> |
| Department of chemical and surfactants technology          | <b>121</b> |

## GENERAL ACTIVITIES

### INVITED CONFERENCES

- R. Neubert  
*College of Pharmacy, Martin Luther University Halle-Wittenberg, Germany.*  
New insights into the morphologic and molecular structure of the stratum corneum - the basis for influencing drug penetration  
10/04/2008
- J.W. Wiechers  
*International Federation of Societies of Cosmetic Chemists, The Netherlands*  
Delivery of cosmetically active ingredients  
22/05/2008
- G.J.T. Tiddy  
*University of Manchester, UK*  
Structures and molecular self-assembly mechanisms of chromonic liquid crystals: New nanomaterial templates with controlled morphology?  
28/05/2008
- L.M. Beltramini  
*Universidad de Sao Paulo, Brasil*  
Investigating specificity of D-galactose-binding lectins using membrane model systems  
02/06/2008
- D. González  
*Universidad de la República, Montevideo, Uruguay*  
Biocatalysis práctica y su aplicación en síntesis quimioenzimáticas  
19/06/2008
- J. Puig  
*Universidad de Guadalajara, México*  
Improving hydration swelling and mechanical properties of hydrogels with polymer nanoparticles  
26/06/2008
- B. F. Chemlka  
*University of California-Santa Barbara, Santa Barbara, USA*  
Functionalization of self-assembled block-copolymer/inorganic oxide films  
26/06/2008
- J.M. de la Fuente  
*Universidad de Zaragoza*  
Biofunctionalization of nanoparticles and surfaces for biotechnological applications  
15/07/2008
- T. Kano  
*Lion Corporation, Japan*  
Chemical products from palm oil  
21/07/2008
- D. Clausse  
*Université de Technologie de Compiègne, France*  
Mass transfer kinetics in emulsions  
24/07/2008
- T. Imae  
*National Taiwan University of Science and Technology, Taiwan*  
Advanced fabrication of metallic nanostructures and their ordered array  
26/08/2008
- L.K. Shrestha  
*Yokohama National University, Japan*  
Structural control of reverse micelles: A SAXS study  
14/09/2008
- M. Sabés  
*Universidad Autónoma de Barcelona.*  
Proyecto de estación de imagen y aplicaciones biomédicas para el sincrotrón ALBA  
05/12/2008
- P. Botta  
*Universidad de Mar del Plata, Instituto Nacional de Tecnología y Materiales, Argentina*  
Synthesis of nanocrystalline inorganic oxides by mechanochemical activation of solids  
24/04/2009
- C.E. Hoppe  
*Universidad de Mar del Plata, Instituto Nacional de Tecnología y Materiales, Argentina*  
Strategies for the dispersion of inorganic nanoparticles in crosslinked polymer matrices  
24/04/2009
- N. Gathergood  
*Dublin City University, Ireland.*  
The abc of green chemistry: atom economy, biodegradation and catalysis  
06/05/2009
- C. La Mesa  
*University of Roma «La Sapienza», Italy.*  
Self-assembly of attractive colloids: a kinetic study  
07/05/2009
- U. Masaki  
*National Taiwan University of Science and Technology, Taiwan*  
Preparation methods for nanomaterials  
17/09/2009
- K. Aramaki  
*Yokohama National University, Japan*  
Recent progress on liquid crystal based gel emulsions and wormlike micelles  
17/09/2009
- J. F. Armando Soltero Martínez  
*Universidad de Guadalajara, Centro Universitario de Ciencias Exactas en Ingenierías, México*  
Reología de Fluidos Complejos  
15/10/2009
- A. Canelas Pais  
*Universidade de Coimbra, Portugal*  
Computational and experimental studies in biological systems  
23/10/2009

M. C. Cabot

*John Wayne Cancer Institute, Santa Monica,  
California (USA)*

Targeting ceramide metabolism. Therapeutic approaches in prostate and pancreatic cancer and acute myeloid leukemia.

10/11/2009

M. P. Calcagno P. de López

*Universidad de los Andes, Mérida, Venezuela*

El género *Pteridium* en Venezuela: mecanismos químicos de defensa y sus consecuencias en la salud animal y humana

09/12/2009

### I WORKSHOP CBN'09 (19-20/10/2009)

Eritja, R.

*Synthesis and properties of modified oligonucleotides*

Esquena, J.

*Research lines of the Surface Chemistry Group*

Fabrega, C.

*Structure-based discovery of novel non-nucleosidic DNA alkyltransferase inhibitors: virtual screening, in vitro and in vivo activities.*

Fernández, F.

*Improvement on surface plasmon resonance detectability for fluoroquinolone antibiotic residue by using nanogold probes*

Garibotti, A.

*Functionalization of two-dimensional DNA arrays with potential applications*

Grijalvo, S.

*Synthesis of novel oligonucleotide-peptide conjugates containing guanidinium and lipophilic groups in their 3'-termini*

Muriano, A.

*Electrochemical magneto immunosensing antibiotic residues in honey samples*

Solans, C.

*Colloid and Interfacial Chemistry Group*

Tort, N.

*Fluorescence and SPR microarrays based on haptene-oligonucleotide bioconjugates*

### SCIENCE WEEK 2008 (14-21 Nov)

Josefina Casas

*Suïcidi cel·lular: rituals per a la supervivència*

Ramon Eritja

*ADN i ordinadors*

Àngel Meseguer

*Hi haurà química entre nosaltres?*

Aurora Pinazo

*Tensioactius: Molècules necessàries per a la vida*

Carlos Rodríguez-Abreu

*Cuando la ciencia imita a la naturaleza*

Josep Lluís Torres

*Radicals lliures i enveliment saludable*

Gregori València

*És un gas!*

Pilar Vinardell

*Métodos alternativos a la experimentación animal*

### SCIENCE WEEK 2009 (13-20 Nov)

Josefina Casas

*Suïcidi cel·lular: rituals per a la supervivència*

Ramon Eritja

*ADN i ordinadors*

Àngel Meseguer

*Hi haurà química entre nosaltres?*

Ramon Pons

*Sabons: de bombolles a cristalls líquids (la importància de la nanoestructura)*

Aurora Pinazo

*Tensioactius: Molècules necessàries per a la vida*

Josep Lluís Torres

*Radicals lliures i enveliment saludable*

Gregori València

*Free Range Chemistry*

### EXPOQUIMIA 2008 (22 Oct)

#### JORNADA SOBRE NUEVOS RETOS DE LA QUÍMICA EN EL SIGLO XXI

«Química y diversidad: potencial y perspectivas de los biocatalizadores en la preparación de productos de alto valor añadido». Dr. Pere Clapés, Investigador Científico del CSIC.

«Tensioactivos: oportunidades y retos en química sostenible». Dra. María Rosa Infante, Profesora de Investigación del CSIC.

«Tecnologías de la química moderna y su influencia en las biociencias». Dr. Àngel Meseguer, Profesor de Investigación del CSIC.

«Ensamblaje de bioreceptores y transductores: una nueva generación de dispositivos analíticos basados en materiales híbridos». Dra. Pilar Marco, Profesora de Investigación del CSIC.

### VISITA IES ERNEST LLUCH (19/02/2009)

Eritja, R.

*Síntesis i propietats del DNA*

Haro, I

*Pèptids sintètics en Biomedicina*

# DEPARTMENT OF BIOLOGICAL CHEMISTRY AND MOLECULAR MODELLING

## Research Projects

Estudio de nuevos receptores de biomoléculas mediante el uso de estrategias de química combinatoria dinámica asistida por plantillas CSIC (I3-200780I001)  
Principal Investigator: I. Alfonso  
2007-2008

Química supramolecular heterocíclica. Sólidos nanoestructurados. Aspectos biomédicos y medioambientales  
MEC (CTQ200615672C05-02)  
Coordinator: Enrique Gracia-España (U.Val.)  
Principal Investigator: Santiago V. Luis (UJI)  
IQAC participant: I. Alfonso  
2006-2009

Líquidos iónicos quirales: nuevos disolventes, reactivos y catalizadores benignos para procesos químicos  
Bancaja-UJI (PI1A2007-11)  
Principal Investigator: E. García-Verdugo (UJI)  
IQAC participant: I. Alfonso  
2008-2009

Mecanismos de las reacciones de transferencia de hidrógeno en la química de la atmósfera.  
Transferencia de átomo de hidrógeno (HAT) versus transferencia de electrón acoplada a proton  
MEC (CTQ2005-07790-C02-01)  
Coordinator, Principal Investigator: J. M. Anglada  
2006-2008

Reacciones de oxidación de interés en química atmosférica, en química ambiental y en procesos biológicos. Estudio teórico  
MICINN (CTQ2008-06536)  
Principal Investigator: J. M. Anglada  
2009-2011

Preparación y evaluación de inhibidores de colina-quinasa con potencial actividad antitumoral  
MICINN (PET2008\_0312)  
Principal Investigator: J. Bujons  
2009-2011

Biotecnología de materiales lignocelulósicos:  
Retos moleculares enzimáticos, químicos y moleculares para su aplicación industrial y medioambiental  
MEC (BIO2007-29806- Special action)  
Principal Investigator: G. Caminal  
2008-2009

Caracterització i millora del procés per a l'obtenció de llevats en el marc del projecte d'investigació CAVAQUALITY  
Codorniu S.A.  
Principal Investigators: G. Caminal, G. González  
2008-2009

Nuevos desarrollos en Ingeniería Bioquímica: Optimización de procesos de producción de proteínas recombinantes y de síntesis enzimática  
MEC (CTQ2005-01706/PPQ)  
Principal Investigator: J. López-Santín (UAB)  
IQAC participant: G. Caminal  
2005-2008

Suport a Grups de Recerca Consolidats.  
Generalitat de Catalunya (2006SGR-00698)  
Grup de Enginyeria de Bioprocessos i Biocatàlisi Aplicada  
Coordinators: F. Valero, J. López-Santin (UAB)  
IQAC participant: G. Caminal  
2006-2008

Desarrollo de procesos para la degradación por hongos de contaminantes orgánicos persistentes y emergentes en aguas  
MEC (CTM2007-60971/TECNO)  
Principal Investigator: M. T. Vicent (UAB)  
IQAC participant: G. Caminal  
2007-2010

Presencia de contaminantes orgánicos prioritarios y emergentes en lodos de EDAR y su biodegradación por hongos  
MMA (010/PC08/3-04.1)  
Principal Investigator: M. T. Vicent (UAB)  
IQAC participant: G. Caminal  
2008-2010

Procesos biotecnológicos integrados para la obtención de compuestos bioactivos  
MICINN (CTQ2008-00578/PPQ)  
Principal Investigator: J. López-Santín (UAB)  
IQAC participant: G. Caminal  
2008-2011

Implementing an enzyme engineering technology platform for the provision of Taylor-made enzymes for biocatalytic synthesis (engbiocat)  
ERA- IB, MICINN (EUI2008-03615)  
Coordinator: M. Struhalla (c-Lecta GmbH)  
UAB Project Leader: J. López-Santín (UAB)  
IQAC participant: G. Caminal  
2009-2012

