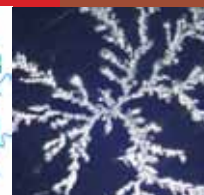
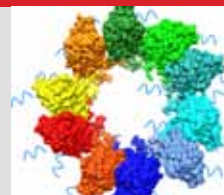


IQAC BIENNIAL SCIENTIFIC REPORT

2018-2019

Institute for Advanced Chemistry
of Catalonia (IQAC)

"Where chemistry helps"

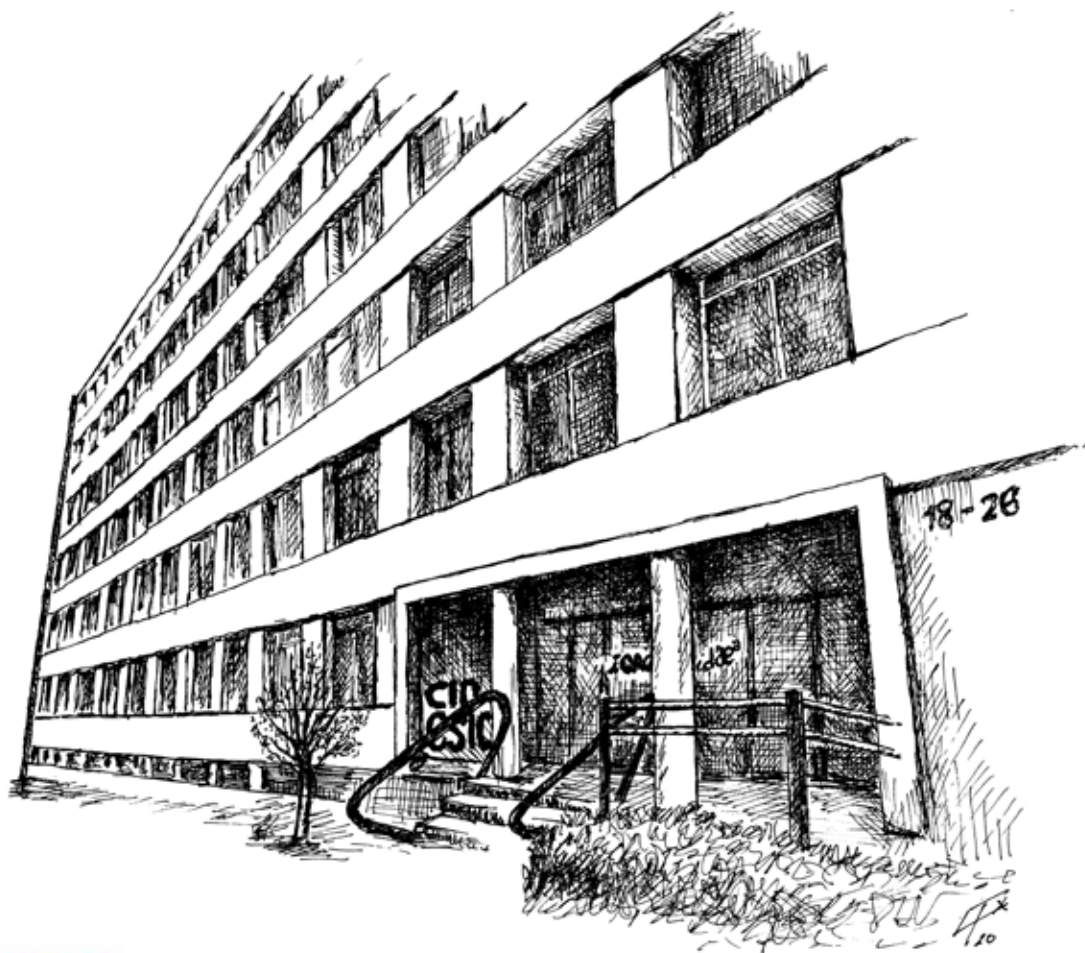


 **iQAC**



CSIC

CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS



2020 - Institute for Advanced Chemistry of Catalonia (IQAC)
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Text and images content: IQAC staff
Graphic design and layout: **2San**

Photos:
(on this page)
(on the top of the cover)
(on the bottom of the cover)

Ink drawing of the CID façade. Author: Lluís Fajarí Agudo (IQAC and CID)
IQAC Nuclear Magnetic Resonance Spectroscopy Facility. Author: Naiara Solozábal Mirón (IQAC)
From the photographic exhibition "There's a light that never goes out". Author: Silvia Panarello (IQAC)

BIENNIAL SCIENTIFIC REPORT 2018 - 2019



Institute for Advanced Chemistry of Catalonia
"Where chemistry helps"

Director's foreword



The Institute for Advanced Chemistry of Catalonia (IQAC) is one of the research centers of the Spanish National Research Council (CSIC). Together with the Institute for Environmental Assessment and Water Research (IDAEA), IQAC is located in the Center for Research and Development (CID), which provides IQAC and IDAEA with administrative support and general services (informatics, library, maintenance, purchase, etc.).

The IQAC was created in 2007 with the mission to perform multidisciplinary research of excellence in Chemical Sciences with the broad goal of improving the quality of life. The general strategy to achieve this mission involves the application of chemical approaches to address and solve societal challenges, mainly those related to human health, the sustainability of chemical processes and products, and the needs for novel materials for different applications. Since its establishment, IQAC has been in a permanent attitude to keep a balance between basic and applied science, as well as to transfer its knowledge and technology results to the productive sector.

Research at IQAC is organized in four inter-related Research Programmes aiming at: the development of methods and strategies for the synthesis of molecules of high added value (Methods & Strategies); the discovery of chemical and molecular entities of therapeutic, biological and biomedical interest (Tools & Hits); the study of molecules with surfactant properties, including synthesis, biophysical studies

and applications (Surfactants) and the generation and use of nanobiotechnology knowledge for the prevention, diagnostic and treatment of diseases (Nanomedicine). The overall studies are founded on varied transversal key enabling capabilities of IQAC researchers. Among them, computation, which looks into the behavior and properties of molecules to understand their reactivity, dynamics and function, deserves a special mention. Administratively, the research programs are organized in two departments: Biological Chemistry, and Surfactants and Nanobiotechnology.

Research at IQAC is complemented with a range of diverse Scientific and Technical Platforms, which offer their capabilities to both internal and external users. Regarding the IQAC services, I would like to remark that one of them is certified according to AENOR (ISO9001) and three of them have achieved the TECNIO accreditation. Furthermore, both the animal facility and the cell culture facility (P2) of CID are certified by the Generalitat de Catalunya. This report is a compilation of our activities during the years 2018-2019. We have maintained the numbers while increasing the quality of our scientific publications and have started to experience a slight raise in funding.

During the last two years, IQAC has incorporated 4 new PIs, who strengthen and complement the existing IQAC capacities thus contributing to enhancing our competitiveness and excellence. On the other hand, 8 PIs and one Technician retired after a life devoted to scientific research.

Regarding infrastructures, IQAC has improved its facilities and services with the acquisition of new equipment and the remodeling of old laboratories. Regarding the former, we got a new 400 MHz NMR instrument and a purification system with UV-MS-ELS detectors, both through the attraction and securing of competitive funding. Furthermore, thanks to the specific CSIC call addressed at its scientific and technical facilities (FAS), we have been able to renew obsolete instruments and buy new equipment to increase some of our services capabilities. Finally, by means of the CSIC specific call for Infrastructures (PAI) we have been able to remodel three outdated laboratories.



The IQAC was created in 2007
with the mission to perform
multidisciplinary research of
excellence in Chemical Sciences
with the broad goal of improving
the quality of life



IQAC is strongly committed to offer training for undergraduates, graduate students and doctoral researchers in order to provide them with the knowledge and skills needed to undertake their professional careers. Within this strategic goal, 71 students performed their Bachelor's degree (43) and Master's degree (28) projects in our laboratories and 12 graduate students presented their Ph. D. theses during 2018-2019. Moreover, 31 doctoral researchers were hosted in our laboratories to continue their training.

During this biennium, IQAC has participated in a range of science outreach activities, such as some included in the 2018 and 2019 Science Week and additional workshops and visits to elementary and high schools. Additionally, we have continued with our offer of attractive seminars and have held our yearly IQAC workshops, where we combine two invited plenary lectures by invited speakers with oral communications and a poster session all presented by IQAC personnel of all levels.

On November 2019 we were gifted with the first evaluation meeting with our External Scientific Advisory Board. They were extremely kind and helpful, providing us with comments and suggestions to efficiently improve our Institute performance, as well as with insightful advices on organizational aspects of the research groups and scientific facilities.

All the achievements of this biennium emerge from the enthusiasm, commitment and hard work of our skillful professionals, including scientific, technical and administrative staff, to whom I am deeply indebted.

Gemma Fabriàs
IQAC Director

I am writing this presentation while the Covid19 pandemic is keeping most of us secluded at home. The SARS-CoV-2 virus has hit hard our world, which is now facing important challenges for the future. The virus has taken lives and caused a deep damage to our economies. The importance of a strong public health and the relevance of scientific research have become clear. Let's hope to look back two years from now to see that our societies have changed for better.

Photo: IQAC Entrance. Author: Lluís Fajari Agudo (IQAC)

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THE INSTITUTE

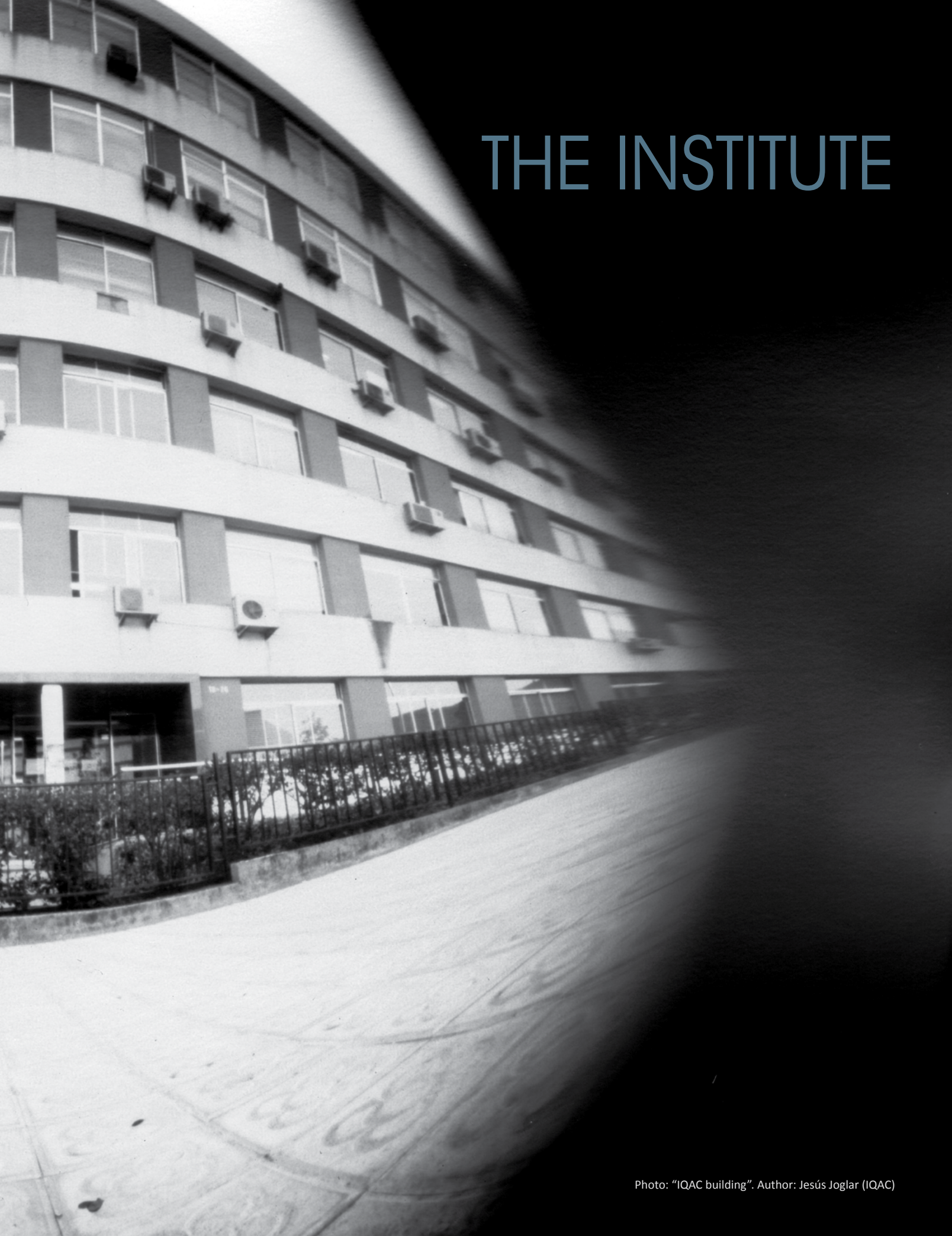


Photo: "IQAC building". Author: Jesús Joglar (IQAC)



Signature

History

The Institute for Advanced Chemistry of Catalonia (IQAC) inherits the long and fruitful research tradition in Organic Chemistry and Chemical Technology initiated by mid-1900's. In 1967, after a productive activity in the University of Barcelona, Prof. Pascual Vila and his co-workers moved into the CSIC Institute of Organic Chemistry of Barcelona, placed at CID. At the same time, CSIC scientists working in the field of tanning and textile Technology, such as Prof. A. Barella, Prof. R. Audivert and Prof. E. Gratacos, were also incorporated into CID to later create the Institute for Chemical and Textile Technology. These moves fostered the emergence and further consolidation of the two main research areas at CID: Organic Chemistry and Chemical Technology. During many years the CID has been the referent of the CSIC Chemistry in Catalonia.

Not only many graduate students and post-docs trained in this Center have moved to relevant positions in academic institutions and in private sectors, but CID has been the seed of outstanding research centers in Catalonia. In 1996, a joined action of the bioorganic, theoretical


and technological groups together with teams working on chemical issues related to the environment led to the creation of the Institute for Chemical and Environmental Research of Barcelona (IIQAB). During the ten-year period of IIQAB, the Institute became a referent in the fields of Environmental Chemistry, Biological Chemistry, Theoretical and Computational Chemistry, Sustainable Chemistry and selected items of Chemical Technology. Some of these fields have remained active and have been reinforced at IQAC since its creation in 2007.

The apparent heterogeneity of the active research areas at IQAC is clearly compensated by the wide opportunities of their mutual interaction, making IQAC a solid and modern Institute that looks at the future leaning on three key pillars: the robustness of the Chemistry tradition in our Centre, the enthusiasm and expertise of its personnel and the firm willingness warmly welcome staff scientists not trained in the Institute, providing them with the best possible conditions to carry out their research in a competitive, friendly and collaborative environment.

Location



Institute for Advanced Chemistry of Catalonia (IQAC)
C. Jordi Girona, 18-26
08034 - Barcelona

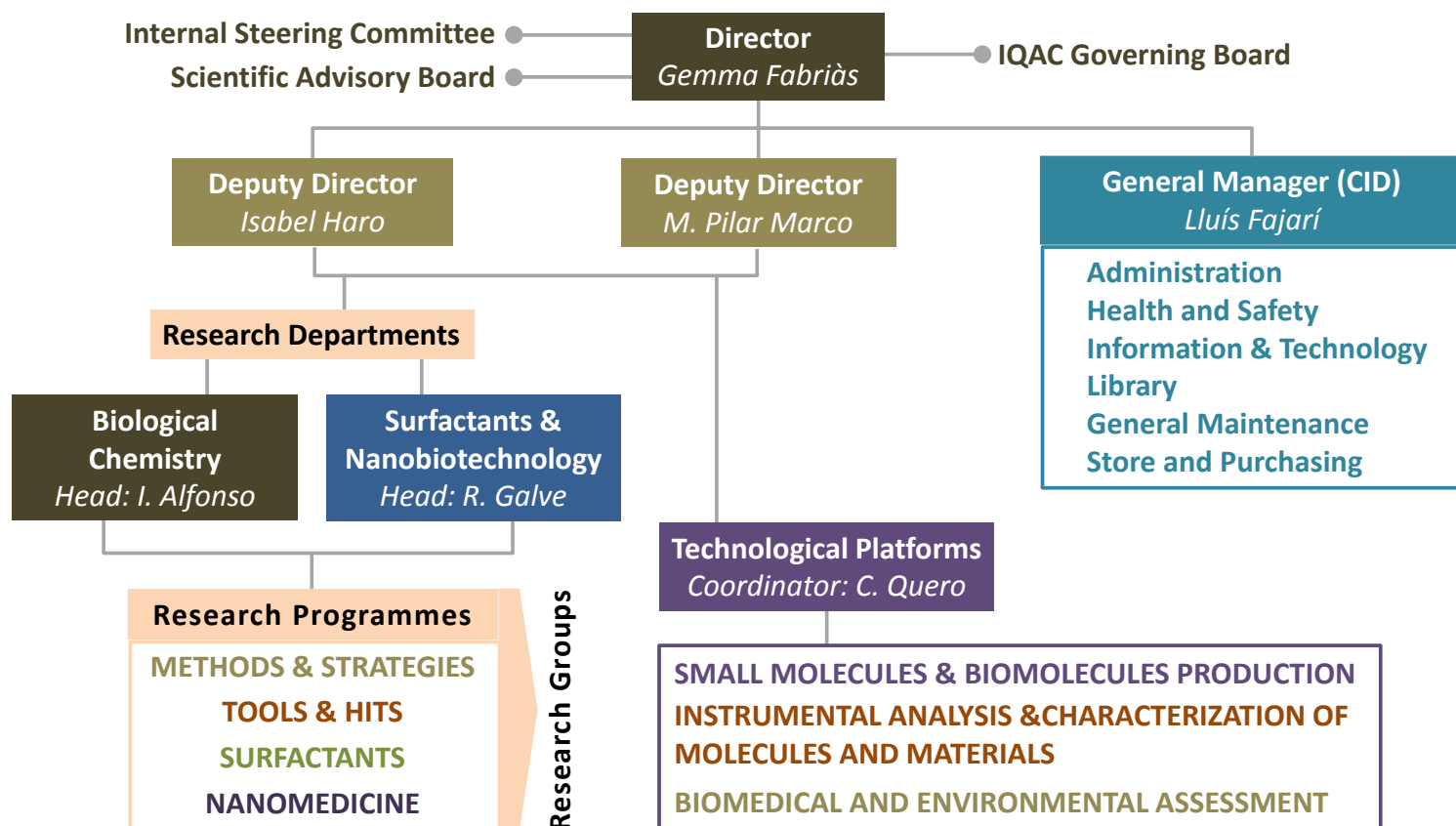
 41° 23' 15.5" N, 2° 06' 53.6" E

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Fax: +34 93 204 59 04

@ info@iqac.csic.es
 www.iqac.csic.es



Organisation



Internal Steering Committee

Gemma Fabriàs Domingo	Amadeu Llebaria Soldevila
M. Pilar Marco Colás	Roger Galve Bosch
Isabel Haro Villar	Olga López Serrano
Ignacio Alfonso Rodríguez	Ramon Pons Pons

IQAC Governing Board

Gemma Fabriàs Domingo	Ignacio Alfonso Rodríguez
Lluís Fajari Agudo	Olga López Serrano
M. Pilar Marco Colás	Jaume Caelles Balcells
Isabel Haro Villar	Meritxell Martí Gelabert
	Ignacio Pérez Pomeda

Scientific Advisory Board

Prof. Arben Merkoçi — Institut Català de Nanociència i Nanotecnologia. Bellaterra, Spain.

Dr. Carmen Almansa — Esteve Laboratories. Barcelona, Spain.

Prof. Anna M Papini — University of Firenze. Firenze, Italy.

Prof. Paul A. Millner — Faculty of Biological Sciences, University of Leeds, England.

Prof. Jesús Jiménez Barbero — CIC bioGUNE. Derio, Spain.

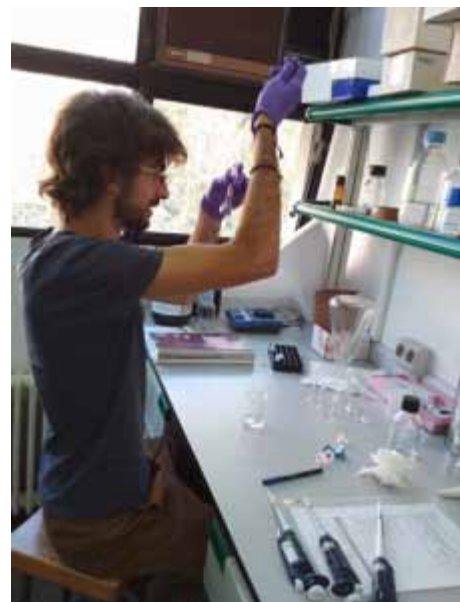
Prof. Pau Ballester — Institut Català d'Investigació Química. Tarragona, Spain.

Prof. Dganit Danino — Technion. Israel Institute of Technology. Haifa, Israel.

IQAC-CSIC "Víctor Carrer" Extraordinary Doctorate Awards

On February 28, 2019, the IQAC-CSIC "Víctor Carrer" extraordinary doctorate awards were established, granting an honorary diploma to the family of the doctoral student for their work on the Doctoral Thesis "Skin Permeability Methodologies for Topical Absorption Prediction".

Unfortunately Víctor Carrer had a traffic accident the night before his oral presentation and lost his life a few days later. Faced with the impossibility of naming him a doctor, an honorary act was held, establishing this award in his honor.



This award will be awarded annually at the IQAC Conference for the best Thesis carried out at the IQAC during the previous year.

Thus, this year a € 500 gift voucher will then be delivered to the best thesis work presented during 2019.

Retired and Ad Honorem members

Ad Honorem

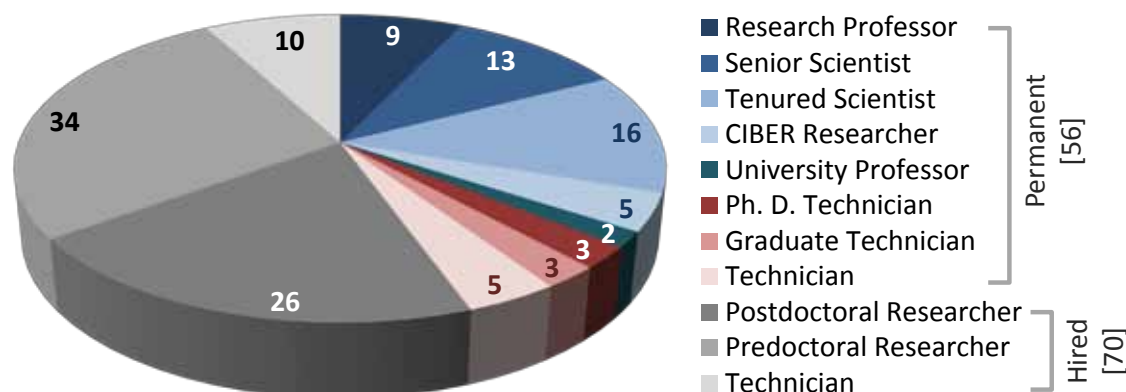
Jerónimo Blanco Fernández	30/12/2018
Ángel Guerrero Pérez	30/12/2018
Àngel Messeguer Peypoch	31/12/2019
Conxita Solans Marsà	31/12/2019

Retired

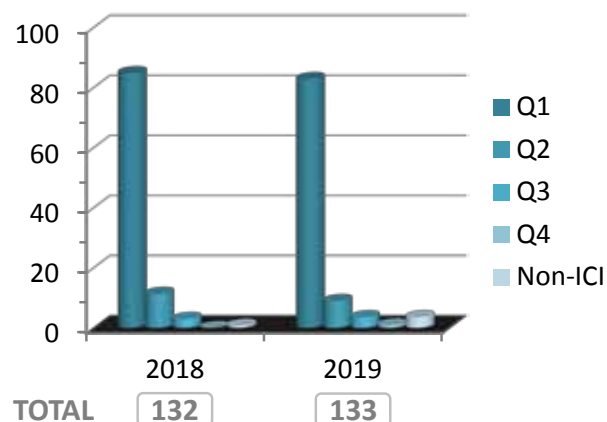
Isabel Yuste Hernández	26/10/2019
Nuria Rubio Vidal	31/03/2018
Lluís Julià Bargés	19/12/2018
Agustín Marsal Monge	09/02/2019
Francesc Comelles Folch	01/02/2018

IQAC in numbers

Personnel



Publications



Funding

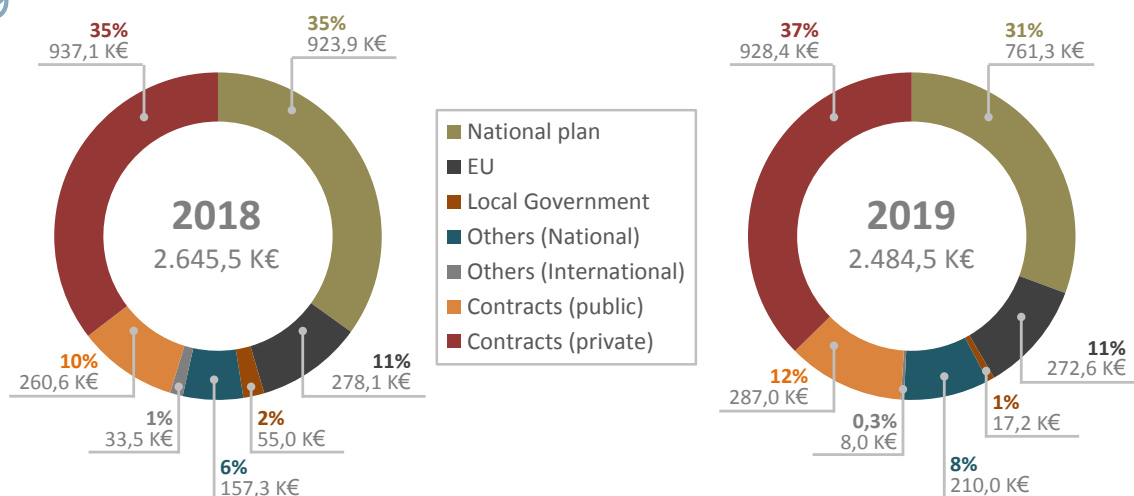




Photo:
From the photographic exhibition "There's a light that never goes out".
Author: Silvia Panarello (IQAC)