Suport a Grups de Recerca Consolidats.  
Generalitat de Catalunya (2009SGR281).  
Grup de Enginyeria de Bioprocessos i Biocatàlisi Aplicada  
Coordinators: F. Valero, J. López-Santin (UAB)  
IQAC participant: G. Caminal  
2009-2012

|  |   |
|--|---|
| <p>Suport a Grups de Recerca Consolidats.<br/> Generalitat de Catalunya (2009-SGR 656)<br/> Grup de Degradació de Contaminants Industrials i<br/> Valorització de Residus<br/> Coordinator: M. T. Vicent (UAB)<br/> IQAC participant: G. Caminal<br/> 2009-2014</p>  | <p>Suport a Grups de Recerca Consolidats.<br/> Generalitat de Catalunya (2009 SGR 871)<br/> Grup d'Ecologia Química<br/> Principal Investigator: A. Guerrero<br/> 2009-2013</p>   |
| <p>Analysis of the role of fucosyl- and<br/> sialyltransferases in the metastatic behaviour<br/> of cancer cells<br/> Fundació La Marató de TV3 (20060293)<br/> Coordinator: C. de Bolós. (IMIM, PRBB).<br/> IQAC Subproject: Chemo-enzymatic synthesis of<br/> iminoacyclitol derivatives with fucosyltransferase<br/> activity.<br/> Subproject leader: P. Clapés<br/> 2006-2008</p> | <p>Elastómeros para su aplicación en la química de<br/> dendrímeros cristales líquidos y preparación<br/> de materiales con propiedades electrónicas y<br/> magnéticas<br/> MEC (CTQ2006-15611-C02-02/BQU)<br/> Principal Investigator: M. D. Velasco (UB)<br/> IQAC participant: L. Juliá<br/> 2007-2009</p> |
| <p>Desarrollo de métodos quimo-enzimáticos para la<br/> síntesis estereoselectiva de iminociclitoles activos<br/> frente a glicosidasas y glicosiltransferasas.<br/> MEC (CTQ2006-01345/BQU)<br/> Principal Investigator: P. Clapés<br/> 2006-2009</p>   | <p>Suport a Grups de Recerca Consolidats.<br/> Generalitat de Catalunya (2005SGR00111)<br/> Grup de Química Teòrica i Computacional<br/> Coordinator: S. Olivella<br/> 2006-2008</p>  |
| <p>Cascade chemoenzymatic processes -<br/> new synergies between chemistry and<br/> biochemistry<br/> EC COST Action: CM0701<br/> WG04 "Aldolases in multi-step synthesis of<br/> natural products and analogues"<br/> WG Coordinator: P. Clapés<br/> 2008-2012</p>  | <p>Suport a Grups de Recerca Consolidats.<br/> Generalitat de Catalunya (2009SGR1472)<br/> Grup de Química Teòrica i Computacional<br/> Coordinator: S. Olivella<br/> 2009-2013</p>   |
| <p>Aislamiento y caracterización de diterpenos<br/> neo-clerodánicos<br/> CSIC 200480E596<br/> Principal Investigator: J. Coll<br/> 2009</p>   | <p>Estudio prospectivo de control integrado de<br/> acrídidos plaga mediante feromonas.<br/> Diputación General de Aragón (2007x0832)<br/> Principal Investigator: C. Quero<br/> 2007-2009</p>  |
| <p>Caracterización e inhibición de enzimas<br/> involucrados en el catabolismo de feromonas de<br/> insectos.<br/> CICYT (AGL2006-13489-C02-01)<br/> Coordinator, Principal Investigator: A. Guerrero<br/> 2006-2009</p>   | <p>Möbius aromaticity: a new challenge for<br/> computational chemistry<br/> Marie Curie Reintegration Grant<br/> (PERG05-GA-2009-249310)<br/> Principal Investigator: M. Torrent Sucarrat<br/> 2009-2012</p>   |
| <p>Control biorracial de plagas del género Coroebus<br/> MMA-CSIC (2006X0827)<br/> Principal Investigator: A. Guerrero<br/> 2006-2010</p>  | <p>Determinación de fitohormonas y metabolitos en<br/> vid.<br/> Ferrer &amp; Bobet SL<br/> Principal Investigator: J. L. Torres<br/> 2005-2008</p>   |
| <p>Biosynthetic chemical communication<br/> EC-STREP (Contract N° 032275, CT-2006)).<br/> Coordinator: Marina Cole (U. of Warwick, UK).<br/> IQAC Project Leader: A. Guerrero<br/> 2007-2010</p>   | <p>Mecanismos de acción de ingredientes<br/> polifenólicos de origen natural como<br/> componentes funcionales en productos de<br/> la pesca y de la acuicultura.<br/> MEC (AGL2006-12210-C03-02/ALI)<br/> Coordinator: I. Medina (IIM).<br/> Principal Investigator: J. L. Torres<br/> 2006-2009</p>         |
| <p>Biosynthetic chemical communication (Ayuda<br/> complementaria)<br/> MEC (AGL2007-30957-E/AGR)<br/> Principal Investigator: A. Guerrero<br/> 2008-2010</p>  | <p>Consultoría y apoyo tecnológico en los procesos<br/> para la generación de sustancias a partir de<br/> procedimientos limpios /white biotechnology/, su<br/> análisis y valoración biológica<br/> BIOGLANE (20081114)<br/> Principal Investigator: J. L. Torres<br/> 2008-2009</p>                         |

Consultoría y apoyo tecnológico para el desarrollo del proceso y aplicaciones en relación con la patente «Chemoenzymatic process for the preparation of iminocyclitols»  
BIOGLANE  
Principal Investigator: J. L. Torres  
2009-2010

Mecanismo de acción de los ácidos grasos poliinsaturados de origen marino en el síndrome metabólico y sinergismo con polifenoles e iminocyclitoles  
MICINN (AGL2009-12374-C03-03)  
Coordinator: I. Medina (IIM).  
Principal Investigator: J. L. Torres  
2009-2012

Purificación y actividad espermicina, citotóxica y anticancerosa de extractos de plantas medicinales de Túnez  
MAE (A/018100/08)  
Principal Investigator: J. L. Torres  
2009

Suport a Grups de Recerca Consolidats.  
Generalitat de Catalunya (2005SGR00204)  
Grup de Bioquímica Integrativa i Teràpia del Càncer  
Principal Investigator: Marta Cascante (UB)  
IQAC Participant: J. L. Torres  
2005-2008

Actividad biológica de los polifenoles, durante el procesado y conservación del tomate transformado. Efecto del procesado en la biodisponibilidad de los polifenoles de las salsas de tomate  
MICINN (AGL2007-66638-C02-01/ALI)  
Principal Investigator: R.M. Lamuela-Raventós (UB)  
IQAC Participant: J. L. Torres  
2007-2010

## Patents

Clapés, P., Joglar, J., Castillo, J.A., Lozano, C.  
Chemoenzymatic process for the preparation of iminocyclitols  
Bioglane S.L.N.E. , CSIC  
WO2008025826A1  
6/03/2008  
ES

Clapés, P., Joglar, J., Concia, A. L., Castillo, J. A., Lozano C.  
Procedimiento quimo-enzimático para la síntesis de 1-deoxi-D-xilulosa  
CSIC, Bioglane S.L.N.E.  
200900254  
29/01/2009  
ES

LLebaria, A., Casas, J., Egido, M., Díaz, L., Bujons, J., Delgado, A.  
Derivados de aminocyclitoles, procedimiento de obtención y usos  
CSIC, UB  
P200931193  
18/12/2009  
ES

Juliá, L., Velasco, D., Castellanos, S., Puigdollers, J., Alcubilla, R.  
Radicales orgánicos como componentes semiconductores  
CSIC, UB, UPC  
P200931217  
21/12/2009  
ES

de la Torre, R., Farré, M., Covas, M., Fitó, M., Almeida, B., Rodríguez de Fonseca, F., Decara del Olmo, J. M., Macías González, M., Romero Cuevas, M., Joglar, J., Clapés, P.  
Derivados de amida de ácidos grasos con anfetaminas para el tratamiento de desórdenes alimenticios  
IMIM, IMABIS, CSIC  
P200931269  
24/12/2009  
ES

## Ph. D. Thesis

- Acin, P.  
Identificación de feromonas y proteínas implicadas en la percepción feromonal de lepidópteros plaga  
Directors: Rosell, G., Quero, C.  
UB. Facultat de Biología (European Thesis)  
19/03/2009  
Excelente «cum laude»
- Bru, M.  
Síntesis y preparación de nuevos macrociclos pseudopeptídicos quirales. Aplicaciones en química supramolecular  
Directors: Alfonso, I., Luis, S.V.  
Universidad Jaume I de Castellón  
09/09/2008  
Excelente «cum laude»
- Castro Ruiz, A.  
Análisis de metabolitos secundarios biológicamente activos de especies vegetales  
Director: Coll, J.  
UB. Facultat de Química.  
11/12/2009  
Excelente «cum laude»
- Lizárraga, D  
Genomic, metabolomic and growth modifications on colon cancer cells triggered by natural polyphenolics  
Directors: Torres, J.L., Cascante, M., Centelles, J.J.  
UB. Facultat de Biología  
17/04/2008  
Excelente «cum laude»
- Mansergas, A.  
Estudio teórico de reacciones de oxidación de interés en la química de la troposfera  
Director: Anglada, J.M.  
UB. Facultat de Química  
27/11/2008  
Excelente «cum laude»
- Rayó, J.  
Nous inhibidors de les proteïnes implicades en la percepció feromonal d'insectes: Síntesi, activitat biològica i estudis d'optimització estructural  
Directors: Guerrero, A., Bosch, M.P.  
UB. Facultat de Química  
03/04/2009  
Excelente «cum laude»
- Touriño, S.  
Contribución al establecimiento de las bases científicas para el uso de fibra dietética antioxidante y fracciones polifenólicas en la prevención del cáncer.  
Director: Torres, J.L.  
UB. Facultat de Farmàcia  
29/07/2009  
Sobresaliente «cum laude»

## Masters-D.E.A.

- Fernández Cachón, M.  
Caracterización del efecto antitumoral de los extractos de la corteza de Hamamelis virginiana  
Directors: Cascante, M., Centelles, J.J., Torres, J.L.  
UB. Facultat de Química.  
03/10/2008
- Fernández Castañé, A.  
IPTG as inducer: HPLC-MS analysis of IPTG in Escherichia coli culture samples  
Directors: López-Santín, J., Caminal, G.  
UAB. Escola d' Enginyeria.  
10/07/2008
- Furstenau, B.  
Estudios dirigidos a la identificación de feromonas del género *Coroebus* para un control biorracial de plagas  
Directors: Guerrero, A., Rosell, G.  
UB. Facultat de Química.  
26/09/2008
- Gago, R.  
Estudios de inhibición de la percepción feromonal en insectos. Síntesis y actividad biológica de nuevos análogos de feromonas  
Directors: Guerrero, A., Bosch, M.P.  
UB. Facultat de Química.  
16/02/2009
- Marcos Benteo, E.  
Estructura, reactividad e implicaciones biológicas del fósforo pentacoordinado  
Directors: Crehuet, R., Anglada J.M.  
UB. Facultat de Química.  
17/05/2008
- Rodríguez Rivero, A.  
Síntesi d'agonistes per el receptor A2A de l'adenosina  
Directors: Guerrero, A., Bosch, M.P.  
UB. Facultat de Química.  
18/02/2008
- Rodríguez Rivero, A.  
Potencials agonistes per el receptor A2A de l'adenosina. Síntesi i activitat biològica (DEA).  
Directors: Guerrero, A., Bosch, M.P.  
UB. Facultat de Química.  
30/09/2008
- Rodríguez Rodríguez, C.  
Colonization of sewage sludge by *Trametes versicolor* for treatment of emerging pollutants.  
Directors: Marco-Urrea, E., Caminal, G  
UAB. Escuela de Ingeniería.  
20/07/2009

## Academic Activities

- Alfonso, I.  
Química Supramolecular  
Máster en Química Sostenible (Interuniversity)  
UJI  
2008, 2009
- Caminal, G., Benaiges, M.D.  
Biotransformacions  
Master en Biotecnologia avançada  
Mòdul: Enginyeria de Processos Bioteclògics  
UAB.  
2008
- Caminal, G.  
Producció de proteïnes recombinants amb E. coli.  
Master en Biotecnologia avançada  
Mòdul: Disseny de Bioprocessos.  
UAB.  
2008
- Clapés, P.  
Biocatalytic cascade reactions for asymmetric synthesis based on carboligation  
Máster en Biotecnologia molecular  
UB. Facultat de Biología.  
2008, 2009
- Clapés, P.  
Enzims en síntesi orgànica  
Máster en Biotecnologia molecular  
UB. Facultat de Biología.  
2008
- Juliá, L.  
Electrònica molecular. Materials. Processos de transferència electrònica. Conductors orgànics  
Materials luminiscents. Dispositius orgànics d'emissió de llum (OLED's).  
Master en Nanomateriales y Nanotecnología  
UB. Facultat de Química  
2008, 2009
- Torres, J.L.  
Natural actives as nutritional supplements.  
Extraction and enzymatic synthesis  
Máster en Biotecnologia molecular  
UB. Facultat de Biología.  
2008, 2009
- Torres, J.L.  
Análisis químico preliminar y determinación de actividad antioxidante de compuestos polifenólicos  
Instituto Nacional de la Biodiversidad,  
Santo Domingo de Heredia, Costa Rica.  
2008

## Congress Organization

- Anglada J. M.  
Organizer  
Summer School on Atmospheric Chemistry  
Barcelona  
6-9/07/2009
- Anglada J. M  
Organizing Committee  
Theoretical chemistry: modeling reactivity from gas phase to biomolecules and solids. Celebrating 25 years of the theoretical chemistry network of Catalonia, Spain  
Barcelona  
29/06-3/07/2009
- Caminal, G.  
Organizing Committee  
XI Meeting. Biotecnologia de materiales lignocelulósicos: Retos moleculares, enzimáticos y químicos para su aplicación industrial y medioambiental  
Sitges, Barcelona  
05/2008
- Coll, J.  
Scientific Committee  
Congrès International sur les Plantes Aromatiques et Médicinales  
Marrakech, Morocco  
26-28/03/2009
- Olivella, S.  
Organizing Committee  
Cinquena Trobada de Joves Investigadors dels Països Catalans  
Vic, Barcelona  
28-29/01/2008

## **Invited Conferences**

Ignacio Alfonso

Nuclear Magnetic Resonance as a powerful tool for studying the supramolecular chemistry of amino acid-containing synthetic macrocycles.  
(IV Reunión bienal del GERMN / I Reunión Ibérica de RMN)  
Universidad de Sevilla  
23/09/2008

Ignacio Alfonso

Química constitucional dinámica con pseudopéptidos: aplicaciones en síntesis y en la preparación de nanoestructuras autoensambladas  
Universidad Jaume I, Castellón  
26/11/2009

Pere Clapés

Enzyme Catalyzed Asymmetric Aldol Additions: Carbohydrates and iminosugars from DHAP to unphosphorylated donor analogues  
Institut Químic de Sarria. Barcelona  
15/12/2009

Josep Coll

Recent advances on the chemistry of allelochemicals from Ajuga genus  
CIPAM 2009. Marrakech, Morocco  
27/03/2009

Ramon Crehuet

Interacciones entre dinámica y catálisis en los enzimas. ¿Qué pueden aportar los cálculos computacionales?  
Instituto de Biomedicina de Valencia  
09/04/2008

Àngel Guerrero

Carboxylesterase inhibition by fluorinated chemicals. Synthesis and biological activity  
XIII Asian Symposium on Medicinal Plants, Spices and other Natural Products  
Indian Institute of Chemical Technology, Hyderabad, India  
5/11/2008

Àngel Guerrero

Long chain fluorinated ketones as inhibitors of esterases. Synthetic aspects and photochemical stability studies  
Indian Institute of Technology, Mumbai, India  
10/11/2008

Àngel Guerrero

Pheromones and antagonists in pest control. Identification, synthesis and biological activity  
National Chemical Laboratory, Pune, India  
11/11/2008

Àngel Guerrero

New potential agonists for the human A2A aadenosine receptor. Synthesis and pharmacological activity  
Ranbaxy Laboratories Ltd. Gurgaon, Delhi, India  
14/11/2008

Miquel Torrent-Sucarrat

On the applicability of the local softness and hardness  
Workshop on Theoretical Chemistry 2009, Platja d'Aro, Spain  
09/07/2009

Miquel Torrent-Sucarrat

The Aplicability Of The HSAB Principle  
ICCMSE 2009, Rhodes, Greece  
01/10/2009

Josep Lluís Torres

¿Pueden los antioxidantes naturales alargar la vida?  
Jornadas Antioxidantes Naturales y Salud. Red de Estudio de Compuestos Naturales con Poder Antioxidante.  
A Coruña  
16/07/2008

Josep Lluís Torres

Crea!Empresa  
Parc Científic Barcelona  
10/11/2009

## **Editorial Activity in Journals**

Josep Coll

Editorial Advisory Board  
Natural Product Communications  
Since 2006

Àngel Guerrero

Editorial Advisory Board  
Current Medicinal Chemistry.  
Since 2008

Àngel Guerrero

Editorial Advisory Board  
The Open Natural Products Journal  
Since 2008

## DEPARTMENT OF BIOMEDICINAL CHEMISTRY

### Research Projects

- Drug discovery for transthyretin cardiac amyloidosis  
Fundació Marató de TV3 (080530)  
Principal Investigator: G. Arsequell  
2009-2011
- Patogénesis de la enfermedad pulmonar obstructiva crónica: papel de los esfingolípidos como reguladores de la apoptosis alveolar y potencial terapéutico de colecciones combinatorias de lípidos.  
Fundació La Marató de TV3 (040730)  
Coordinator, Principal Investigator: J. Casas  
2005-2008
- Patogénesis de la enfermedad obstructiva crónica: papel de los esfingolípidos bioactivos en la regulación de la apoptosis de las células alveolares y evaluación de quimiocinas lipídicas para una potencial utilización terapéutica  
Fundació Marató de TV3 (040731)  
Coordinator: J. Casas  
Subproject Principal Investigator: A. Delgado  
2005-2008
- Una nueva aproximación contra el Virus de la Inmunodeficiencia Humana-1: Perturbación de microdominios de membrana mediante inhibidores de la dihidroceramida desaturasa. Estudios biofísicos y biológicos.  
CSIC, Proyecto Intramural Frontera (200580F0211)  
Coordinator, Principal Investigator: G. Fabriàs.  
2005-2008
- Suport a Grups de Recerca Consolidats  
Generalitat de Catalunya (2005SGR01063)  
RUBAM  
Principal Investigator: G. Fabriàs  
2006-2009
- Bases biológicas y biofísicas de los efectos de los inhibidores de la dihidroceramida desaturasa en el proceso de entrada del virus de la inmunodeficiencia humana.  
Fundación para la Investigación y la Prevención del Sida en España (FIPSE) (AIDS Prevention and Research Foundation), 36550/06  
Coordinator: Santos Mañes (NCB, CSIC)  
Principal Investigator: G. Fabriàs  
2007-2009
- Dihidroceramida desaturasa, ceramidasa lisosomal y autofagia: nuevo modo de acción de algunos agentes antitumorales  
MICINN (SAF2008-00706)  
Principal Investigator: G. Fabriàs  
2009-2011
- Suport a Grups de Recerca Consolidats  
Generalitat de Catalunya (2009 SGR 1072)  
RUBAM  
Principal Investigator: G. Fabriàs  
2009-2013
- Síntesis de péptidos del virus de la hepatitis G (GBV-C/HGV) y evaluación de su antigenicidad mediante sueros coinfectados con el virus de la inmunodeficiencia humana (HIV)  
CSIC (CSIC-I3 200880/081)  
Principal Investigator: M. J. Gómara  
2008-2009
- Péptidos sintéticos del Gbv-C/Hgv. Aplicación en el diagnóstico de infección por el virus de la hepatitis G y en el diseño de potenciales agentes terapéuticos contra el Hiv  
MEC (CTQ2006-15396-02-01)  
Coordinator, Principal Investigator: I. Haro  
2006-2009
- Caracterización fenotípica, genética e inmunohistoquímica de los pacientes con artritis reumatoide con y sin anticuerpos anti-péptidos citrulinados  
Coordinator: J. A. Gómez Puerta (IDIBAPS, Hospital Clínic, Barcelona)  
Fundació Clínic (S/R)  
IQAC Participant Group Leader: I. Haro  
2008
- Pèptids i proteïnes: estudis fisicoquímics  
Generalitat de Catalunya (AGAUR)  
Coordinator: M. Asunción Alsina (UB)  
IQAC Participant Group Leader: I. Haro  
2009
- Artritis reumatoide con y sin anticuerpos séricos frente a péptidos sintéticos citrulinados: Estudio comparativo fenotípico, genotípico e inmunohistológico  
MICINN. Instituto de Salud Carlos III  
Coordinator: R. Sanmartí (IDIBAPS, Hospital Clínic, Barcelona)  
IQAC Participant Group Leader: I. Haro  
2009-2011
- Estudio estructural de dominios peptídicos del GB virus C con capacidad inhibitoria del HIV-1 y de aptámeros de RNA que se unen a la proteína PrP PGE. Acción Integrada con Italia (IT2009-0067)  
Principal Investigators: I. Haro, E. Ragg  
2009-2010
- Diseño, síntesis y actividad biológica de análogos estructurales de esfingolípidos. Aplicaciones al estudio de la biosíntesis diferencial en mamíferos y hongos  
MEC (CTQ2005-00175/BQU)  
Principal Investigator: A. LLebaria  
2006-2008
- Molecular bases of neuropathic pain: An integrated approach to analyze the role of Group-III metabotropic glutamate receptors.  
Fundació La Marató de TV3 (S/R)  
IQAC Participant Group Leader: A. LLebaria  
2008-2010

Diseño y síntesis de nuevos ciclitoles para el estudio de procesos de señalización, biosíntesis y metabolismo  
MICINN (CTQ2008-01426)  
Principal Investigator: A. Llebaria  
2009-2011

Dianes moleculars dels antiinflamatoris no esteroïdals: implicacions en el dolor crònic.  
Fundació La Marató de TV3 (072610)  
Coordinator: A. Lleó Bisa (Hospital de Sant Pau, Barcelona)  
IQAC Participant Group Leader: G. Valencia  
2008-2010

Disseny racional, síntesi i caracterització d'anàlegs d'opiorfina i M6G: vers un millor coneixement dels mecanismes del dolor.  
Fundació La Marató de TV3 (070430)  
Coordinator, Subproject Principal Investigator: G. Valencia  
2008-2010

Procesos estequiométricos y catalíticos con reactivos electrófilos: Avances en el diseño de metodologías sintéticas eficientes basadas en metales de transición y yodo.  
MICINN (CTQ200761048/BQU)  
Principal Investigator: J. Barluenga (U. de Oviedo)  
IQAC Participant Group Leader: G. Valencia  
2008-2010

## Patents

Llebaría, A., Casas, J., Egido, M., Delgado, A., Serrano, P.  
Cyclohexane substitute for activating beta-glycosidase enzyme for production of pharmaceutical composition for treatment of Gaucher disease and cancer  
CSIC y UB  
ES2289853  
01/02/2008  
ES

Haro, I., Gómara, M.J., Pérez, M.L., Sanmartí, R.  
Polipéptido quimérico fibrina-filagrina citrulinado capaz de detectar los anticuerpos generados en la artritis reumatoide  
CSIC y Fundació Clínic  
PCT/ES08/070087  
30/04/2008  
ES

Haro, I., Gómara, M.J.  
Uso de péptidos de la proteína E1 del virus de la hepatitis G para inhibir la actividad del virus VIH-1  
CSIC  
P020093045  
06/04/2009  
ES

Haro, I., Gómara, M.J.  
Uso de péptidos de la proteína E2 del virus de la hepatitis G para inhibir la actividad del virus VIH-1  
CSIC  
P020093044  
06/04/2009  
ES

Fabrias, G., Casas, J., Abad, J. L., Camacho, L., Delgado, A.  
Amidas de 2-amino-1,3-propanodioles y su uso como inhibidores de ceramidasas  
CSIC y UB  
P200930404  
02/07/2009  
ES

Haro, I., Gómara, M.J., Sanmartí, R., Pérez, M.L.  
Polipéptido quimérico fibrina-filagrina citrulinado capaz de detectar los anticuerpos generados en la artritis reumatoide  
CSIC y Fundació Clínic  
2307421  
10/09/2009  
ES

Llebaría, A., Casas, J., Egido, M., Díaz, L., Bujons, J., Delgado, A.  
Derivados de aminociclitoles, procedimiento de obtención y usos  
CSIC, UB  
P200931193  
18/12/2009  
ES

## **Ph. D. Thesis**

Pérez, M.L.

**Péptidos sintéticos citrulinados en la artritis reumatoide: Significación, diagnóstico y pronóstico**

Directors: Haro, I., Ercilla, G.

UB. Facultat de Biología

19/12/2008

Excelente «cum laude»

## **Masters**

Fernández, L.

**Péptidos sintéticos del GBV-C/HGV. Aplicación en el diagnóstico de infección por el virus de la hepatitis G y en el diseño de potenciales agentes terapéuticos contra el HIV**

Directors: Haro, I., Gómara, M.J.

UB, Facultat de Química

30/09/2008

Reina, E.

**Determinació de l'activitat de l'enzim esfingosina-1-fosfat liasa.**

Director : Fabrias, G.