DEPARTMENTS, RESEARCH AND RESEARCH GROUPS

BIOLOGICAL CHEMISTRY

Synthetic Methodology & New Building Blocks
Theoretical & Computational Chemistry
Biotransformation & Bioactive Molecules
Supramolecular Chemistry
Plasma Chemistry

Development of methods and strategies for the synthesis of molecules of high added value

Synthesis & Biomedical Applications of Peptides
Research Unit on BioActive Molecules
Unit of Glycoconjugate Chemistry
Medicinal Chemistry
Chemical Biology
Nutraceuticals & Free Radicals

Discovery of chemical and molecular entities of therapeutic, biological and biomedical interest

SURFACTANTS & NANO BIOTECHNOLOGY

Cosmetic & Textile Innovations
Biophysics of Lipids & Interphases
Physical Chemistry of Surfactant Systems
Biocompatible Surfactants & Ionic Liquids

Surfactants: synthesis, biophysical studies and applications

Surface Chemistry
Nucleic Acids Chemistry
Colloidal & Interfacial Chemistry
Nanobiotechnology for Diagnostics
Multivalent systems for nanomedicine

Generation and use of nanobiotechnology knowledge for the prevention, diagnostic and treatment of diseases

BETTER

PROGRAMMES RESEARCH GROUPS

PROGRAMMES

KEY ENABLING CAPABILITIES

METHODS & STRATEGIES

TOOLS & HITS

SURFACTANTS

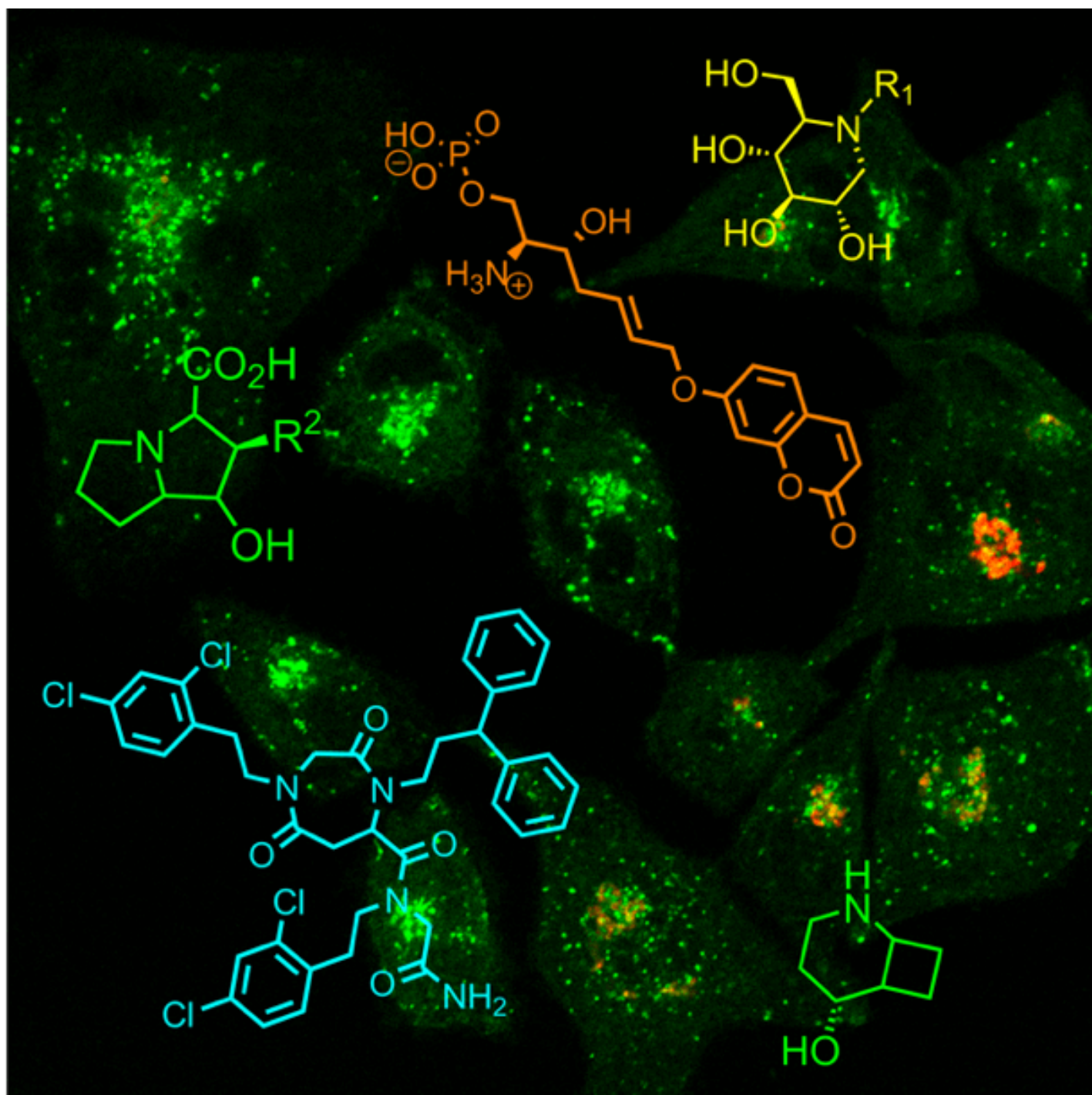
NANOMEDICINE

Chemical Synthesis
Biotechnology
Biochemistry & Cell Biology
Formulation Science & Technology
Nanotechnology
Physical Chemistry

COMPUTATION

Looking into the behavior and
properties of molecules to understand
their reactivity, dynamics and function

LIFE



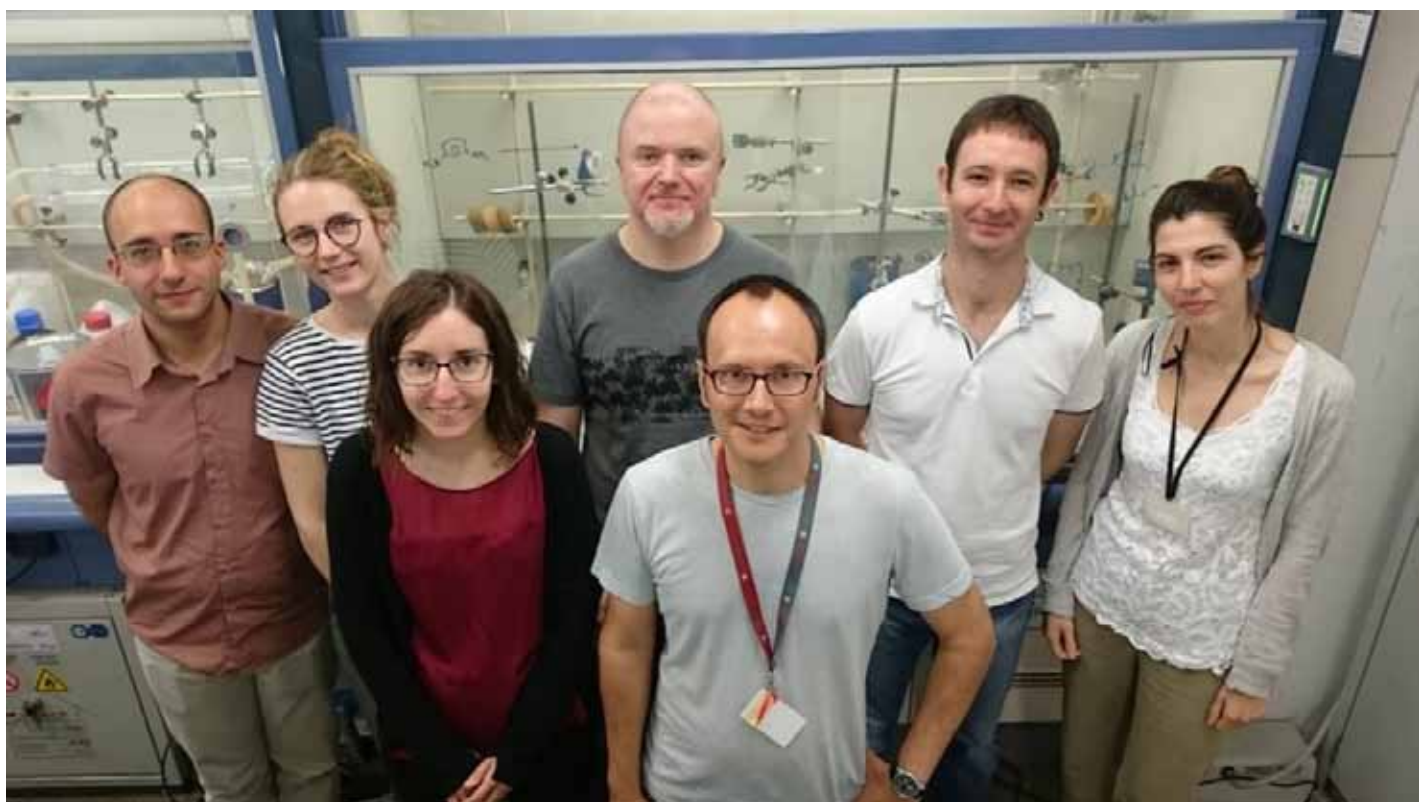
BIOLOGICAL CHEMISTRY DEPARTMENT

RESEARCH GROUPS • Supramolecular Chemistry • Medicinal Chemistry • Chemical Biology • Biotransformations and Bioactive Molecules • Synthesis and Biomedical Applications of Peptides (USiBAP) • Research Unit of Bioactive Molecules (RUBAM) • Theoretical and Computational Chemistry • Nutraceuticals and Free Radicals • Unit of Glycoconjugate Chemistry • Plasma Chemistry • Synthetic Methodology and New Building Blocks •

The Department of Biological Chemistry is focused on the multidisciplinary field of Chemistry in the frontiers with Biology. We aim to perform top scientific research in chemistry to answer important and general questions related to life, in a broad sense. As a common goal, we generate new knowledge at the molecular level to face societal challenges, also providing young researchers with top-notch training so as to prepare them for a successful professional career in science. Thus, starting from basic and fundamental research, we also pursue to find key applications of our results to solve real problems. To that, many varied aspects in the biological chemistry field are covered by the different research groups of the department, from purely theoretical approaches, to the development of new synthetic strategies toward the assembly of challenging molecular and supramolecular structures, including the use of state-of-the-art chemical and biocatalytic reactions. The understanding of intermolecular interactions, mainly within the biomolecular field is also a key goal of our department. This fundamental research is supported by the different chemical entities mastered by the scientists belonging to the department, going from peptides, lipids or carbohydrates, to fully synthetic organic molecules or metabolites and nutraceuticals. This has allowed us to find new applications in the fields of biomedicine and medicinal chemistry, such as new bioactive compounds, research and diagnostic tools or potential therapeutic solutions to diseases.

Department Head: - Ignacio Alfonso Rodríguez

Supramolecular Chemistry



The Supramolecular Chemistry group aims to study non-covalent interactions in chemical systems, using these interactions to implement function. We are interested in all topics related to supramolecular chemistry, such as molecular recognition, self-assembling, templated synthesis, molecular motions and dynamic processes. The group specifically works in three main research lines:

1. Molecular recognition of biologically relevant species,
2. Dynamic combinatorial chemistry and systems chemistry,
3. Stereoselective organocatalysis.