IQAC

15/07/2009

## **Conferences**

I. Haro, M.L. Pérez, M.J. Gómara, R. Sanmartí  
Pèptids sintètics citrulinats derivats de la fibrina amb utilitat per la diagnosi d'artritis reumatoide  
Societat Catalana de Reumatologia. Acadèmia de Ciències Mèdiques i de La Salut de Catalunya i de Balears  
Barcelona  
01/02/2008

I. Haro  
Els pèptids serveixen per diagnosticar malalties  
Escola Bell-Iloc del Pla, Girona  
20/02/2008

## **Editorial Activity in Journals**

Haro, I  
Editorial Advisory Board  
**Current Medicinal Chemistry**  
2009

# DEPARTMENT OF CHEMICAL AND BIOMOLECULAR NANOTECHNOLOGY

## Research Projects

Estudio de la formación y estabilidad de formulaciones detergentes líquidas  
Prolutec  
Principal Investigator: N. Azemar  
2006-2008

Desarrollo de formulaciones líquidas para la detergencia textil de uso industrial.  
MICINN (PETRI) (PET2007-0385)  
Principal Investigator: N. Azemar  
2008-2010

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

Desarrollo de plataformas nanobio-analíticas basadas en reconocimiento molecular mediante detección óptica y/o electrónica  
MEC. NAN2004-09415-C05-03.  
Coordinator: J. Samitier (IBEC, Barcelona)  
IQAC Participant Group Leader: R. Eritja  
2005-2009

Síntesis racional de moléculas con afinidad al ADN de doble cadena constituidas por diversas unidades activas por el mecanismo de intercalación.  
OTRI (PTR1995-0976-OP).  
Principal Investigator: F. Albericio (UB)  
IQAC Participant Group Leader: R. Eritja  
2006-2008

Suport a Grups de Recerca Consolidats Generalitat de Catalunya (2005SGR00693).  
Grupo de Síntesis y estructura de biomoléculas  
Principal Investigator: E. Pedroso (UB)  
IQAC Participant Group Leader: R. Eritja  
2006-2008

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

Grupo de Química de Ácidos Nucleicos  
CIBER Bioingeniería, Biomateriales y Nanomedicina (CB06/01/0019)  
Principal Investigator: R. Eritja.  
2006-2013

Conjugados carbohidrato-ARN inhibidores como nuevos agentes antivirales, interferente (siARN), antisentido, aptámeros y ribozimas  
CSIC Proyecto intramural de frontera PIF06-045  
Principal Investigator: J. C. Morales (CSIC, Sevilla)  
IQAC Participant Group Leader: R. Eritja  
2007-2008

Síntesis y propiedades de oligonucleótidos modificados de interés biomédico y estructural (OMIBE).  
MEC (BFU-2007-63287)  
Principal Investigator: R. Eritja.  
2007-2010

Síntesis de RNA interferente unido a lípidos Sylentis (20080909)  
Principal Investigator: R. Eritja  
2008

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

Self-assembled guanosine structures for molecular electronic devices.  
European Community- COST Action MP0802 (proposal OC-2007-2-1520)  
Coordinator: L. Spindler (Josef Stefan Institute, Ljubljana, Slovenia)  
IQAC Participant Group Leader: R. Eritja  
2008-2012

Suport a Grups de Recerca Consolidats Generalitat de Catalunya (2009SGR208).  
Grupo de Síntesis y estructura de biomoléculas  
Principal Investigator: E. Pedroso (UB)  
IQAC Participant Group Leader: R. Eritja  
2009-2011

Obtención de sistemas meso/macroporosos, a partir de emulsiones altamente concentradas y aplicación en procesos de sorción.  
MEC (CTQ2005-08241-C03-01/PPQ)  
Coordinator, Principal Investigator: J. Esquena  
2005-2008

Application of inulin based surfactants in latex formation and stabilization  
ORAFI  
Principal Investigators: J. Esquena, C. Solans  
2006-2008

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|---|--|
| Adquisición de un equipo de rayos X a ángulos pequeño y grande (SAXS-WAXS) (CTQ2007-28961-E/BQU)<br>Principal Investigator: J. Esquena<br>2007-2008.  | Fundamental studies of rubber latex<br>Malasyan Rubber Board<br>Principal Investigator: J. Esquena<br>2008-2011  |
| Estudio comparativo de las propiedades y efectos de plasmas y post-descargas sobre fibras textiles y materiales poliméricos.<br>Acción Integrada España-Francia (HF2006-0095)<br>Principal Investigators: J. Esquena, J. P. Sarrete<br>2007-2008  | Advances in functional organic-inorganic nanocomposites by cooperative self-assembly FP7-PEOPLE IRSES 2008<br>Coordinator/Principal Investigator: J. Esquena<br>2009-2011  |
| Formulación de nuevas emulsiones de parafina de elevada estabilidad<br>PETRI-MICINN, Repsol YPF (PET2006-0582)<br>Principal Investigator: J. Esquena<br>2007-2009   | Diseño de inhibidores de los mecanismos de reparación del ADN como coadyuvantes en quimioterapia.<br>Fondo de Investigaciones Sanitarias, PI06/1250<br>Principal Investigator: C. Fàbrega<br>2007-2009   |
| Preparación y caracterización de nuevas membranas de microfiltración y ultrafiltración a partir de materiales meso/macroporosos obtenidos en emulsiones altamente concentradas, para su aplicación en tratamientos de aguas<br>AECL (Spain-Morocco Project A-4986-06)<br>Principal Investigators: J. Esquena, M. El Amrani<br>2007-2009 | Inmunosensores basados en nanoestructuras resonantes como dispositivos de alarma frente a hormonas androgénicas (HINAN).<br>Fundación Areces<br>Coordinator/Principal Investigator: S. Soria (ICFO)<br>IQAC participant: Roger Galve<br>2005-2008  |
| Investigación en nuevos conceptos de carreteras más seguras y sostenibles.<br>CDTI (CENIT2007-1014)<br>Coordinator: C. Cortés (I+D+I, Serviá Cantó, Girona)<br>Principal Investigator: J. Esquena<br>2007-2010  | Microarray de epítopos: una herramienta para el diagnóstico y la investigación de las respuestas alérgicas a antibióticos b-lactámicos (b-Array)<br>Plan Nacional de I+D+I (SAF2008-03082)<br>Principal Investigator: R. Galve<br>2009-2011  |
| Preparación y caracterización de materiales meso/macroporosos, para su aplicación en procesos de purificación de aguas.<br>CSIC- CNCPRST, Morocco (2007MA0009)<br>Principal Investigators: J. Esquena, M. El Amrani<br>2008-2009  | Desarrollo de plataformas nanobio-analíticas basadas en reconocimiento molecular mediante detección óptica y/o electrónica (NanoBioMol).<br>MEC. EC Nanotechnology Strategic Action. NAN2004-09415-C05-02.<br>Coordinator/Principal Investigator: J. Samitier (IBEC, Barcelona).<br>Principal Investigator: M. P. Marco<br>2006-2008 |
| Preparación y caracterización de hidrogeles y estudio de su utilización en la funcionalización de sustratos textiles<br>AITEX (20080322)<br>Principal Investigator: J. Esquena<br>2008-2010   | CIBER-BBN<br>Ministerio de Sanidad y Consumo. ISC III.<br>Acciones CIBER. Programa Consolider (iniciativa Ingenio 2010).<br>Director: Manuel Doblaré (Zaragoza)<br>Coordinator/Principal Investigator (Applied molecular receptor group): M. P. Marco<br>2006-2009   |
| Obtención de materiales porosos avanzados (mesoporosos y meso/macroporosos) por autoagregación en sistemas tensioactivos<br>CSIC Proyecto intramural de frontera (2008 80F0091)<br>Principal Investigator: J. Esquena<br>2008-2010  | Desarrollo de un dispositivo inmunosensor basado en la resonancia de plasmón localizado de nanopartículas de metales nobles para la detección de substancias prohibidas en el deporte (dWatch Array).<br>MEC. EC Sport Strategic Action (DEP2007-73224-C03-01).<br>Coordinator/Principal Investigator: M. P. Marco<br>2007-2010      |
| Obtención y caracterización de estructuras meso/macroporosas a partir de emulsiones altamente concentradas: control de la porosidad dual y aplicaciones en medio ambiente.<br>MICINN (CTQ2008-06892-C03-01)<br>Coordinator/Principal Investigator: J. Esquena<br>2008-2011  |  |

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| Micro/Nanotecnologías para la inmunodetección multiplexada de microorganismos patógenos (MICROPLEX)<br>CIBER Project Intramural<br>Coordinator/Principal Investigator: M. P. Marco<br>2008-2009   | Desarrollo de nuevas estructuras con actividad antioxidante e inhibidora del envejecimiento<br>Lipotec, S.A. (20070831Pr1)<br>Principal Investigator: A. Messeguer<br>2008-2009  |
| Micro/nanopartículas magnéticas para el diagnóstico clínico (NANOMAG).<br>CIBER Project<br>Coordinator/Principal Investigator: Francisco del Pozo (UAM)<br>Participant Group Leader: M. P. Marco.<br>2008-2009  | Nuevos inhibidores de la interacción TCR-nck<br>Genoma España<br>Project Supervisor: B. Alarcón (CBM-CSIC)<br>Subproject Supervisor: A. Messeguer<br>2008-2010   |
| Micro/nanotecnologías para la inmunodetección multiplexada de microorganismos patógenos (Microplex)<br>Proyecto CIBER inter area<br>Principal Investigator: M. P. Marco<br>2008-2009  | The Spanish Ion Channel Initiative<br>MICINN Consolider Program<br>IQAC Participant Group Leader: A. Messeguer<br>2009-2013  |
| CONTaminants in Food and Feed: Inexpensive DEtectioN for Control of Exposure ( <i>Confidence</i> ).<br>EC, VII- Framework Programme. Food, Agriculture and Fisheries and Biotechnology.<br>Proposal No.: 211326 – CP (Collaborative Project)<br>Coordinator/Principal Investigator: Jacob de Jong (RIKILT, The Netherlands)<br>Participant Group Leader: M. P. Marco<br>2008-2012 | Diseño y síntesis de análogos químicos de inhibidores de quinasas<br>Allinky Biopharma<br>Principal Investigator: A. Messeguer<br>2009-2011  |
| Nanobioanalytical platforms for improved diagnosis of infections caused by pathogens (Nanomediag)<br>Plan Nacional de Internacionalización de la I+D (EUI2008-00175)<br>Coordinator/Principal Investigator: J. Samitier (IBEC, Barcelona).<br>Principal Investigator: M. P. Marco<br>2009-2011  | Modulación química de rutas de señalización celular de relevancia en enfermedades degenerativas: generación de cabezas de serie MEC/MICINN<br>Principal Investigator: A. Messeguer<br>2009-2011  |
| Suport a Grups de Recerca Consolidats Generalitat de Catalunya (2009SGR1343)<br>Applied molecular receptor group<br>Principal Investigator: M. P. Marco<br>2009-2013  | Estudios sobre laminina- decorina y cromanos antiradicalarios.<br>Min. Industria, Turismo y Comercio. Cenit-Nanofarma.<br>Coordinator: A. Messeguer<br>Subproject Principal Investigator: Francisca Reig Isart<br>2006-2008                                |
| Red española de esclerosis múltiple (REEM)<br>MICINN, Instituto de Salud Carlos III<br>IQAC Participant Group Leader: A. Messeguer<br>2007-2010.  | Propiedades catalíticas de nanopartículas y clústeres atómicos metálicos organizados por sistemas autoensamblados anfífilicos<br>MEC (RyC) (08-18-000X-711)<br>Principal Investigator: C. Rodríguez-Abreu<br>2006-2011                                     |
| Compuestos con actividad farmacológica relevante en la modulación de la proteína Apaf-1<br>Laboratorios Salvat (20080540)<br>Principal Investigator: A. Messeguer<br>2008-2009  | Cristales líquidos cromónicos de interés industrial como plantillas orientables para la fabricación de nuevos materiales nanoestructurados.<br>CSIC-The Royal Society, UK (2007GB004)<br>Principal Investigators: C. Rodríguez, G. Tiddy<br>2008-2009      |
| Intervenció farmacològica sobre el receptor TRPV1 per atenuar el dolor crònic<br>Fundació Marató de TV3 (20080123)<br>Coordinator: A. Ferrer-Montiel (U. of Elx)<br>IQAC Principal Investigator: A. Messeguer<br>2008-2010  | Nuevos materiales funcionales obtenidos por incorporación de nanoestructuras inorgánicas en matrices poliméricas.<br>CSIC-CONICET, Argentina (2007AR0031)<br>Principal Investigators: C. Rodríguez Abreu, R. Williams<br>2008-2009                         |
|   | Síntesis y propiedades fisicoquímicas de nuevos compuestos anfífilicos con carácter complejante derivados de azúcares y benzimidazolonas.<br>CSIC-CNCPRST, Morocco (2007MA00559)<br>Principal Investigators: C. Rodríguez Abreu, B. Lakhrissi<br>2008-2009 |