Staff

Group leader:
Ignacio Alfonso Rodríguez (IC)

Research staff:
Ciril Jimeno Mollet (CT)
Jordi Solà i Oller (CT)
Àngel Messeguer Peypoch (Ad Honorem)

Postdocs:
Daniel Carbajo López

Predocs:
María Lafuente Fabra
Anna Serra Pont
Lucía Tapia Pérez

Technicians:
Cristian Lastre López

Research projects

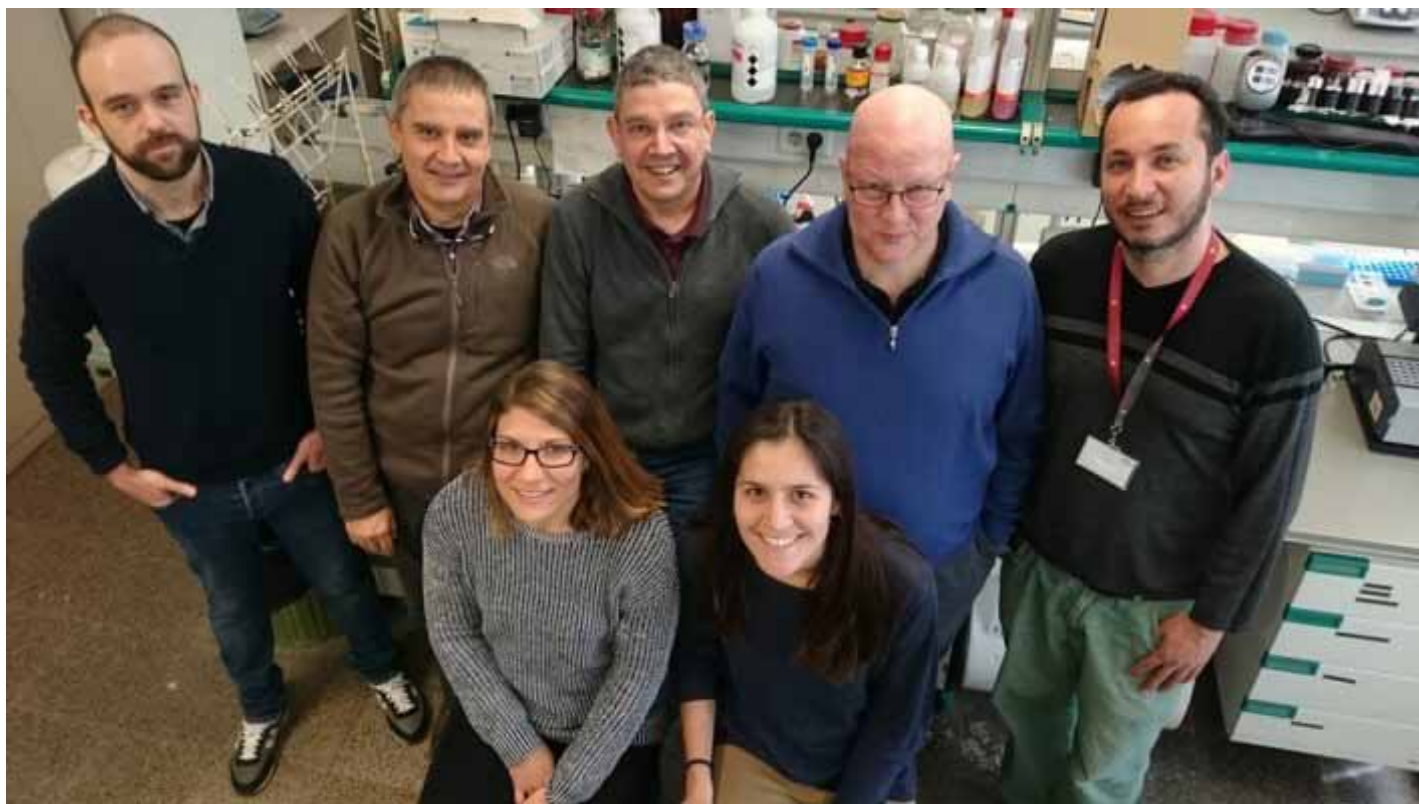
Supramolecular approaches to chemical biology and catalysis: pseudopeptidic receptors, dynamic combinatorial libraries and bio-inspired organocatalysts (SUPRABIOCAT). Ministerio de Economía y Competitividad (CTQ2015-70117-R). 01/01/2016-31/12/2018. 122.210€ + FPI. PI: I. Alfonso, J. Solà.

Supramolecular Chemistry and Catalysis (SUPRACAT). Generalitat de Catalunya, Grupo Pre-Consolidado (2017 SGR 208). 01/01/2018-31/12/2020. 15.000€. PI: I. Alfonso.

Renovación y mejora del espectrómetro de 400 Mhz del servicio de rmn del IQAC-CSIC. Ministerio de Ciencia, Innovación y Universidades (EQC2018-004579-P). 01/01/2018-31/12/2019. 466.773,76€ (25% IQAC, 25% CSIC, 50% FEDER). PI: I. Alfonso.

SUPRAmolecular approaches to FUNctional systems (SupraFUN). Ministerio de Ciencia Innovación y Universidades/ Agencia Estatal de Investigación (RTI2018-096182-B-I00). 01/01/2019-31/12/2021. 142.296€. PI: I. Alfonso, J. Solà.

Biotransformation and Bioactive Molecules



The research of our group is focused on the development and optimization of new and existing biocatalyst for carbon-carbon bond formation (carbolidgases). Carbolidgases have the potential to efficiently access complex molecular scaffolds from simple starting materials, with unparalleled stereoselectivity and without a need for tedious and time-consuming iterative steps for protection and deprotection of sensitive or reactive functional groups.

Three goals are pursued:

1. to develop new cost-efficient and eco-friendly processes for the chemical manufacturing
2. to produce new compounds (i.e. new structure types generating molecular diversity) accessible for investigations in drug discovery
3. to engineer the biocatalyst for improving its substrate tolerance, stereoselectivity, and catalytic properties (i.e. towards non-natural reactions) to broaden its window of applicability.

The research includes computational models for ligand-protein interaction essential for biocatalyst optimization by structure-guided protein engineering.

Staff

Group leader:

Pere Clapés Saborit

Research staff:

Jordi Bujons Vilàs

Jesús Joglar Tamargo

Postdocs:

Karel Hernández Sánchez

Angela Mourelle Insua

Mathias Pickl

Predocs:

Carlos José Moreno Fontalba

Roser Marín Valls

Research projects

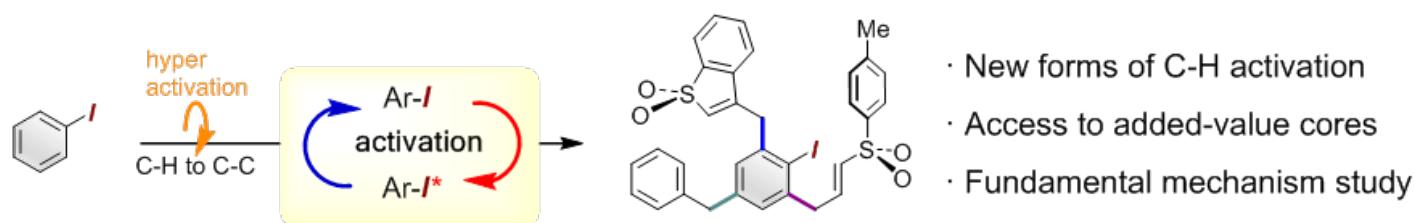
Catalizadores Híbridos Organoenzimáticos. RTI2018-094637-B-I00. Pedro Clapés Saborit (IQAC-CSIC) and Jordi Bujons Vilàs (IQAC-CSIC). Ministerio de Ciencia, Innovación y Universidades. 01/01/2019 - 31/12/2021. 121.000,00€.

Plataforma enzimática para la síntesis de aminoalcoholes y aminoácidos no proteinogénicos quirales (Tralaminol). PCI2018-092937. Pedro Clapés Saborit (IQAC-CSIC). Proyectos de Programación Conjunta Internacional ERA-CoBiotech. Coord: Wolf-Dieter Fessner (Technische Universität Darmstadt, Organic chemistry dept, Germany). Ministerio de Ciencia, Innovación y Universidades. 01/04/2018 - 31/03/2021. 150.000,00€.

Sustainable industrial processes based on a C-C bond-forming enzyme platform. Carbazymes-635595. H2020-BIOTEC-2014-2015/H2020-LEIT-BIO-2014-1. Pedro Clapés Saborit (IQAC-CSIC). Coord: Wolf-Dieter Fessner (TUD). 01/04/2015-31/03/2019. 1.145.190,00€ (IQAC-CSIC).

Desarrollo de biocatalizadores para la formación de enlaces carbono-carbono orientados a transformaciones estratégicas de interés industrial. CTQ2015-63563-R. Pedro Clapés Saborit (IQAC-CSIC) MINECO. 01/01/2016 - 31/12/2018. 100.430,00€

Synthetic Methodology and New Building Blocks



Our group works in the field of synthetic methodology, with emphasis on the development of new oxidative and coupling reactions. The group specializes in the usage of certain highly-reactive molecular entities, including those based on hypervalent iodine, boron and silicon, aiming to explore their reactivity with and without the use of metal catalysts. We are driven both by our curiosity regarding the fundamental properties and reactivity of these species, and by their great synthetic potential for a rapid build-up of complex molecules.

Staff

Group Leader

Alexandr Shafir

Postdoc

Anton Cunillera Martin

Graduate students

Wei Wen Chen

Master Students

Laura Rodríguez

Undergraduates (TFG):

Albert López de Moragas

Oriol Angurell Garreta

Inés Sedó Agustí

Guillem Sanz

Research projects

Main group chemistry: from high energy intermediates to rapid building block assembly. BISI Bonds. Ministerio de Economía Industria y Competitividad: CTQ2017-86936-P. IP: Alexandr Shafir (IQAC) and Ana Belén Cuenca (IQS-URL). 2018 – 2020

Photo:

From the photographic exhibition "There's a light that never goes out".

Author: Silvia Panarello (IQAC)



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Theoretical and Computational Chemistry



The computational and theoretical chemistry group (CTCG) investigates the behavior and properties of molecules in order to understand their reactivity, their dynamics and their function.

We use the methods and tools of the theoretical and computational chemistry to do research in chemical reaction mechanisms biochemistry and biophysics, with special interest in atmospheric chemistry, protein dynamics and enzyme catalysis.

Staff

Group leader.
Dr. Josep M. Anglada Rull

Research staff
Dr. Ramon Crehuet Simon

Master students
Adrià Villacrosa Ribas
Gil Murria Aranda
Pedro Juan Buigues Jorro
Oriol Esquivias Bautista

Research projects

Cloud droplets as atmospheric catalysts: insights from computer simulations. Proyecto internacional de Cooperación científica CNRS – CSIC (Proyecto PIC2015FR1). 01/01/2016 - 31/12/2018. IP: Josep M. Anglada

Proteínas intrínsecamente desordenadas: cerrando la brecha entre simulaciones y experimentos (CTQ2016-78636-P) Ministerio de Economía y Competitividad. 30/12/2016 - 29/12/2020 IP: Ramon Crehuet

Integración de datos de SAXS en simulaciones biomoleculares mediante técnicas de Machine Learning. Salvador de Madariaga, 01/08/2018 - 30/01/2019. IP: Ramon Crehuet

Laboratory of Molecular Biophysics, Ajuts Suport a Grup de recerca consolidats, (2017 SGR 324), 01/01/2018 - 31/12/2020. IP: Xavier Salvatella (IRB-Barcelona).

Plasma Chemistry



Plasma Chemistry Group research is focused on the technological applications of non-thermal plasmas (low and atmospheric pressure). The activity and interest of the group deals with different plasma processes:

- Surface functionalization: tailoring of adhesion and wetting properties.
- Plasma treatment in liquids: elimination of contaminants in wastewater and plasma initiated polymerization for development of stimuli sensitive polymer coatings.
- Plasma sterilization: elimination of spores, fungi, bacteria.
- Plasma in agriculture: modulate seed germination.
- Development of atmospheric plasma configuration for advances technologies: dielectric barrier discharges, jet plasma and surface plasma.
- Laser processing: metallic circuits onto transparent substrates for plasma sources (Surface dielectric barrier discharge plasmas).

Staff

Group leader
Dr. Ricardo Molina Mansilla

Technicians
Alberto Vilchez González

Undergraduate students
Alba Lalueza Sánchez

Research projects

Study of the ageing of polymeric solutions treated with plasma for electrospinning applications. IP: Ricardo Molina, MINECO. 2018.

Nanostructured multilayered architectures for the development of optofluidic responsive devices, smart labels and advanced surface functionalization. IP: Francisco Yubero, Ángel Barranco. MINECO. 2017-2019.

Environmental and process control with responsive devices with nanostructured layers manufactured by innovative vacuum and plasma technologies. IP: Agustín R. González-Elipe, Alberto Palmero. MINECO. 2014-2018.

Contracts

Treatment and characterization of textile materials treated with plasma and polycarboxyl acids. Technology Transfer Contract with a Catalan Technological Center. 2019-2020. 9.000€. IP: Ricardo Molina

Medicinal Chemistry



The group is devoted to the discovery of small molecules with activity on biologically relevant processes, including medicinal chemistry and chemical biology. The research projects are in the borderline between chemistry and biology with the goal to find molecules useful to study basic processes and mechanisms and to develop new therapeutics for diseases. Main research topics include photopharmacology, immunotherapy and chemical methods for native protein labelling.

Besides its basic research activities, the group is actively involved in R+D+i industrial projects concerted with companies working mainly in chemicals, pharmaceuticals, diagnostics, biotechnology and biosciences. The lab is providing research support and chemical expertise and advice to academic groups or companies in custom synthesis, process development, medicinal chemistry and analytical methods development.

Staff

Group leader

Amadeu Llebaria Soldevila

Research staff

Lourdes Muñoz Rubio

Postdocs

Carme Serra Comas

Juanlo Catena Ruiz

Roser Borràs Tuduri

Laia Josa Culleré

Xavier Gregori Durán

Predocs

Alessia Sclaro

Maria Ricart Ortega

Silvia Panarello

Gloria Somalo Barranco

Anna Duran Corbera

Technicians

Teresa Sarrias Solà

Carolina Cera Ribas

Undergraduate students

Gisela Trenchs Mir

Master students

Arnau Rué Casamajó

Carles Martínez Juvés

Research projects

Exploring Pain using Light-controlled ligands for Optical Regulation of Endogenous Receptors (EXPLORER). Agence Nationale de la Recherche (ANR), France. 01/10/2016 - 30/09/2020. ANR-16-CE16-0010.

Photoactivable molecules for the precise regulation of the activity of biological receptors with light. Ministry of Economy, Industry and Competitiveness. 01/01/2018 - 31/12/2020. CTQ2017-89222-R.

Amygdala synaptic neuromodulatory mechanisms and role of mGlu4 in Autism Spectrum Disorder (MAGNOLIA). ERA-NET NEURON JTC 2017 "Synaptic Dysfunction in Disorders of the Central Nervous System"; Ministry of Science, Innovation and Universities. 01/09/2018 - 01/09/2021. PCI2018-093047

Light-regulated drugs to restore sight (DRUG4SIGHT). Health Research 2018 La Caixa Foundation. 01/10/2019 - 01/10/2022. LCF/PR/HR19/52160010.

Contracts

Study of molecules for GPCR receptor switching with light. Research agreement with the Julius-Maximilians-Universität Würzburg (Germany). 2018 - 2021. 228.000€. IP: Amadeu Llebaria.

Dynamics and control of metabotropic glutamate receptor activity for an improved efficacy. Research agreement with the Institut de Génomique Fonctionnelle (IGF-CNRS) (France). 2018 - 2020. 60.000€. IP: Amadeu Llebaria.

Provision of ligand-directed endogenous receptor ligands. Contract with a french bioassays company. 2018 - 2021. 24.484,32€. IP: Amadeu Llebaria.

Design and synthesis of photoswitchable compounds. Research agreement with Purdue University and an International pharmaceutical company. 2019- 2020. 122.822€. IP: Amadeu Llebaria.

Chemical Biology



LIPIDS & PROTEINS. Basic research and novel strategies for the treatment of cancer and neurodegenerative disorders. Our current research deals with the synthesis of molecular probes to explore biological processes with a special focus on lipidated proteins and lipid-protein interactions and the development of methods for protein synthesis and modification.

Staff

Group leader:
Gemma Triola Guillem
Juan Bautista Blanco Canosa

Predocs:
Carla Busquets Cortés
Mireia Quintana Agustí
Ana Bilbao Girona

Undergraduate students:
Alejandro Díaz Moreno
Amin Boulahfa Lamdaghi

Master students:
Iván Sánchez Campillo
Adrià Soler Palazón
Ignasi Villarroya Arenas
Joan Barceló Mir

Research projects

"Estudio de proteínas modificadas lipídicamente: Sonic Hedgehog, LC3 y heterogeneidad lipídica". RTI2018-096323-B-100. Ministerio de Ciencia, Innovación y Universidades. Gemma Triola and Juan B. Blanco. 01/01/2019 - 31/12/2021

Max Planck Partner Group on Chemical Biology
Max Planck Society. Gemma Triola. 01/05/2014-31/04/2019

Intramural CSIC 2018 (OEP2016)

Transautophagy. Unión Europea, Cost Action CA15138. 2016-2019

ERNEST. Unión Europea, Cost Action CA18133. 2019-2023

Synthesis and Biomedical Applications of Peptides (USiBAP)



The overall objectives of the Unit of Synthesis and Biomedical Applications of Peptides (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 peptide inhibitors of viral entrance and fusion**, as new futures of anti-HIV-1 drugs. This approach is of great interest, on the one hand, because they can be applied in combined therapies or when resistance to other antiretroviral drugs is detected; and on the other, since they act before the virus enters the cell, they can have the same potential as the immunity induced by a vaccine: pre-exposure prophylaxis.

USiBAP is also working in designing novel **peptides for the diagnosis and prognosis of rheumatoid arthritis** (RA) containing several post-translational modifications (i.e. citrullination and/or homocitrullination). There is growing interest in improving the precision of the tests for the diagnosis of RA and also for the early differentiation of RA from other rheumatic diseases that affect articulations and connective tissue. As an objective in this line of research, we aim to identify new antigen

peptides, derived from proteins present in rheumatoid synovial fluid in order to thereby identify those patients who require more aggressive therapies right from the moment of diagnosis of the disease. That would allow greater control of the disease and, consequently, less harm to the articulations and a better prognosis.

Finally, another line of research is related with **peptide controlled-release nanosystems for the administration of drugs**. The objective of this line of research includes the development of new systems of administration based on liposomes and nanoparticles that are targeted via the use of peptides.

Staff

Group leader

Isabel Haro Villar

Research staff

María José Gómara Elena
María José Bleda Hernández

Predocs

Cristina García Moreno
Ruth Galindo Camacho

Undergraduate students

Andrea Llaves López (Biology)
Clara Tejada Illa (Biochemistry)
Marc Sibil Giralt (Chemistry)
Martí Recort Fornals (Chemistry)
Blanca Plana Robles (Biology)
Marta Remolà Grabulós (Biotechnology)
Elias Romero Cavagnaro (Chemistry)
Pau Ferrerons Calbet (Chemistry)

Post-graduate students

Teresa Silvestri
Bianca Fiorillo
Antonia Scognamiglio
Sara Miralles Comins (JAE-Intro)

Master students

Pablo Terroba Seara
Lupita Ivonne García Rojas
Cristina Duran Rebenaque

Research projects

Diseño, síntesis y aplicaciones biomédicas de péptidos: inhibidores de entrada del HIV-1 y diagnóstico de la artritis reumatoide. (CTQ2015-63919-R). MINECO/FEDER. CSIC. Dra. Isabel Haro. 2016-2018. 111.320€

Red de Investigación en Inflamación y Enfermedades Reumáticas (RIER). Ministerio de Economía, Industria y Competitividad. Programa Redes Temáticas de Investigación Cooperativa en salud (RETICS). Coord: Dr. Jose L. Pablos (Hospital 12 Octubre), PI: Dr. Juan D. Cañete (particip. I. Haro, M.J. Gómara IQAC-CSIC). 2017-2020. 198.869€ (IDIBAPS/IQAC-CSIC)

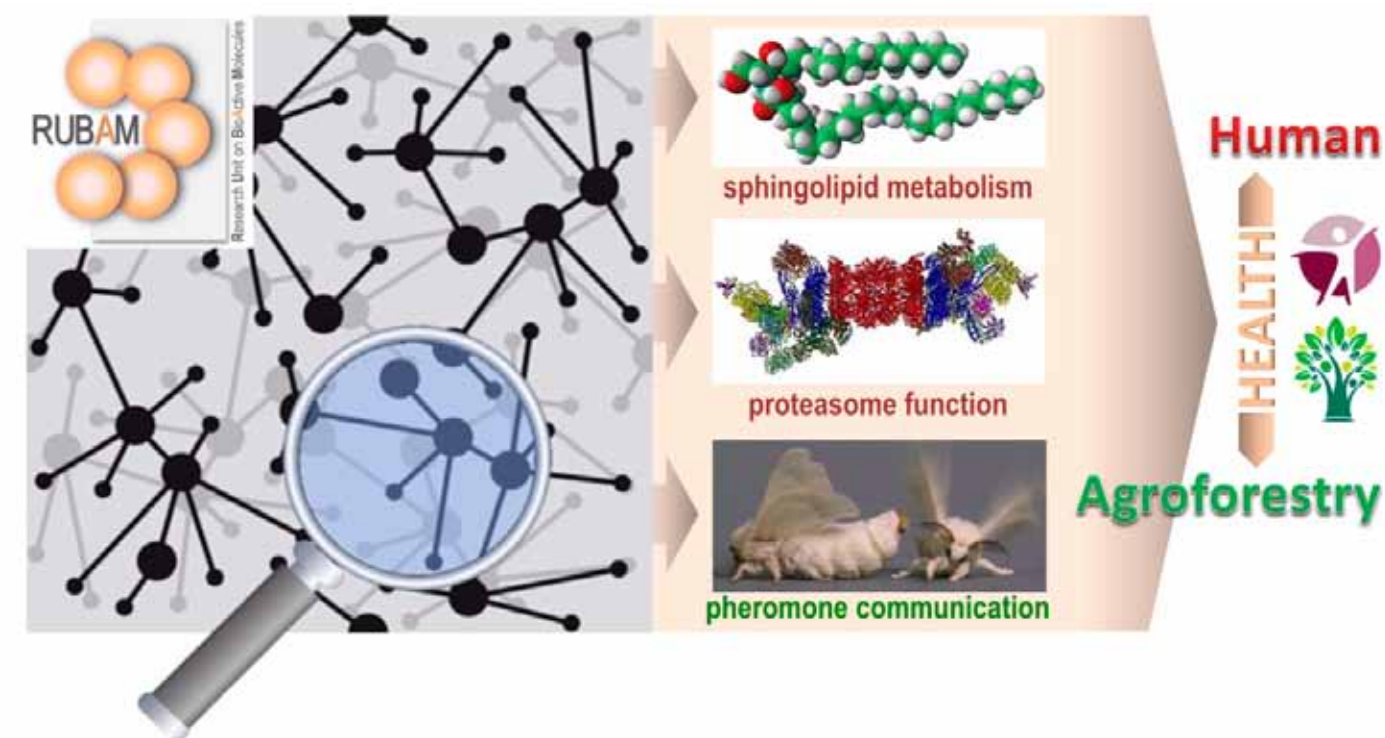
Novel approaches based on synthetic peptides for the diagnosis and treatment of rheumatoid arthritis and for the pre-exposure prophylaxis of HIV-1 infection. RTI2018-094120-B-I00. MINECO/FEDER. CSIC. Coord: Dra. Isabel Haro. 2019-2021. 120.879€

Contracts

Clinical trial: effects of abatacept on the progression to rheumatoid arthritis in patients with palindromic rheumatism. Research agreement with Hospital Clinic de Barcelona and a multinational pharmaceutical company. 2018-2020. 411.016€. IP: Raimon Sanmartí (H. Clinic) and Isabel Haro (IQAC).

Estudio de biomarcadores de respuesta terapéutica al tratamiento con abatacept en pacientes con artritis reumatoide. Research agreement with Hospital Universitario Vall de Hebron. 2019-2020. 25.827,45€. IP: Isabel Haro

Research Unit on BioActive Molecules (RUBAM)



The Research Unit on BioActive Molecules works on the discovery of small molecules with activity on biologically relevant processes, with special interest on those related to human and agroforestry health. Regarding the former, our research lines include the design and development of chemosensors of sphingolipid metabolism to be applied in diagnostics, high throughput library screening (including drug repurposing) and as specific cellular organelle stains. Additionally, manipulation (inhibition or enhancement) of enzymes of sphingolipid metabolism is also addressed with therapeutic purposes. Furthermore, the Unit also aims at the discovery of molecules active on proteasome-mediated degradation processes, with a focus on conceptually novel proteolysis targeting chimeras (Protacs) towards proteins of therapeutic relevance. In the agroforestry field, the Unit works on the development of novel eco-friendly approaches for controlling insect pests of agricultural and forest importance, aiming at those chemical cues involved in intraspecific communication, especially sex pheromones.

Staff

Group leader

Gemma Fabriàs Domingo

Research staff

José Luis Abad Saiz

Josefina Casas Brugulat

Antonio Delgado Cirilo

Carne Quero López

Postdocs

Mireia Casasampere Ferrer

Jose Maria Álvarez Calero

Sergio López Romero

Predocs

Eduard Izquierdo García

Nuria Bielsa Vilardaga

Mazen Aseeri

Technicians

Eva Dalmau Alsina

Alexandre Garcia Barrena

Undergraduate students

Francesc Estrany Castillo

Ignacio Corral Raxach

Miriam González Pérez

Ester Martí Selva

Adriana Muñoz Nebot

Anna Gómez Ballester

Anna Argemí Gil (practicum)

Master students

Alexander Vazquez Pardo

Jon Gil Martínez.

Guillem Pons Barcons

Laura Bassas Serra

Sofía Iglesias Valle

Eleonora Marangio (Erasmus)

Invited researchers

Alican Kurtulus

Research projects

Chemical Probes to Study Sphingolipid Metabolism and Functions: Design, Synthesis, Validation and Applications. José Luis Abad (IQAC), Josefina Casas (IQAC), Antonio Delgado (IQAC), Gemma Fabriàs (IQAC) (IP). Ministerio de Economía Industria y Competitividad: CTQ2017-85378-R. 2018 - 2020

ER stress-mitochondrial cholesterol axis in obesity-associated insulin resistance and comorbidities MitoCholERaxis. José C. Fernández Checa (IIBB) (IP), Carmen García Ruiz (IIBB), Nuria Bielsa (IQAC), Josefina Casas (IQAC), Gemma Fabriàs (IQAC). Fundación BBVA. 2018 - 2021

European Network of Multidisciplinary Research and Translation of Autophagy knowledge. Fina Casas (IQAC), Gemma Fabrias (IQAC). European Union, COST Action. 2016-2020

Knowing the enemy: a mechanistic approach to fight against OPIDN. José Luis Abad (IQAC), Josefina Casas (IQAC), Antonio Delgado (IQAC), Gemma Fabrias (IQAC), Demetrio Raldua, (IDAEA) (IP). North Atlantic Treaty Organization (NATO). 2015 – 2018

CHEMometric and High-Throughput Omics Analytical Methods for Assessment of Global Change Effects on Environmental and Biological Systems. ENTIDAD FINANCIADORA: ERC (advanced grant). Romà Tauler. 01/04/2014 – 31/03/2018.