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| <p>Obtención por organización espontánea de nuevos nanocomuestos híbridos orgánico-inorgánicos para aplicaciones avanzadas en recubrimientos multifuncionales.</p> <p>MICINN (CTQ2008-01979)</p> <p>Principal Investigators: C. Rodríguez-Abreu, C. Solans</p> <p>2009-2011</p>   | <p>Estudio de sistemas nanoestructurados para aplicaciones tecnológicamente avanzadas: Formulación y textiles inteligentes</p> <p>MEC (CTQ2005-09063-C03-02/PPQ)</p> <p>Coordinador: J. M. Gutierrez (UB)</p> <p>Principal Investigator: C. Solans</p> <p>2005-2008</p>              |
| <p>Nanoestructuras magneto-plasmónicas para biosensores de alta sensibilidad (NanoBioMag).</p> <p>MEC. EC Nanotechnology Strategic Action.</p> <p>NAN2004-09195-C04-04.</p> <p>Coordinator/Principal Investigator: J. Rivas (U. Santiago de Compostela)</p> <p>Principal Investigator: F. Sánchez.</p> <p>2006-2008</p>   | <p>Suport a Grups de Recerca Consolidats.</p> <p>Generalitat de Catalunya (2005SGR-0018)</p> <p>Grup de Tensioactius</p> <p>Principal Investigator: C. Solans</p> <p>2006-2008</p>   |
| <p>Aproximación integral al desarrollo de tecnologías para detectar residuos de Antibióticos de uso veterinario para mejorar la eficacia del control desde la granja a la mesa (PANOPTES)</p> <p>AGL2005-07700-C06-01.</p> <p>Coordinator/Principal Investigator: F. Sánchez.</p> <p>2006-2008</p>  | <p>Etude sur l'exploration de systèmes formulatoires contenant des agents cosmétiques encapsulés et libérables de façon contrôlée</p> <p>Empresa Sector Cosmético</p> <p>Principal Investigator: C. Solans</p> <p>2007-2008</p>  |
| <p>Desarrollo de una plataforma de biosensores para aplicaciones en la industria agroalimentaria (MEATSENS).</p> <p>Ministerio de Industria (PROFIT). FIT-330100-2007-138.</p> <p>Coordinator/Principal Investigator: Irene Larroy (CRIC)</p> <p>Participant Group Leader: F. Sánchez.</p> <p>2007-2009</p>   | <p>Phase behaviour of the actives in laundry products in solution and on the surface of fabric</p> <p>Procter &amp; Gamble</p> <p>Principal Investigator: C. Solans</p> <p>2007-2008</p>   |
| <p>Desarrollo de una plataforma de biosensores para aplicaciones en la industria agroalimentaria</p> <p>Ministerio de Industria, Turismo y Comercio.</p> <p>Acción Estratégica de Telecomunicaciones y Sociedad de la Información. Subprograma AVANZA. (TSI-020100-2008-494)</p> <p>Coordinator/Principal Investigator: Irene Larroy (CRIC)</p> <p>Participant Group Leader: F. Sánchez.</p> <p>2008-2009</p> | <p>Surface coating characterization</p> <p>Procter &amp; Gamble</p> <p>Principal Investigator: C. Solans</p> <p>2007-2009</p>  |
| <p>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.</p> <p>Control y seguridad alimentaria (Detecta)</p> <p>AGL2008-05578-C05-01</p> <p>Principal Investigator: F. Sánchez-Baeza</p> <p>2009-2011</p>  | <p>Centre de Suport a la Innovació Tecnològica (Centre IT), TECNIO ACC1Ó (GENERALITAT DE CATALUNYA)</p> <p>Grupo QCI-CSIC</p> <p>Principal Investigator: C. Solans</p> <p>2007-2010</p>  |
| <p>Colloid and Interface Science for Nanotechnology Action COST D43: ESF WG 4: Nanostructured and bio-inspired materials</p> <p>Coordinator: M. Borkovec (U. Geneva)</p> <p>Principal Investigator: C. Solans</p> <p>2006-2010</p>  | <p>Grupo QCI-CSIC del CIBER-BBN, ISCIII.</p> <p>Principal Investigator: C. Solans</p> <p>From 2008</p>   |
|   | <p>Adquisició d'equipament per a plataforma de caracterització de líquids nanoestructurats</p> <p>CIBER-BBN, ISCIII</p> <p>Principal Investigator: C. Solans</p> <p>2008-2009</p>  |
|   | <p>Supporting mechanistic understanding of polymer-surfactant residue behaviour by modelling concentrate (HDL product) to dilute (wash) microstructures and properties with phase diagrams</p> <p>Procter &amp; Gamble</p> <p>Principal Investigator: C. Solans</p> <p>2008-2009</p> |
|   | <p>Functional polyester material for delivery of bioactives</p> <p>Firmenich</p> <p>Principal Investigator: C. Solans</p> <p>2009-2010</p>   |
|   | <p>Phase behavior of surfactants and polymers of fabric and hair care interest</p> <p>Procter &amp; Gamble</p> <p>Principal Investigator: C. Solans</p> <p>2009-2010</p>   |

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|---|--|
| Generalising concepts for formation and stabilization of nanoemulsions by low energy methods<br>Acción Integrada CSIC/UT Germany<br>Principal Investigators: C. Solans, M. Gradzielsky<br>2009-2010 | Suport a Grups de Recerca Consolidats<br>Generalitat de Catalunya (2009SGR961)<br>Principal Investigator: C. Solans<br>2009-2013   |
| Embedding of organic-inorganic hybrids of fibrous carbon materials in self- assembling systems<br>CSIC-The NSC Taiwan<br>Principal Investigators: C. Solans, P. D. Hong<br>2009-2010                | Phase behavior of surfactants and polymers of fabric care interest<br>Empresa Sector Detergencia<br>Principal Investigator: C. Solans<br>2009-2010   |
| Revisió i valorització inicial de l'estoc de coneixement acumulat al Centre QCI ACC1Ó (CIDEM-COPCA)<br>Principal Investigator: C. Solans<br>2009-2010   | Phase behavior of surfactants and polymers of fabric and hair care interest<br>Empresa Sector Detergencia<br>Principal Investigator: C. Solans<br>2009-2010  |
| Integrating nanomaterials in formulations EU (FP7-NMP-2008-CSA-2)<br>Coordinator: F. Siperstein (U. Manchester)<br>Principal Investigator: C. Solans<br>2009-2012                                   | Sintesis de materiales inorganicos nanoestructurados por el metodo de reacciones en microemulsiones del tipo aceite en agua (INNOCASH)<br>FECYT-MICINN<br>Principal Investigator: C. Solans<br>2009-2010 |

## Patents

|   |  |
|---|--|
| Cotter, T., Doonan, F., Sanvicens Diez, N., O'Driscoll, C., Messeguer Peypoch, A.R.<br>Treatment of retinal degeneration<br>University College Cork, National University of Ireland, Cork<br>Priority Data 05.08.2008 (S2008/0647)<br>Publication Date: 11.02.2010 (Pub. No.: WO/2010/016044)<br>International Application No.: PCT/IE2009/000055 | Aymamí, J., Albericio, F., Aviñó, A., Farrera, J., Royo, M., Navarro, I., Eritja, R.<br>New polymers and their use as fluorescent labels<br>Crystax Pharmaceuticals, S.L.<br>PCT/EP2008/058922<br>09/07/2008<br>European Union |
| Ramón, J., Sánchez, F., Marco, M.P.<br>Haptenos. Usos y método inmunoquímico para la detección de bromopropilato<br>CSIC<br>P200803612<br>18/12/2008<br>ES  | Ramón-Azcon, J., Sánchez-Baeza, F., Marco, M.P., Bratov, A., Abramova, N., Ipatov, A.<br>Sistema y procedimiento multianalítico basado en mediciones impedimétricas<br>CSIC<br>P200931164<br>15/12/2009<br>ES                  |
| Bertrán, E., Molina, R.<br>Reactor de plasma<br>CSIC<br>P200803269<br>17/11/2008<br>ES  | Ramón, J., Sánchez-Baeza, F., Marco, M.P.<br>Haptenos, usos y método inmunoquímico para la detección de bromopropilato<br>CSIC<br>PCT/ES2009/000578<br>18/12/2009<br>PCT, International-NO US                                  |
| Solans, C., Sánchez-Domínguez, M., Boutonnet, M.<br>Procedimiento para la obtención de nanopartículas por reacción en microemulsiones del tipo aceite-en-agua (O/W)<br>CSIC<br>PCT/ES2009/070223 (en estudio)<br>12/06/2009<br>PCT INTERNACIONAL  |  |

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|--|---|
| Esquena, J., Solans, C., Vílchez, S., Erra, P., Miras, J.<br>Materiales poliméricos macroporosos o meso/macroporosos obtenidos en emulsiones concentradas y altamente concentradas<br>CSIC<br>P200930038<br>03/04/2009<br>ES | Villoslada, P., Moreno, B., Messeguer, A., Messeguer, J., Navarro, G.<br>New peptoids agonists of nerve growth factor and their use as medicaments<br>CSIC<br>09169045.3<br>31/08/2009<br>ES                      |
| Messeguer, A., Moure, A., García-Pinacho, D., Masip, I.<br>Compuestos inhibidores de Apaf-1<br>CSIC<br>ES200901757<br>30/07/2009<br>ES   | Villoslada, P., Moreno, B., Messeguer, A., Messeguer, J., Navarro, G.<br>New 3-oxypiperazinium derivatives agonists of nerve growth factor and their use as medicaments<br>CSIC<br>09169036.2<br>31/08/2009<br>ES |
| Bayona, J.M., Molina, R., Erra, P., Bertan, E., Jover, E., Reyes, C.<br>Método de eliminación de trihalometanos y/o contaminantes emergentes mediante plasma<br>CSIC<br>P200900215<br>26/01/2009<br>ES                       | Vicent, M.J., Pérez-Payá, E., Cascales, L., Messeguer, A.<br>Conjugado polimérico para el tratamiento de infecciones bacterianas<br>CSIC<br>200930218<br>28/05/2009<br>ES   |
| Esquena, J., Solans, C., Vílchez, S., Erra, P., Miras, J.<br>Materiales poliméricos macroporosos o meso/macroporosos obtenidos en emulsiones concentradas y altamente concentradas<br>CSIC<br>P200930038<br>03/04/2009<br>ES | Planas, A., Messeguer, A.<br>Uso de un compuesto para el tratamiento de una lesión producida por una repercusión post-isquémica<br>CSIC<br>P0200900756<br>01/03/2009<br>ES  |

## PhD Thesis

Font, H.

Mètodes immunoquímics per a la detecció de pesticides i antibiòtics que contenen el grup arilsulfonamida en aliments

Diretors: Marco, M. P., Sánchez, F.

UB. Facultat de Química

26/01/2008

Excelente «cum laude»

Martínez-Cabot, A.

La síndrome de l'oli tòxic: Contribució a la seva etiologia mitjançant estudis xenobioquímics sobre el 3-N-(fenilamino)-1,2-propandiol

Director: Messeguer, A.

UB. Facultat de Química

10/01/2008

Excelente «cum laude»

Moore Fernández, A

Modulación química de rutas de señalización celular: Optimización de compuestos hits identificados a partir de quimiotecas

Director: Messeguer, A.

UB. Facultat de Química

04/11/2009

Excelente «cum laude»

Obregon, R.

Materiales con memoria molecular para el análisis de residuos de antibióticos

Diretors: Sánchez-Baeza, F., Marco, M. P.

UB. Facultat de Química

29/09/2009

Sobresaliente «cum laude»

Obiols Rabasa, M.

Preparation and colloidal properties of latex dispersions stabilized using hydrophobically modified inulin polymeric surfactant

Diretors: Esquena, J., Solans, C.

UB. Facultat de Química

23/03/2009

Excelente «cum laude»

Pey, C.M.

Estudi, optimització i escalat de nano-emulsions o/w preparades per inversió de fases

Diretors: Solans, C., González, C., Maestro, A.

UB. Facultat de Química

06/06/2008

Excelente «cum laude»

Ramón, J.

Estudio y desarrollo de técnicas inmunoquímicas y biosensores para el control de contaminantes agroalimentarios

Diretors: Marco, M. P., Sánchez, F.

UB. Facultat de Química

19/12/2008

Excelente «cum laude»

Solé, I.

Formació de nano-emulsions en sistemes amb tensioactius iònics mitjançant mètodes de condensació o de baixa energia

Diretors: Gutiérrez, M., Solans, C., González, C.,

Maestro, A.