Estudios dirigidos al conocimiento de la comunicación química en acrídidos-plaga de la Península Ibérica. Posible incidencia en sistemas de control integrado". Carmen Quero, Gloria Rosell, Angel Guerrero Pérez (IP). MINECO (AGL2015-66469-R). 2016-2018

Desarrollo de nuevos métodos de control de plagas de *Leptoglossus occidentalis*. Carmen Quero López. CDTI-MINECO (IDI-20180250). 2018 -2020

Contracts

Obtención de atrayente para el control de moscas de la fruta de la especie *Bactrocera oleae* y Obtención de atrayente para el control de moscas de la fruta de la especie *Rhagoletis cerasi*. Carmen Quero. SEDQ SL. 2013-2018

Treballs dirigits a la caracterització d'extractes feromonal de *Coraeus undatus*, per a la síntesi de feromones de *Matsucoccus feytaudi*, per l'assessorament sobre control integral d'altres plagues forestals i per a la divulgació dels resultats dels treballs realitzats. Angel Guerrero and Carmen Quero. Generalitat de Catalunya. Expedient AG-2017-222. 2017 -2018

Treball tècnic per a la caracterització d'extractes feromonal de *Coraeus undatus*, per a la síntesi de feromones de *Matsucoccus feytaudi*, *Leptoglossus occidentalis*, *Paysandisia archon* i per a l'assessorament sobre control integrat d'altres plagues forestals i per a la divulgació dels resultats dels treballs realitzats. Carmen Quero. Generalitat de Catalunya (Expedient AG-2019-20061). 2019 - 2020

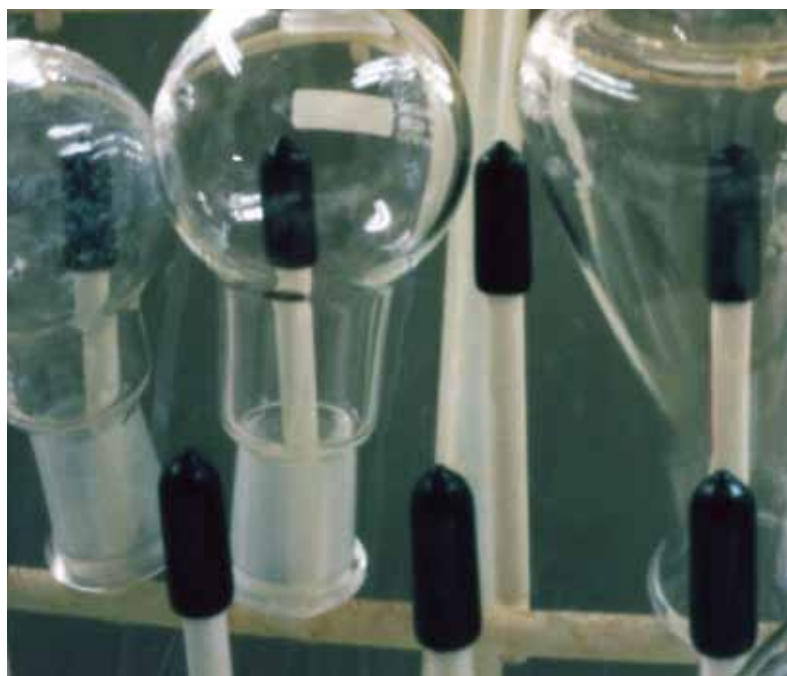




Photo: "Cristalo-mitosis. A new concept". FotoCelDe contest. Author: Cristian Lastre López (IQAC)

Photo: "Glassware". FotoCelDe contest. Author: Jesús Joglar (IQAC)



Nutraceuticals and Free Radicals



Research at NFR involves the thorough evaluation of health promoting agents such as nutraceuticals and functional food components. The nutraceuticals (e.g. antioxidant polyphenols, omega-3 polyunsaturated fatty acids, iminosugars) are natural products obtained either from agricultural and fishery by-products or by environmentally friendly biosynthetic procedures. The group is mainly centered on the prevention of the modern epidemics of obesity and diabetes. We pay particular attention to insulin resistance, low-grade inflammation and oxidative stress, which are factors in the early stages of diabetes. The study of free radicals, their reactivity, their use as probes for antioxidant activity and their control or elimination by nutraceuticals is a central goal of our research. The antioxidant activity is measured by Electron Paramagnetic Resonance spectroscopy with the spin trapping and radical scavenging methodology.

We focus on in vivo studies with rat models of pre-diabetes in which we test combinations of different nutraceuticals that show complementary activities. The study of the relationship between intestinal microbiota, gut integrity and the health status of the host is also a primary goal in our recent studies. Preventive strategies of the future may include the maintenance of a balanced gut microbiota.

Staff

Group leader
Josep Lluís Torres

Research staff
Luis Juliá Bargés
Lluís Fajará Agudo

Postdocs
Sara Ramos Romero

Predocs
Mercè Hereu Planas

Undergraduate students
Alex Guillamón Thiéry
Adriana Alí Cladellas

Master students
Cristina Busquets Roca
Sebastian Robroeks
Roger Barrull Pérez

Research projects

Effect of marine omega 3 PUFA and iminosugars to avert metabolic disorders derived of hypercaloric diets: role of lipid mediators and fagomine. AGL2013-49079-C2-2-R. Ministerio de Economía y Competitividad, Programa de I+D+i orientada a los Retos de la Sociedad. CSIC (IQAC-IIM), Universitat Rovira i Virgili. 01/01/2014-31/12/2018. 220.000€ (IQAC-CSIC). PI: Dr. Josep Lluís Torres. Part.: Luis Juliá, Lluís Fajará, Sara Ramos-Romero, Mercè Hereu.

Functional effect of natural iminosugars on a rat model of diet induced prediabetes. From the mechanism of action to food design. AGL2017-83599-R. Ministerio de Economía, Industria y Competitividad, Programa de I+D+i orientada a los Retos de la Sociedad. CSIC (IQAC-CSIC), Universitat Rovira i Virgili. 01/01/2018-31/12/2020. 187.550€. PI: Dr. Josep Lluís Torres. Part.: Luis Juliá, Lluís Fajará, Sara Ramos-Romero, Mercè Hereu.

Nuevos materiales orgánicos y su uso para la modulación y transformación de la energía. CTQ2015-65770-P. Dirección General de Investigación Científica y Técnica, Ministerio de Economía y Competitividad. CSIC (IQAC-CSIC). 2016-2018. 53.900€. PI: Dolores Velasco Castrillo. Part.: Luis Juliá, Lluís Fajará.

Unit of Glycoconjugate Chemistry



The aim of the Unit is to study biochemical or medicinal chemistry issues by using chemical methodologies. Most frequently used tools are peptide and carbohydrate chemistry, halogenation reactions, aqueous organometallic catalysis and proteomic techniques. Traditional fields of interest are enzyme catalysis, pain and immunity related mechanisms (glycobiology), and drug discovery projects to search for transthyretin amyloidosis inhibitors and more recently, for Alzheimer's Disease (AD) interfering compounds. These activities are carried out in multidisciplinary projects involving computer scientists, biochemical, biological, pharmacological, conformational (NMR), crystallographic and nuclear chemistry groups at national and international level.

Staff

Group leader

Gemma Arsequell Ruiz

Research staff

Gregorio Valencia Parera

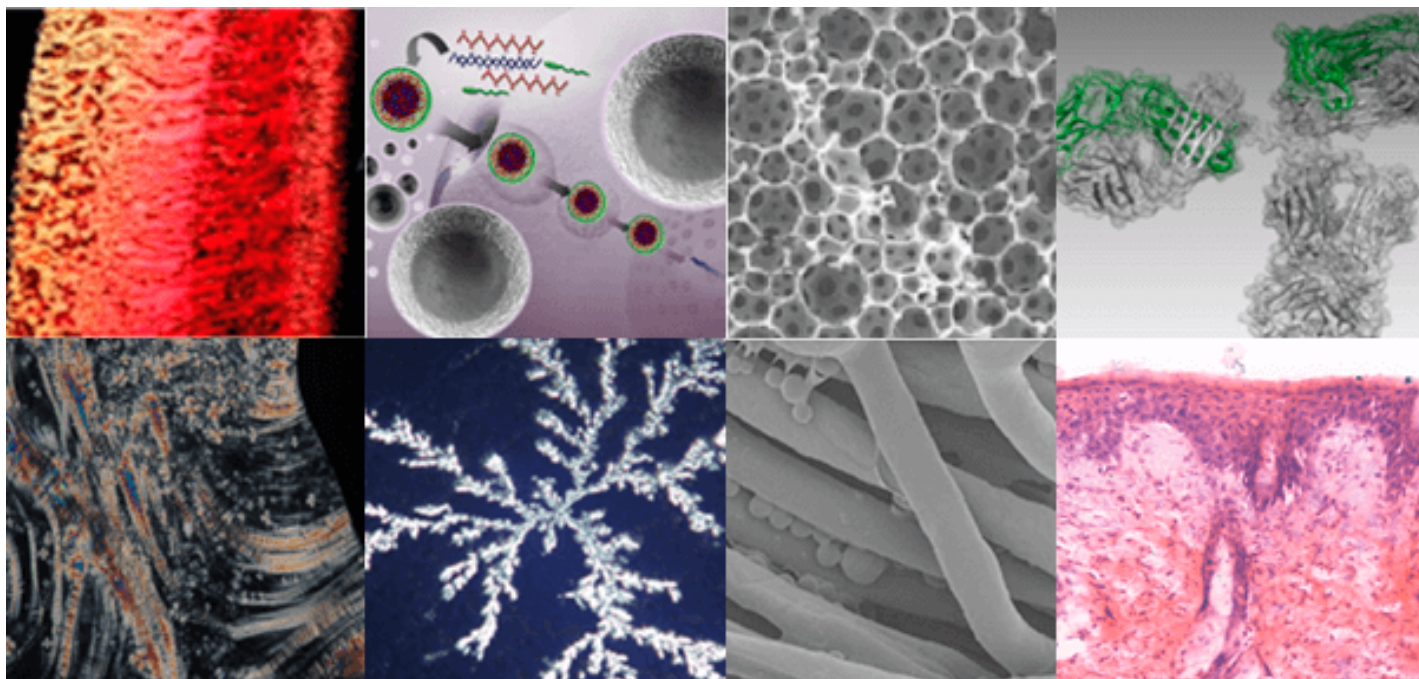
Predocs

Ellen Yadira Cotrina Celis

Research projects

Addition And Substraction Transformations For The Catalytic Valorization Of Unsaturated Systems. Ministerio de Economía, Industria y Competitividad. PLAN NACIONAL CTQ2016-76840-R. PI: José Manuel González Díaz. University of Oviedo. 30/12/2016 - 29/12/2019. Programa estatal de investigación, desarrollo e innovación orientada a los retos de la sociedad. Plan estatal de investigación científica y técnica y de innovación 2013-2016. Call: convocatoria de 2016.

Rational screening programme for stabilising compounds of the transthyretin-A β binding as potential modulating drugs of Alzheimer disease. Fundació Marató de TV3 (2013): Neurodegenerative diseases call. 2015-2017. Extended to June 2019. Dr. Gemma Arsequell Ruiz. IQAC-CSIC. Barcelona.



SURFACTANTS AND NANOBIO TECHNOLOGY DEPARTMENT

RESEARCH GROUPS • Nanobiotechnology for Diagnostics (Nb4D) • Nucleic Acids Chemistry • Colloidal and Interfacial Chemistry • Multivalent Systems for Nanomedicine (MS4N) • Surface Chemistry • Biocompatible Surfactants and Ionic Liquids (BSILs) • Physical Chemistry of Surfactant Systems • Biophysics of Lipids and Interphases (BLI) • Cosmetic and Textile Innovations (CTI) • Sustainable Processes and Materials Characterization (until 02/2019) • Cell Therapy (until 12/2018) •

The research in the Department of Surfactants and Nanobiotechnology (TNT) is devoted to the study of biomolecules, nanomaterials and supramolecular systems, from structural and functional perspectives. Our aim is improve human health, food safety and the environment. Our research focuses on the synthesis, characterization, detection and application of bioactive molecules of high scientific interest (antibodies, oligonucleotides, proteins, lipids, antimicrobial surfactants and ionic liquids), as well as on the preparation of nanostructures and their biofunctionalization. The department's research also focuses on theoretical and practical aspects for the development of chemical products and processes, specifically concerning to the physical-chemistry and biocompatibility of surfactants.

The department has developed expertise on the following fields:

- Design of biosensors based on antibodies as analytical tools for applications in diagnostic, food safety and environment.
- Study of oligonucleotides. Design of new nucleic acid derivatives with structural properties to control gene expression by antisense and RNA interference mechanisms.
- Surfactant and lipid systems based on complex supramolecular nanostructures, application as templates, nanoreactors, delivery systems and membrane models.
- New nanostructured materials with controlled size and morphology, using self-assemblies and colloidal templates.
- Cell therapy treatments, antitumor therapies using stem cells for the local delivery of therapeutic agents.
- Development of multivalent systems for biomedicine and chemical biology. Drug delivery systems for colorectal and triple negative breast cancer and lysosomal diseases. Development on peptide-based targeting moieties.
- Cosmetic and textile application of vehicles to encapsulate active ingredients and promoting their penetration into different substrates.
- Study of lipokeratinic tissues as skin and hair
- Physical chemistry of surfactants and systems based on surfactants and other amphiphilic molecules.
- Development of biocompatible and biodegradable amino acid based surfactants and ionic liquids with antimicrobial and antifungal properties.
- Development and application of clean technologies to achieve sustainable processes in the tanning and textile industries by the application of the statistical modelling to optimize material properties.

The Department integrates consolidated and multidisciplinary research teams, with a proven capacity to secure funds from public organizations and companies. Part of the research groups belong to the Biomedical Research Networking Center in Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), and three of those groups belong to TECNIO, a network of centers for innovation and technological transfer to the industrial sector. Furthermore, the department is also active in generating intellectual property via patents and in creating an Spin-off company.

Department Head: Olga López Serrano

Nucleic Acids Chemistry



Synthetic oligonucleotides are used abundantly in 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 2018-2019 deal with

1. the use of modified oligonucleotides in DNA/RNA therapeutics,
2. the effect of modified nucleosides in the structural and biological properties of oligonucleotides, and
3. the use of modified oligonucleotides in biosensors

Staff

Group leader

Ramon Eritja Casadellà

Research staff

Anna Maria Aviñó Andrés

Santiago Grijalvo Torrijo

Carme Fàbrega Clavería

Postdocs

Adele Alagia

Andreia F. Jorge

Ariadna Lobo Ruiz

Predocs

Anna Clua Villas

Undergraduate students/ Visitors

Laia Oviedo López

Marc Guasch Albanieue

Laura Reyes Fraile

Victor Martínez De Julián

Virginia Martín Nieves

Maria Ortega Lahosa

Ayuda a los grupos de investigación de Catalunya. Grupo de Química de ácidos nucleicos. Comissionat per a Universitats i Recerca. Generalitat de Catalunya (2017SGR114). IP: Ramon Eritja, IQAC-CSIC. 2018-2022.

Desarrollo y validación de nuevos sistemas de administración inteligente de ARNs en la médula espinal lesionada: aplicación en una terapia neuroprotectora basada en miR-138. Junta de Castilla-La Mancha, 2017, SBPLY/17/180501/000376. IP: Manuel Nieto Díaz, Hospital Nacional de parapléjicos SESCAM. R. Eritja. 2018-2021.

Nuevos agentes antifúngicos a base de microRNA a medida para la protección de cultivos. MINECO, Proyectos Explora, BIO2017-92113-EXP. IP: Blanca San Segundo de los Mozos, Centre de recerca en agrigenómica (CRAG), R. Eritja, Consorci CSIC-IRTA-UAB. 2018-2020.

Delivery of antisense RNA therapeutics (DARTER). C.C.E.E. COST Action CA17103. Coordinador: Dr. Virginia Arechavala-Gomez. Biocruces Bizkaia Health Research Institute. 2018-2021.

Monitoring of Acquired Brain Injury and recovery of biomarkers by the combined label-free NanoSensing of multiple circulating molecules (ABISens). Euronanomed-III (ERA-Net cofund action on Nanomedicine), Acción complementaria de Programación Conjunta Internacional (AC18/00046). IP: Laura Lechuga, ICN2-CSIC. 2019-2021.

Research projects

Ácidos Nucleicos sintéticos para aplicaciones biomédicas. MINECO, Plan Nacional Retos de la Sociedad, CTQ2014-52588-R. IP: Ramon Eritja, IQAC-CSIC. 2015-2018.

Nanoestructuras de ADN para transfección celular. MINECO, Explora project, CTQ2014-61758-EXP. IP: Ramon Eritja (IQAC-CSIC). 2015-2018.

Estudio de las estructuras de ADN con potencial biomédico (MEDAS). MINECO, Plan Nacional Retos de la Sociedad, CTQ2017-84415-R. IP: Ramon Eritja (IQAC-CSIC). 2018-2020.

Síntesis de nucleótidos con actividad biomédica. Research agreement with a pharmaceutical Spanish company. 2018. 20.000€. IP: Ramon Eritja.

Contracts

Colloidal and Interfacial Chemistry



Our group is focused on the molecular self-assembly in soft matter as a vehicle for the bottom-up fabrication of nanomaterials, with minimum use of energy. We are interested in nanostructured systems such as surfactants, polymers, micelles, gels, liquid crystals, foams, microemulsions and nano-emulsions; they can find direct applications or be used as templates, structure directing agents or nanoreactors for the synthesis of nanoparticles, nanocomposites or nanoporous solids. Through state-of-the-art techniques, we intend to understand the fundamental mechanisms of aggregation, colloidal forces and interfacial interactions and their impact on material domain size, structure, stability and other properties. We aim to use molecular information and physicochemical parameters to predict, control and program hierarchical self-organization at multiple scales and with increasing complexity, for materials with new or improved properties and applications.

Currently, the main research lines of the group are: (a) Molecular self-assembly of chromonic molecules and their applications in functional materials (b) Formulation of nano-emulsions and derived particles for applications in theranostics. (c) Nanomaterials from bioresources.

Staff

Group leader:

Carlos Rodríguez Abreu

Research staff:

Conxita Solans Marsà

Santiago Grijalvo Torrijo

Postdocs:

Gabriela Calderó Linnhoff

Marta Monge Azemar

Technical staff:

José Antonio Durán

Predocs:

Adrià Pérez Calm

Undergraduate students:

Pol Puigseslloses i Sánchez

Nestor Murciano Durán

Santiago Pons Allés

Santiago Herrera Restrepo

Master students:

Maxime Fruh

Theranostic ultrasound active nanocarriers for the non-invasive drug delivery to brain tumors. Intramural CIBER-BBN. Instituto de Salud Carlos III. Spain. PI: Gabriela Calderó Linnhoff, Carlos Rodríguez-Abreu. 01/01/2018-31/12/2019.

Nanocarriers for of antibiotics against multidrug-resistant microorganisms Intramural CIBER-BBN. Instituto de Salud Carlos III. Spain. PI: Carlos Rodríguez-Abreu. 01/01/2018-31/12/2019

Novel drug delivery system for X-linked adrenoleukodystrophy. Intramural CIBER-BBN. Instituto de Salud Carlos III. Spain. PI: Carlos Rodríguez-Abreu. 01/01/2018-31/12/2019.

Development of targeted nanotherapy against melanoma and HER2 breast cancer. Intramural CIBER-BBN. Instituto de Salud Carlos III. Spain. PI: Carlos Rodríguez-Abreu. 01/01/2018-31/12/2019.

Contracts

Formulation and characterization of personal care products. Contract with a multinational company. 2017-2018. 90.000 €. PI: Carlos Rodríguez.

Formulation and characterization of personal care products. Contract with a multinational company. 2017-2018. 36.800 €. PI: Carlos Rodríguez.

Formulation and characterization of personal care products. Contract with a multinational company. 2018. 40.000 €. PI: Carlos Rodríguez.

Formulation and characterization of personal care products. Contract with a multinational company. 2019. 50.000 €. PI: Carlos Rodríguez.

Research projects

Segregación molecular a múltiples escalas en sistemas no tensioactivos para la obtención de materiales avanzados (CTQ2017-84998-P). MINECO/FEDER. Spain. PI: Jordi Esquena Moret, Carlos Rodríguez-Abreu. 206.910 €. 01/01/2018-31/12/2020.

Celullose-based hybrid nanomaterials for energy applications (I-LINK1188). CSIC. Spain. PI: C.Rodríguez. 20.000 €. 01/01/2018-31/12/2019.

Surface Chemistry



The Research focuses on the formation and characterization of new (nano) structured systems, and evaluate their possible applications in new technological processes. The field of study is systems with presence of interfaces, whether liquid dispersions (emulsions, microgels, etc.), soft materials (hydrogels) or solid porous materials (solid foams). Structured liquid systems obtained by molecular self-aggregation, as well as by molecular segregation processes, are studied, and mainly in the nanometric size range..

The main reasearch lines include:

- Study of the formation and stabilization of new water-in-water (W/W) dispersions.
- Formation and study of hydrogels and microgels, with stimuli-sensitive properties; and
- Preparation and characterization of porous materials with complex textures, for applications as drug delivery devices.

Staff

Group leader:

Jordi Esquena Moret

Research staff:

M. José García Celma (Invited Professor (UB))

Postdocs:

Susana Vílchez Maldonado

Jonathan Miras Hernández

Predocs:

Adrià Pérez Calm

Esteban Figueroa Becerra

Undergraduate students:

Néstor Salinas González

Clara Jaén Flo

Carla Ramírez Ventura

Isaac Expósito Martínez

Oriol Sansalvadó Carbonés

Mathilde Michaux

Master students:

Clara García Vallicrosa

Carmen Hervés Carrete

Jordi Soley Cascales

Katayun Ameli

Research projects

Diseño y aplicaciones de nuevos micro/nanogeles biocompatibles obtenidos mediante métodos de condensación avanzados (MICRONANOGELES) (CTQ2014-52687-C3-1-P). Jordi Esquena Moret. 159.000€. 01/01/2015-31/12/2017, extended to 31/12/2018.

Development of innovative formulations for the delivery of actives in the skin. Spanish Pharmaceutical Company (Industrial Ph.D.). M^a José García-Celma. 71.646€. 11/02/2016-10/02/2019.

Estrategias de formación y estabilización de emulsiones agua-en-agua para aplicaciones farmacéuticas y alimentarias innovadoras (CTQ2016-80645-R) MINECO (Programa Estatal de Investigación, Desarrollo e Innovación orientada a los retos de la Sociedad). Carmen González Azón, M^a José García-Celma. 100.000€. 2017-2019.

Segregación molecular a múltiples escalas en sistemas no tenioactivos para la obtención de materiales avanzados (CTQ2017-84998-P) MINECO/FEDER. Jordi Esquena Moret, Carlos Rodríguez-Abreu. 206.910€. 01/01/2018-31/12/2020

Contracts

Principios activos nanoencapsulados para el acondicionamiento del cabello, la reparación-reconstrucción, el brillo y el mantenimiento del color. Contract with a Spanish cosmetic company. 2017-2020. 82.353€. IP: María José García-Celma.

Obtención de emulsiones estables. Contract with a Spanish cosmetic company. 2018-2019. 21.200 €. IP: Jordi Esquena.

Caracterización de una formulación. Contract with a Spanish pharmaceutical company. 3.000€. 2018. IP: Jordi Esquena.

Comparative study of micellar solutions containing an active agent. Contract with a Spanish pharmaceutical company. 2018. 7.146€. IP: M^a José García-Celma.

Obtención de emulsiones estables. Contract with a Spanish pharmaceutical company. 2019-2020. 27.357€. IP: Jordi Esquena.

Estudio de la obtención de nuevas formulaciones y materiales de polímeros biocompatibles. Contract with a Spanish biomaterials company. 2019-2020. 40.000 €. IP: Jordi Esquena.

Nanobiotechnology for Diagnostics (Nb4D)



The Nanobiotechnology for Diagnostics Group has focused on the development of novel molecular diagnostic tools to provide alternatives to the actual limitations existing in several fields but particularly in the clinical and food safety areas.

Objective: Perform research of excellence addressed at solving specific problems and developing know-how and expertise in basic chemical science and perform research at the chemistry-biology interface.

Our mission is to improve the diagnostic efficiency using technologies based on new micro and nano(bio) technologic approximations that will improve the standard of living of the society.

Our vision is to be an important group, internationally renowned, that contributes with innovative technological alternatives to overtake the actual limitations in the diagnostic field in clinics, food safety and in the environment.