UB. Facultat de Química

19/01/2008

Excelente «cum laude»

## Masters

|  |  |
|--|--|
| Aubery Torres, C. D.<br><b>Síntesis de nanopartículas de óxidos mixtos por el método de reacción en microemulsión (DEA)</b><br>Directors: M. Sánchez, C. Solans<br>UB. Facultat de Química<br>07/07/2008 | Vila, E.<br><b>Aproximación al desarrollo de un inmunoensayo para la detección de derivados antiestrogénicos</b><br>Directors: M. P. Marco, J. P. Salvador<br>UB. Facultat de Química<br>06/02/2009  |
| Martínez, M.<br><b>Obtención y caracterización de emulsiones bituminosas concentradas</b><br>Directors: J. Esquena, C. Solans<br>UB. Facultat de Química<br>06/07/2009                                   | Vilanova, N.<br><b>Microcápsulas de sílice preparadas a partir de sistemas tensioactivos para la liberación de substancias activas</b><br>Director: Rodríguez-Abreu, C.<br>UB. Facultat de Química<br>05/02/2009                               |
| Rodríguez, E.<br><b>Uso de compuestos anfifílicos no convencionales en la formación de nanoestructuras (DEA)</b><br>Directors: C. Rodríguez, C. Solans<br>UB. Facultat de Química<br>19/09/2008          | Vílchez, A.<br><b>Preparación de TiO<sub>2</sub> meso/macroporoso a partir de emulsiones altamente concentradas y evaluación de su eficiencia fotocatalítica</b><br>Directors: J. Esquena, C. Solans<br>UB. Facultat de Geología<br>06/07/2009 |
| Tort, N.<br><b>Hormones anabolitzants: un model pel desenvolupament d'una plataforma de multidetecció universal</b><br>Directors: M. P. Marco, J. P. Salvador<br>IIQAB/CSIC<br>15/02/2008                | Vílchez Maldonado, S.<br><b>Preparación de nanoparticulas poliméricas biodegradables y su incorporación sobre sustratos textiles</b><br>Directors: G. Calderó, R. Molina<br>UB. Facultat de Química<br>06/07/2009                              |

## **Academic activities**

Interés del comportament fàsic de sistemes tensioactius en formulació  
PARTTICIPÉ (Programas de reuniones de transferencia de tecnología entre la Industria y los centros de investigación españoles)  
Societat Espanyola de Químics Cosmètics SEQC,  
Barcelona  
C. Solans  
28/02/2008

Centre de Química Col·loïdal i Interficial (QCI).  
Presentation.  
PARTTICIPÉ (Programas de reuniones de transferencia de tecnología entre la Industria y los centros de investigación españoles)  
Societat Espanyola de Químics Cosmètics SEQC,  
Barcelona  
J. Nolla  
28/02/2008

Teoría de las emulsiones  
Jornada Científico-técnica de «Emulsiones: Tecnología, Reología y Procesos»  
Societat Espanyola de Químics Cosmètics SEQC,  
Barcelona  
J. Esquena  
16/06/2008

Emulsiones  
Programa Interuniversitario de Doctorado «Ciencia y Tecnología de Coloides e Interfases»  
J. Esquena  
19/06-2008; 11/06/2009

Aplicaciones en materiales porosos  
Programa Interuniversitario de Doctorado «Ciencia y Tecnología de Coloides e Interfases»  
C. Rodríguez Abreu  
26/06/2008

Master in Cosmetics and Dermopharmacy.  
Practical lessons  
«Centro de Estudios Superiores de la Industria Farmacéutica» (CESIF).  
J. Esquena, J. Nolla, M. Obiols, M. Sánchez  
23/09-09/10/2008; 22/06-23/07/2009

Comportamiento físico de sistemas tensioactivos  
Emulsiones y microemulsiones: Preparación, propiedades y aplicaciones industriales  
Col·legi Oficial de Químics de Catalunya  
C. Rodríguez-Abreu  
02/11/2008

Emulsiones y microemulsiones  
Emulsiones y microemulsiones: Preparación, propiedades y aplicaciones industriales  
Col·legi Oficial de Químics de Catalunya  
J. Esquena  
03/11/2008

## **Congress Organization**

Solans, C.  
17th. Int. Symp. on Surfactants in Solution. 27: Symposium to the honour of the late Prof. H. Kunieda.  
Organization Committee  
Berlin (Germany)  
17-22/08/2008

Messeguer, A.  
Cinquena Trobada de Joves Investigadors dels Països Catalans  
Organization Committee President  
Vic (Barcelona)  
28-29/01/2008

Galve, R., Calderó, G.  
I Jornadas NQB  
Organization Committee  
IQAC, Barcelona  
20/10/2009

## **Invited Conferences**

- R. Eritja  
Use of DNA derivatives in nanosciences  
11 Encuentro Peptídico Ibérico (EPI-11)  
Santiago de Compostela  
06/03/2008
- C. Rodríguez-Abreu  
Surfactant self-aggregation and phase behaviour  
Université de Kénitra, Morocco  
18/03/2008
- C. Solans  
Microemulsions  
Université de Kénitra, Morocco  
18/03/2008
- R. Eritja  
Development of new RNA derivatives for RNA interference studies  
Universidad del País Vasco. Facultad de Medicina.  
12/04/2008
- C. Rodriguez-Abreu  
Viscoelastic surfactant systems: From soft to hard matter  
University of Manchester, UK  
30/07/2008
- C. Solans  
Surfactant self-assembly as a biomimetic approach to control size and shape in nanomaterial synthesis  
22nd European Colloid and Interface Society (ECIS) Conference  
Cracovia, Poland  
04/09/2008
- C. Rodríguez-Abreu  
From self-aggregation to nanostructured solids  
Surfactant Templated Porous Materials: Synthesis and Characterisation Workshop.  
CECAM (Centre Européen de Calcul Atomique et Moléculaire) Zurich, Switzerland.  
08/09/2008
- C. Solans  
Surfactant self-assembly: application to the preparation of innovative nanostructured materials  
Firmenich S. A. Geneva, Switzerland  
20/10/2008
- R. Eritja  
Use of DNA derivatives in the fabrication of devices and sensors  
6èmes Journées Maghreb-Europe, MADICA 2008,  
Rabat, Morocco  
31/10/2008
- C. Rodríguez-Abreu  
Autoorganización en sistemas tensioactivos y su aplicación en la preparación de sólidos nanoestructurados  
IICTM. Consejo Nacional de Investigaciones Científicas y Técnicas. Mar del Plata. Argentina.  
24/11/2008
- C. Solans  
Highly Concentrated (Gel) Emulsions  
Yokohama National University, Yokohama, Japan  
27/02/2009
- C. Solans  
Surfactant self-assemblies: Role in the formation and properties of nano-emulsions and highly concentrated emulsions  
Shiseido, Yokohama, Japan  
02/03/2009
- C. Solans  
Understanding of polymer-surfactant residue behavior: Modeling concentrate to dilute microstructures with phase diagrams  
Procter and Gamble. Cincinnati, USA  
22/06/2009
- M. Alvira  
Triplex and quadruplex DNA: Chemical synthesis of modified DNA structures and study of their stability  
The architecture of life. IRB Ph.D. Symposium.  
Barcelona  
02/11/2009
- J. Esquena  
Emulsions: Formation and properties  
Université de Kénitra, Morocco  
09/12/2009
- R. Molina  
Plasma treatment on polymeric materials  
Université de Kénitra, Morocco  
09/12/2009

## **Editorial Activity in Journals**

- C. Solans  
Coeditor of the Section «Emulsions and Microemulsions»  
*Current Opinion in Colloid and Interface Science.*  
2008

- C. Rodriguez Abreu  
Associate Technical Editor  
*Journal of Surfactants and Detergents*  
2008

# DEPARTMENT OF CHEMICAL AND SURFACTANTS TECHNOLOGY

## Research Projects

Formulación de los lípidos internos de la lana para una efectiva aplicación tópica.  
CSIC. Proyecto Intramural 2004 OE 373  
Principal Investigator: L. Coderch  
2007-2008

Evaluation of the antioxidant effect in «ex vivo» skin of a marine extract.  
AgResearch Limited, Lincoln, New Zealand  
Principal Investigator: L. Coderch  
2007-2008

Extracción y análisis lipídico de la epidermis y dermis de piel canina de diferentes razas  
Univet (20071186)  
Principal Investigator: L. Coderch  
2007-2008

Eficacia de antioxidantes en cabello humano  
Provital (20090985)  
Principal Investigator: L. Coderch  
2009-2010

Encapsulación lipídica/polimérica en la producción de tejidos biofuncionales  
MICINN (CTQ2009-13967-C03-01PPQ)  
Coordinator/Principal Investigator: L. Coderch  
2009-2012

Minimización de residuos industriales. Obtención de biopolímeros de elevado valor añadido.  
MCyT (CTM2006-11610)  
Principal Investigator: J. Cot  
2006-2009

Biodegradabilidad y toxicidad acuática de líquidos iónicos como alternativa a disolventes orgánicos convencionales  
MEC (CTQ2007-60364)  
Principal Investigator: M. T. García  
2007-2010

Preparación y estudio de sistemas tensioactivos derivados de aminoácidos para su potencial aplicación en química biológica. Estudios de interacción con membranas  
CICYT (CTQ2006-01582)  
Principal Investigator: M. R. Infante  
2007-2009

Tensioactivos biocompatibles en la complejación de biopolímeros  
MEC (Spanish-Portuguese Contract P2007PT0050)  
Principal Investigators: M. R. Infante /M. da Graça Martins  
2008-2009

Contrato de licencia y explotación de la patente ES512643/ PI9500027  
Principal Investigator: M. R. Infante  
2002-2015

Síntesis de derivados hidrofóbicos de la inulina  
RAFTI  
Principal Investigator: M. R. Infante  
2006-2008

Biopolymer based surfactants – stabilization and functionalisation of particles and surfaces  
COST Action n. D36  
Coordinator: M. R. Infante  
2006-2010

Tensioactivos derivados de lisina  
L'OREAL  
Principal Investigator: M. R. Infante  
2007-2009

Síntesis de tensioactivos cationicos de arginina y lisina  
Novo Nordisk A/S  
Principal Investigator: M. R. Infante  
2009

Suport a Grups de Recerca Consolidats  
Generalitat de Catalunya (2009SGR 1331)  
Tensioactius i Química Sostenible  
Principal Investigator: M. R. Infante  
2009-2013

Comportamiento fásico de sistemas bicelares:  
influencia de la composición lipídica  
MCyT (CTQ2007-60409/BQU)  
Principal Investigator: O. López  
2007-2009

Caracterización, propiedades y aplicaciones de las fibras de polí(ácido láctico)  
PN de I+D+I (MAT 2007-66569-C02-02)  
Coordinator: D. Cayuela (UPC)  
Subproject Principal Investigator: A. M. Manich  
2007-2010

Tecnologías limpias en tenería: Recuperación del nitrógeno orgánico de los efluentes de tenería y revalorización del residuo proteico obtenido  
MCyT (CTQ2006-08106/PPQ)  
Principal Investigator: A. Marsal  
2006- 2009

Suport a Grups de Recerca Consolidats.  
Generalitat Catalunya (2005SGR 00066)  
Fisicoquímica i estructuració vesicular de lipids y biopolímers bacterians  
Principal Investigator: J. L. Parra  
2005-2008

Producción de tejidos inteligentes con ceramidas para pieles sensibles.  
DGICYT (CTQ2006-15405-CO3-01PPQ)  
Coordinator/Principal Investigator: J. L. Parra  
2006-2009

Comparación del perfil de penetración cutánea de dos formulaciones de cafeína.  
Provital  
Principal Investigator: J. L. Parra  
2008

Absorción percutánea de un péptido en solución acuosa, etanólica y en una formulación liposómica.  
Lipotec  
Principal Investigator: J. L. Parra  
2008

Suport a Grups de Recerca Consolidats.  
Generalitat Catalunya (2009 SGR 1212)  
Fisicoquímica i estructuració vesicular de lipids i biopolymers bacterians  
Principal Investigator: J. L. Parra  
2009-2014

Tensioactivos del tipo tris-quats: síntesis, propiedades físico-químicas y aplicación de estos compuestos como inhibidores de corrosión MEC (2007MA0010). Convenio Cooperación con Marruecos  
Principal Investigators: L. Pérez/ M. El Achouri  
2008-2009

## Patents

De la Maza, A., Barbosa-Barros, L., López, O., Cebrian, J., García-Antón, J.M., Almiñana, N. Composición cosmética o dermofarmacéutica de micelas mixtas  
Lipotec, S.A.  
P200800596  
01/10/2008  
European Union

Ramos-Stanbury, L., Pérez, L., Infante, M.R. Utilisation d'au moins un compose dérivé de lysine pour le conditionnement des fibres keratiniques, composition cosmétique le contenant et procédé de conditionnement des fibres  
L'Oreal  
FR0857287  
27/10/2008  
France

Bertrán, E., Molina, R. Reactor de plasma  
CSIC  
P200803269  
17/11/2008  
ES

Torres, P., Plou, F.J., Ballesteros, A., Parra, J.L., Cornelles, F., Jiménez, J. Procedimiento enzimático para la obtención de derivados glucosilados de resveratrol con propiedades tensioactivas  
CSIC  
P200930037  
03/04/2009  
ES

Pons, R. Dispositivo para alojar una muestra en el Interior de una cámara de dispersión o difracción de Rayos X  
CSIC  
P200930061  
13/04/2009  
ES

Martí, M., Coderch, M.L., Parra, J.L., de la Maza, A. Colorantes dispersos liposomados  
CSIC  
P200930301  
12/06/2009  
ES

Perez, L., Pinazo, A., Infante, M.R., Angelet, M. N,N Acyloxypropyl Lysine Methyl Ester and N,N Bis (N-Acyloxypropyl) Lysine Methyl Ester Type Compounds and use thereof as Surface-Active Agents with Na Antimicrobial Activity  
CSIC, L'Oreal  
US2009203781A  
13/08/2009  
U.S.A.

Ramos-Stanbury, L., Perez, L., Infante, M.R. Utilisation d'au moins un compose dérivé de lysine pour le conditionnement des fibres keratiniques, composition cosmétique le contenant et procédé de conditionnement des fibres  
L'Oreal  
09174130  
27/10/2009  
European Union

Pons, R., Pinazo, A., Lozano, N., Rivas, L.I., Fernández-Reyes, M.R., Luque, J.R., Pérez, L., Infante, M.R., Morán, C. Formulaciones de lipoaminoácidos catiónicos con menor poder hemolítico basadas en la formación de pares cataniónicos  
CSIC  
P200930990  
13/11/2009  
ES

Pons, R. Complejo tripolifosato-tensioactivo catiónico como ionóforo en eléctrodos selectivos y sus aplicaciones  
CSIC  
P200931149  
11/12/2009  
ES

Pons, R., Pinazo, A., Lozano, N., Rivas, L.I., Fernández-Reyes, M.R., Luque, J.R., Pérez, L., Infante, M.R., Morán, C. Uso de acilgliceroles derivados de arginina como antiprotozoarios  
CSIC  
P200931165  
15/12/2009  
ES

Morales, J.C., Cornelles, F., Parra, J.L. Derivados fenólicos lipófilos como surfactantes  
CSIC  
P200931214  
21/12/2009  
ES

## PhD Thesis

Barbosa, L.  
**Formación, caracterización y aplicación cutánea de sistemas bicelares**  
Directors: López, O., de la Maza, A.  
UB. Facultat de Química  
20/10/2008  
Excelente «cum laude»

Hernández Balada, E.  
**Improvement of conventional leather making processes to reduce the environment impact**  
Directors: Cot, J., Costa, J.  
UB. Facultat de Química  
05/02/2009  
Excelente «cum laude»

Méndez, S.  
**Caracterización y estructuración de lípidos de tejidos queratinicos y efectividad de su aplicación capilar**  
Directors: Coderch, M.L., Parra, J.L.  
UB. Facultat de Química  
13/02/2009  
Excelente «cum laude»

Ramírez, R.  
**Extracción y análisis de ceramidas procedentes de la lana para su aplicación farmacéutica o cosmética**  
Directors: Coderch, M.L., Martí, M.  
UB. Facultat de Química  
27/01/2009  
Excelente «cum laude»

## Masters

Bautista Pérez, M. E.  
**Tecnologías limpias en tenería: recuperación del nitrógeno orgánico de los efluentes de tenería**  
Director: A. Marsal  
CSIC (ME in Biological Chemistry, Environmental and Related Technologies)  
29/07/2008

Colomer, A.  
**Estudio fisicoquímico de la interacción del irinotecan con modelos de membrana**  
Directors: A. Pinazo, F. Reig  
Master IIQAB  
28/10/2008

Colomer, A.  
**Síntesis y propiedades de nuevos tensioactivos catiónicos derivados de lisina**  
Directors: L. Pérez, A. Pinazo  
UB. Facultat de Química  
18/09/2009

Miranda León, J. R.  
**Termofijado, análisis termomecánico y comportamiento a la relajación de la poliamida 66**  
Director: A. M. Manich  
ESIT (INTI) México  
18/06/2008

Morros, J.  
**Obtenció de tensioactius biopolimèrics basats en la Inulina en medi aquós**  
Director: M.R. Infante  
UB. Facultat de Química  
07/07/2008

Yousefi, H.R.  
**Elaboración de nanopartículas de flurbiprofeno estabilizadas con un tensioactivo catiónico derivado de la lisina**  
Directors: L. Pérez, M. L. García  
UB. Facultat de Farmàcia  
16/09/2009

## Academic activities

Tendencias en investigación de preparados cosméticos  
Master en Dermofarmacia y Cosmetología  
UB. Facultat de Farmàcia  
J.L. Parra Juez  
2008

Estadística y planificación de experiencias aplicadas a las ciencias farmacéuticas  
Máster técnico en compliance para la industria farmacéutica y afines  
UB. Facultat de Farmàcia  
A.M. Manich  
2008

## Congress Organization

|  |  |
|--|--|
| Marsal, A.<br>57 Congreso de la Asociación Química Española<br>de la Industria del Cuero (AQEIC)<br>Organizing Committee Member<br>Igualada<br>25-26/04/2008 | Martí, M.<br>35 Simposium de l'AEQCT<br>Organizing Committee<br>Barcelona<br>25-26/03/2009   |
| Marsal, A.<br>Jornada Técnica de la AQEIC: <b>Mantenimiento<br/>de prendas de piel</b><br>Organizing Committee Member<br>Igualada<br>6/11/2008               | Sanchez Leal, J.<br>C.E.D. 38th Meeting<br>Secretary<br>Barcelona<br>02-03/04/2008   |
| Marsal, A.<br>58 Congreso de la AQEIC<br>Organizing Committee Member<br>Peñíscola<br>08-10/05/2009   | Sánchez Leal, J.<br>Technical Workshop: Creatividad en el Perfumado<br>y Aromatización de Productos: Detergentes,<br>Cosméticos, Alimentarios, Farmacéuticos.<br>Organization Committee<br>Barcelona<br>11/06/2008 |
| Martí, M.<br>21st. IFATCC Int. Congress<br>Scientific Committee Member<br>Barcelona<br>06-09/05/2008   | Sánchez Leal, J.<br>Technical Workshop: GHS. Sistema Global<br>Armonizado de Clasificación y de Etiquetado de<br>Productos Químicos<br>Workshop Secretary<br>Barcelona<br>11/11/2008                               |

## **Invited Conferences**

Cot, J.

Taylor-made biomaterials from collagenic wastes:  
feasible link between tanning industry and tissue  
engineering  
XXX Congress of IULTCS. Beijing, R.P. China  
11/10/2009

Infante, M. R.

New surfactants from lysine  
Università La Sapienza. Rome, Italy  
28/05/2008

Infante, M. R.

Biocompatible Surfactants from Renewable  
Hydrophiles  
2nd Workshop on Fats and Oils as Renewable  
Feedstock. Emdem, Germany  
23/03/2009

Infante, M. R.

The role of the amino acid based surfactants as  
DNA delivery systems  
ECIS 2009. 23rd Conference of the European  
Colloid and Interface Society. Symposium in  
Honour of Maria Miguel. Antalya, Turkey  
07/09/2009

Manich, A.M.

Elasticidad y plasticidad de la piel curtida destina-  
da al calzado  
Escuela Superior de Ingeniería Textil, México D.F.,  
México  
26/05/2008

Manich, A.M.

Transiciones térmicas en el termofijado de la  
poliamida  
Escuela Superior de Ingeniería Textil, México D.F.,  
México  
27/05/2008

Manich, A.M.

Termoporometría aplicada al estudio de la  
porosidad de las fibras textiles  
Escuela Superior de Ingeniería Textil, México D.F.,  
México  
28/05/2008

Manich, A.M.

A investigação têxtil no marco Europeio  
Universidade da Beira Interior. Covilhá, Portugal  
03/12/2009

Molina, R.

Plasma treatment on polymeric materials  
Faculty of Sciences, Ibn Tofail University, Kenitra,  
Morocco  
11/12/2009

Parra, J.L.

Absorción percutánea de compuestos aplicados  
tópicamente  
Sociedad Española Químicos Cosméticos.  
Barcelona  
26/02/2008

Pons, R.

Cationic vesicles with biocompatible surfactants  
Graz, Austria  
15/05/2008

Pons, R.

Structural transformations in surfactant systems  
Coimbra, Portugal  
13/11/2008

## **Editorial Activity in Journals**

M.R. Infante

Associate Technical Editor

**Journal of Surfactants and Detergents**  
2008

A. M. Manich

Editorial Board

**Journal of the Textile Institute**  
2009

## **APPENDIX 2: 2008-2009 Publications**

|   |            |
|---|------------|
| 1. List of ISI journals in alphabetical order (and impact factor)                                 | <b>128</b> |
| 2. Publications listed by decreasing impact factor<br>(2009 listed first if papers in both years) | <b>129</b> |
| 3. Publications in non-ISI journals (journals in alphabetical order)                              | <b>138</b> |
| 4. Book chapters  | <b>139</b> |
| 5. Conference Proceedings   | <b>140</b> |

## 1. List of ISI journals in alphabetical order (and impact factor)

| ISI JOURNALS (in alphabetical order)   | 2008         | 2009          |
|--|--------------|---------------|
| Anal. Bioanal. Chem.                   | 2.867        | <b>3.328</b>  |
| Anal. Biochem.                         | 3.002        | 3.088         |
| Anal. Chem.                            | 5.287        | <b>5.712</b>  |
| Anal. Chim. Acta                       | 3.186        | <b>3.146</b>  |
| Angew Chem.-Int. Ed.                   | 10.031       | <b>10.879</b> |
| Apoptosis                              | 3.043        | <b>3.971</b>  |
| Appl. Clay Sci.                        | 1.861        | <b>2.005</b>  |
| Appl. Surf. Sci.                       | <b>1.406</b> | 1.576         |
| Arkivoc                                | 1.253        | <b>1.377</b>  |
| Arthritis Res. Ther.                   | 4.035        | <b>4.485</b>  |
| BBA- Proteins Proteomics               | <b>3.078</b> | 2.233         |
| Biochem. Eng. J.                       | <b>1.872</b> | 1.889         |
| Biochem. Pharmacol.                    | 4.006        | <b>4.838</b>  |
| Biochimie                              | 2.899        | <b>3.071</b>  |
| Bioorg. Med. Chem.                     | 2.662        | <b>3.075</b>  |
| Bioorg. Med. Chem. Lett.               | 2.604        | <b>2.531</b>  |
| Biophys. Chem.                         | 1.913        | <b>2.362</b>  |
| Bioresour. Technol.                    | 3.103        | <b>4.453</b>  |
| Biosens. Bioelectron.                  | 5.061        | <b>5.143</b>  |
| Blood Cells Mol. Dis.                  | 2.555        | <b>2.749</b>  |
| Cancer Lett.                           | 3.398        | <b>3.504</b>  |
| Carbohydr. Polym.                      | <b>1.782</b> | 2.644         |
| Chem. Biodivers.                       | 1.420        | <b>1.659</b>  |
| Chem. Biol.                            | 5.178        | <b>5.603</b>  |
| Chem. Commun.                          | <b>5.141</b> | 5.340         |
| Chem. Eng. J.                          | <b>1.707</b> | 2.813         |
| Chem.-Eur. J.                          | 5.330        | <b>5.454</b>  |
| Chem. Mat.                             | <b>4.883</b> | 5.046         |
| Chem. Phys. Lett.                      | 2.207        | <b>2.169</b>  |
| Chem. Phys. Lipids                     | 2.396        | <b>2.647</b>  |
| Chem. Res. Toxicol.                    | <b>3.508</b> | 3.491         |
| ChemBioChem                            | 3.446        | <b>3.684</b>  |
| ChemMedChem                            | 2.825        | <b>3.150</b>  |
| Chemoecology                           | <b>1.250</b> | 1.446         |
| Chemosphere                            | 2.739        | <b>3.054</b>  |
| ChemPhysChem                           | 3.502        | <b>3.636</b>  |
| Clin. Biochem.                         | 2.072        | <b>1.926</b>  |
| Colloid Surf. A-Physicochem. Eng. Asp. | <b>1.601</b> | 1.926         |
| Colloid Surf. B-Biointerfaces          | 2.109        | <b>2.593</b>  |
| Crystengcomm                           | 3.468        | <b>3.535</b>  |
| Curr. Opin. Colloid Interface Sci.     | <b>4.354</b> | 5.493         |
| Drug Metab. Dispos.                    | 3.907        | <b>3.491</b>  |
| Electrochem. Commun                    | <b>4.186</b> | 4.194         |
| Electrophoresis                        | 3.609        | <b>3.509</b>  |
| Entomol. Exp. Appl.                    | <b>1.483</b> | 1.281         |
| Environ. Int.                          | <b>2.797</b> | 3.516         |
| Eur. J. Med. Chem.                     | 2.301        | <b>2.882</b>  |
| Eur. J. Org. Chem.                     | <b>2.914</b> | 3.016         |
| Fiber Polym.                           | <b>0.659</b> | 0.577         |
| Food Chem. Toxicol.                    | <b>2.186</b> | 2.321         |
| Green Chem.                            | 4.836        | <b>4.542</b>  |
| Helv. Chim. Acta                       | 1.515        | <b>1.396</b>  |
| Inorg. Chem.                           | 4.123        | <b>4.147</b>  |
| Inorg. Chim. Acta                      | 1.713        | <b>1.940</b>  |
| Insect Biochem. Mol. Biol.             | 2.827        | <b>2.626</b>  |
| Int. J. Pharm                          | <b>2.408</b> | 3.061         |
| J. Agric. Food Chem.                   | 2.532        | <b>2.562</b>  |
| J. Am. Chem. Soc.                      | 7.885        | <b>8.091</b>  |
| J. Am. Leather Chem. Assoc.            | 0.506        | <b>0.659</b>  |
| J. Appl. Microbiol.                    | <b>2.501</b> | 2.028         |
| J. Appl. Polym. Sci                    | <b>1.008</b> | 1.187         |
| J. Biol. Chem.                         | 5.581        | <b>5.520</b>  |
| J. Biotechnol.                         | <b>2.565</b> | 2.748         |
| J. Chem. Ecol.                         | 1.941        | <b>2.327</b>  |
| J. Chem. Technol. Biotechnol.          | <b>1.426</b> | 1.682         |

| ISI JOURNALS (in alphabetical order)  | 2008         | 2009          |
|---------------------------------------|--------------|---------------|
| J. Chem. Theory Comput.               | 4.308        | <b>4.274</b>  |
| J. Colloid Interface Sci.             | 2.309        | <b>2.443</b>  |
| J. Comb. Chem                         | <b>3.154</b> | 3.011         |
| J. Hazard. Mater.                     | 2.337        | <b>2.975</b>  |
| J. Label. Compd. Radiopharm.          | 1.142        | <b>0.698</b>  |
| J. Liposome Res.                      | 2.021        | <b>2.089</b>  |
| J. Mater. Sci.                        | 1.081        | <b>1.181</b>  |
| J. Med. Chem.                         | 4.895        | <b>4.898</b>  |
| J. Microsc.-Oxf.                      | 1.565        | <b>1.409</b>  |
| J. Mol. Catal. B-Enzym.               | 1.973        | <b>1.996</b>  |
| J. Mol. Model.                        | <b>1.669</b> | 2.018         |
| J. Nanopart. Res.                     | 2.338        | <b>2.299</b>  |
| J. Nanosci. Nanotechnol.              | 1.987        | <b>1.929</b>  |
| J. Nat. Prod.                         | <b>2.551</b> | 2.843         |
| J. Neurochem.                         | <b>4.451</b> | 4.500         |
| J. Non-Cryst.Solids                   | <b>1.319</b> | 1.449         |
| J. Org. Chem.                         | 3.959        | <b>3.952</b>  |
| J. Pestic. Sci.                       | <b>0.694</b> | 0.769         |
| J. Pharmacol. Exp. Ther.              | 4.003        | <b>4.304</b>  |
| J. Photochem. Photobiol. B-Biol.      | 1.919        | <b>1.838</b>  |
| J. Phys. Chem. B                      | 4.086        | <b>4.189</b>  |
| J. Phys. Chem. C                      | 0.000        | <b>3.396</b>  |
| J. Soc. Leather Technol. Chem.        | 0.422        | <b>0.256</b>  |
| J. Therm. Anal Calorim                | <b>1.483</b> | 1.630         |
| J. Thromb. Haemost.                   | 5.947        | <b>6.291</b>  |
| Langmuir                              | 4.009        | <b>4.097</b>  |
| Luminescence                          | <b>1.317</b> | 1.183         |
| Macromolecules                        | 4.411        | <b>4.407</b>  |
| Microbiol. Res.                       | <b>1.535</b> | 2.054         |
| Microporous Mesoporous Mat.           | 2.210        | <b>2.555</b>  |
| Mini-Rev. Org. Chem.                  | <b>2.000</b> | 1.449         |
| Mol. Divers.                          | 2.708        | <b>2.859</b>  |
| Mol. Pharm.                           | 3.500        | <b>4.565</b>  |
| Nano Lett.                            | 9.627        | <b>10.371</b> |
| Nat. Prod. Commun.                    | <b>0.435</b> | 0.766         |
| Neurochem. Int.                       | <b>2.975</b> | 3.228         |
| Nucleic Acids Res.                    | 6.954        | <b>6.878</b>  |
| Nucleosides Nucleotides Nucleic Acids | <b>0.723</b> | 0.571         |
| Opt. Express                          | <b>3.709</b> | 3.880         |
| Org. Lett.                            | <b>4.802</b> | 5.128         |
| Phys. Chem. Chem. Phys.               | 3.343        | <b>4.064</b>  |
| Physiol. Entomol.                     | <b>1.410</b> | 1.533         |
| Phys. Status Solidi A-Appl. Mat.      | <b>1.214</b> | 1.205         |
| Plant Cell Tissue Organ Cult.         | <b>1.068</b> | 1.017         |
| Plant Mol. Biol.                      | 3.847        | <b>3.541</b>  |
| Plasma Process. Polym.                | 2.132        | <b>2.921</b>  |
| Rapid Commun. Mass Spectrom.          | <b>2.971</b> | 2.772         |
| Regul. Toxicol. Pharmacol.            | <b>1.968</b> | 2.353         |
| Sens. Actuator B-Chem.                | <b>2.934</b> | 3.122         |
| Sens. Lett.                           | 1.587        | <b>1.160</b>  |
| Sep. Purif. Technol.                  | <b>2.142</b> | 2.503         |
| Stem Cells Dev.                       | 3.224        | <b>3.273</b>  |
| Skin Res. Technol.                    | <b>1.253</b> | 1.348         |
| Surf. Interface Anal.                 | 1.036        | <b>1.272</b>  |
| Synthesis                             | <b>2.257</b> | 2.470         |
| Tekstil                               | 0.107        | <b>0.137</b>  |
| Tenside Surfactants Deterg.           | 0.486        | <b>0.515</b>  |
| Tetrahedron                           | 2.869        | <b>2.897</b>  |
| Tetrahedron Lett.                     | <b>2.615</b> | 2.538         |
| Tetrahedron: Asymmetry                | 2.634        | <b>2.796</b>  |
| Text. Res. J.                         | 0.702        | <b>0.779</b>  |
| Theor. Chem. Acc.                     | 2.537        | <b>2.370</b>  |
| Thermochim. Acta                      | 1.562        | <b>1.659</b>  |
| Trac-Trends Anal. Chem.               | 5.827        | <b>5.485</b>  |
| Trends Biotechnol.                    | <b>7.610</b> | 6.624         |
| Water Res.                            | 3.427        | <b>3.587</b>  |

## 2. Publications listed by decreasing impact factor (2009 listed first if papers in both years)

- Asymmetric self- and cross-alcohol reaction of glycolaldehyde catalyzed by D-fructose-6-phosphate aldolase  
Garrabou, X., Castillo, J. A., Guérard-Hélaine, C., Parella, T., Joglar, J., Lemaire, M., Clapés, P.  
*Angew. Chem.-Int. Ed.* 2009, 48, 5521-5525
- A ferromagnetic  $[Cu_3(OH)_2]^{4+}$  cluster formed inside a tritopic nonaaazapryridinophane. Crystal structure and solution studies.  
González-Álvarez, A., Alfonso, I., Cano, J., Díaz, P., Gotor, V., Gotor-Fernández, V., García-España, E., García-Granda, S., Jiménez, H., Lloret, F.  
*Angew. Chem.-Int. Ed.* 2009, 48, 6055-6058
- All organic discotic radical with spin carrying rigid-core showing intracolumnar interactions and multifunctional properties  
Castellanos, S., López-Calahorra, F., Brillas, E., Juliá, L., Velasco, D.  
*Angew. Chem.-Int. Ed.* 2009, 48, 6516-6519
- Shaping supramolecular nanofibers with complementary hydrogen bond-forming nanoparticles  
Puigmartí-Luis, J., Pérez del Pino, A., Laukhina, E., Esquena, J., Laukhin, V., Rovira, C., Vidal-Gancedo, J., Kanaras, A.G., Nichols, R.J., Brust, M., Amabilino, D.B.  
*Angew. Chem.-Int. Ed.* 2008, 47, 1861-1865
- Label-free DNA biosensors based on functionalized carbon nanotube field effect transistors  
Martínez, M.T., Tseng, Y.C., Ormategui, N., González-Domínguez, J.M., Loinaz, I., Eritja, R., Bokor, J.  
*Nano Lett.* 2009, 9, 530-536
- $\alpha,\gamma$ -Peptide nanotube templating of one-dimensional parallel fullerene arrangements  
Reiriz, C., Brea, R.J., Arranz, R., Carrascosa, J.L., Garibotti, A., Manning, B., Valpuesta, J.M., Eritja, R., Castedo, L., Granja, J.R.  
*J. Am. Chem. Soc.* 2009, 131, 11335-11337
- Unique tautomeric and recognition properties of thiokethothymines?  
Faustino, I., Aviñó, A., Marchán, I., Luque, F.J., Eritja, R., Orozco, M.  
*J. Am. Chem. Soc.* 2009, 131, 12845-12853
- Unconventional biradical character of titanium enolates  
Moreira, I. de P.R., Bofill, J.M., Anglada, J.M., Solsona, J.G., Nebot, J., Romea, P., Urpí, F.  
*J. Am. Chem. Soc.* 2008, 130, 3242-3243
- Supramolecular control for the modular synthesis of pseudopeptidic macrocycles through an anion-templated reaction  
Alfonso, I., Bolte, M., Bru, M., Burguete, M.I., Luis, S.V., Rubio, J.  
*J. Am. Chem. Soc.* 2008, 130, 6137-6144
- Theoretical and experimental studies on the mechanism of norbornadiene Pauson-Khand cycloadducts photoarrangement. Is there a pathway on the excited singlet potential energy surface?  
Olivella, S., Solé, A., Lledó, A., Ji, Y., Verdaguer, X., Suau, R., Riera, A.  
*J. Am. Chem. Soc.* 2008, 130, 16898-16907
- Multifunctional nanoparticles-properties and prospects for their use in human medicine  
Sanvicenç, N., Marco, M.P.  
*Trends Biotechnol.* 2008, 26, 425-433
- Conformationally rigid nucleoside probes help understand the role of sugar pucker and nucleobase orientation in the thrombin binding aptamer  
Saneyoshi, H., Mazzini, S., Aviñó, A., Portella, G., González, C., Orozco, M., Marquez, V., Eritja, R.
- Aggregated low density lipoprotein induces tissue factor by inhibiting sphingomyelinase activity in human vascular smooth muscle cells.  
Camino-Lopez, S., Badimon, L., Gonzalez, A., Canals, D., Pena, E., Llorente-Cortes, V.  
*J. Thromb. Haemost.* 2009, 7, 2137-2146
- Impedimetric immunosensor based on a poly(pyrrole-antibiotic model) film for the label-free picomolar detection of ciprofloxacin  
Giroud, F., Gorgy, K., Gondran, C., Cosnier, S., Pinacho, D.G., Marco, M.P., Sanchez-Baeza, F.J.  
*Anal. Chem.* 2009, 81, 8405-8409
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