Staff

Group leader

Prof. M. Pilar Marco Colàs

Research staff

Dr. Roger Galve Bosch
Dr. J. Pablo Salvador Vico
Dr. Núria Pascual Duran

Postdocs

Dr. Lluïsa Vilaplana Holgado
Dr. Montse Rodríguez Núñez
Dr. David Santos Álvarez
Dr. Ana Sanchís Villariz

Predocs

Enrique Montagut Cañete
Klaudia Lilla Kopper
Julian Guercetti
Bárbara Rodríguez Urretavizcaya

Technicians

Astrid Garcia Amenos
Melek Denizli
Fabiola Felipe Salmoral
Laia Joval Ramèntol

Administration

Marlene Mendoza Santana

Former members (2018-2019)

Pablo Martínez Valera
Izaskun Miguel García
Camilo Perales
Johanna Scheper
Josefa Cruz Rodríguez
Raheel Ahmad
Susana Otero Fernández
Miriam Corredor Sánchez

Research projects

New diagnostics for infectious diseases. H2020-MSCA-ITN-2015-675412. M.-Pilar Marco (IP). 01/03/2016-29/02/2020

Smartphones analyzers for on-site testing of food quality and safety. 720325. M.-Pilar Marco (IP). 01/01/2017 - 31/12/2020

Ajuda acreditació tecnio pel grup nb4d. TECDTP16-1-0009. M.-Pilar Marco (IP), Miriam Corredor. 02/05/2017 - 02/05/2018

Grupo de Biotecnología para Diagnósticos (Nb4D). 2017 SGR 1441. M.-Pilar Marco (IP). 01/01/2018 - 31/12/2020

Pyocyanin as a new biomarker for diagnosis of pseudomonas aeruginosa infections. M.-Pilar Marco. 20/06/2018 - 31/12/2019

Ajuda acreditació tecnio pel grup nb4d. TECDTP18-1-0011. M.-Pilar Marco (IP). 01/11/2018 - 30/10/2019

Estrategias inmunoquímicas de diagnóstico y terapia en base al quorum sensing. SAF2015-67476-R. M.-Pilar Marco (IP). 01/01/2016 - 30/06/2019

A new approach for the diagnosis of pseudomonas aeruginosa infections. C116-00031. Lluïsa Vilaplana (IP), Miriam Corredor. 01/09/2016 - 31/10/2018

Quorum sensing as potential biomarker targets to diagnose bacterial infections (QS-MOTION). TV32018-201825-30-31. M.-Pilar Marco (IP), M.-Teresa Martín (coord). 01/11/2018 - 30/10/2021

El quorum sensing una alternativa para mejorar la gestión de la fibrosis quística. RTI2018-096278-B-C21. M.-Pilar Marco (IP), J.-Pablo Salvador (co-IP). 01/01/2019 - 31/12/2021

Personalized and/or generalized integrated biomaterial risk assessment. 760921. M.-Pilar Marco (IP). 01/01/2018 - 31/12/2021

Contracts

Desarrollo de un bioensayo para la determinación de betaglicanos. Research and Development contract with an international biotechnological company. 2018. 12950€. IP: M. P. Marco

Amendment to "production of immunoreagents and antibodies". Technological service contract with an international biotechnological company. 2018-2021. 150.000€. IP: M. P. Marco

Design and synthesis of immunoreagents and antibodies for antibiotics detection. Research and Development contract with an international pharmaceutical. 2018-2020. 166.600 €. IP: M. P. Marco

Creación de una plataforma para desarrollo y producción de anticuerpos entre la ae csic y consorcio centro de investigación biomédica en red bioingeniería, biomateriales y nanomedicina (CIBER-BBN). Agreement between CSIC and CIBER. 2018-2022. 10750€. IP: M. P. Marco

Dispositivo sensor basado en inmunocromatografía con medida electroquímica. Research and Development contract with an international biotechnological. 2018-2022. 6.000€. IP: M. P. Marco

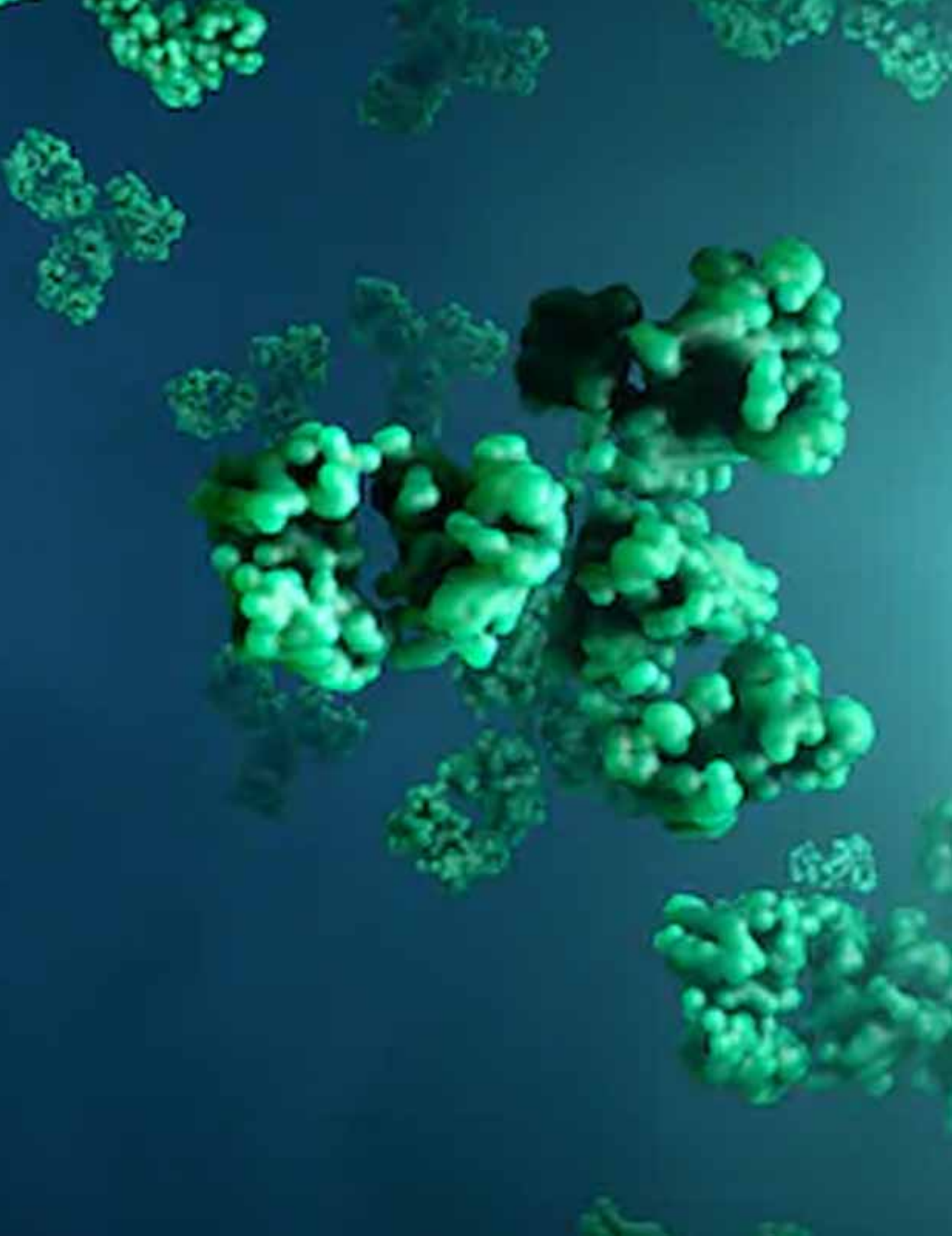
Convenio entre el CSIC y el CIBER. Agreement between CSIC and CIBER . 2018-2022. 20.000€. IP: M. P. Marco

Promoción e impulso de la investigación en el área temática de bioingeniería, biomateriales y nanomedicina - unidad u2 de nanbiosis. Agreement between CSIC and CIBER. 2018-2022. 50.000€. IP: M. P. Marco

Bioconjugate competitors and antibodies for detection of antibiotics. License of biological materials to an international biotechnological company. 2018-2038. 1.297€. IP: M. P. Marco

Síntesis y bioconjugación de haptenos para la obtención de anticuerpos monoclonales como fungicida. Research and Development contract with an international pharmaceutical company. 2018-2020. 65.150 €. IP: M. P. Marco

Development of rat monoclonal antibodies that bind to the murine par2. Contract with a national pharmaceutical. 2019-2020. 15.854 €. IP: M. P. Marco



Multivalent Systems for Nanomedicine (MS4N)



The group of Multivalent Systems for Nanomedicine (MS4N) was installed at the IQAC-CSIC on September 2018. They are devoted to the study of chemical multivalent systems, that are molecules containing multiple functional groups disposed on spatial distributions that are directly associated to their skeleton/scaffold architecture. These functional groups can be modified, in a controlled manner, with diverse biomolecules, drugs or ligands. Due to this versatility, multivalent systems become chemical tools with great potential in areas as chemical biology and nanomedicine, such as drug delivery, diagnosis and biomaterials.

MS4N group explore the use of diverse types of chemical multivalent platforms (oligomers, dendrimers, polymers, micelles and lipid nanovesicles), in:

- the generation of multivalent ligands to study GPCR oligomerization; and
- the development of drug delivery systems for colorectal and breast cancer treatment, protein delivery systems for the treatment of lysosomal diseases and macromolecular compounds that have intrinsically therapeutic properties with application to central nervous system diseases.
- the use of different targeting moieties (peptides, small molecules) or transporters to improve the accumulation of these delivery systems of therapeutic agents on specific cells, tissue or organs, or to facilitate the entry through biological barriers as blood brain barrier.

MS4N group also belongs to the CIBER BBN (CB06/01/0074) a Spanish consortium of the Carlos III Health Institute. The team is also part of a consolidated research group of the Catalan Government (2017SGR1439).

Staff	Research projects
<p>Group leader</p> <p>Miriam Royo Expósito</p>	<p>Multivalent systems for Nanomedicine (MS4N, RTI2018-093831-B-I00). Miriam Royo. Ministerio de Ciencia, Innovación y Universidades, MICINN. 181.500€. 01/01/2019-31/12/2022.</p>
<p>Research staff</p> <p>Daniel Pulido Martínez (Senior CIBER Researcher)</p> <p>Fernando Albericio Palomera (Doctor Vinculado UB)</p> <p>Gerardo Acosta (Senior CIBER Researcher)</p>	<p>Smart multifunctional GLA-nanoformulation for Fabry disease (SMART-4-FABRY. 720942-2). N. Ventosa. European Community Horizon 2020, NMBP-2016-2STAGE-HEALTH. 147.982,7€. 01/01/2017-31/12/2020.</p>
<p>Postdocs</p> <p>Edgar Cristóbal Lecina (CIBER)</p>	<p>Chemical tools to study their interaction with biological barriers and GPCR oligomers" (SAF2014-60138-R). M. Royo. Ministerio de Economía y Competitividad, MINECO. 215.380€. 01/01/2015-30/09/2019.</p>
<p>Master students</p> <p>Raffaella Giordano (Erasmus +)</p>	

Biocompatible Surfactants and Ionic Liquids (BSILs)



The research activities of the BSILs group focuses on the study, design and development of novel biocompatible surfactants and ionic liquids derived from natural amino acids. These compounds are designed according to basic principles of Green Chemistry: Design safe chemicals, use of renewable feedstock, design for energy efficiency, design for biodegradation and, use of waste materials. The new compounds present low toxicity and high biodegradability. Both surfactants and ionic liquids can be applied in a number of industries like food, cosmetics and pharmaceutical industries.

Staff

Group leader:

Aurora Pinazo Gassol

Research staff:

Lourdes Pérez Muñoz

M. Teresa García Ramón

Technicians:

Juan José González Chaparro

Isabel Ribosa Fornoví

Ana de la Fuente Polo

Postdocs:

Fábio Oliveira de Sousa

Predocs:

Anderson do Santos

Zacarias Hafidi

Undergraduate students:

Maria Fernanda Esponda Fontoura

Nuria Agustí Font

Judit Ruiz Ibáñez

Carla Hidalgo Navarro

Master students:

Inés Terrones Fernández

Marina Gual Fornés

Paula Victoria Tysko Gonzales

Albert Carcereny Sánchez

Training students:

Ana Paola García

Visiting Professors:

Susana Morcelle

Research projects

Lourdes Pérez and M. Teresa García. Biocompatible lipoaminoacids and ionic liquids for the development of new strategies of antimicrobial control and biofilm removal. Ministry of Science, Innovation and Universities. Plan Estatal de Investigación Científica y Técnica. 2017-2020

Lourdes Pérez. Biodegradable bis-esterQuats and bis-amideQuats to be used as antimicrobial and anticorrosive compounds. COOPA20264 dentro del Programa I-COOP+ 2018, CSIC, 2019-2020

Physical Chemistry of Surfactant Systems



The general subject of the research is the physical chemistry of systems based on surfactants. This subject lies within the framework of colloids and nanotechnology in its bottom-up approach and is closely related to Soft Matter. We focus on new surfactants' phase behavior, in particular, those derived from biocompatible natural products, dynamics of transformation (emulsification and solubilisation) and the use of them as templates for other uses (drug delivery and synthesis of materials).

The characterization of stable and unstable structures allows for the exploration of applications of simple water-surfactant systems and their complexes with biological molecules or with inorganic molecules. The main techniques are SAXS-WAXS, light scattering, tensiometry, conductivity and selective electrode.

Staff

Group leader

Ramon Pons Pons

Predocs

César González Griñán

Technicians

Jaume Caelles Balcells

Imma Carrera Altarriba

Research projects

Lipoaminoácidos y líquidos iónicos biocompatibles para el desarrollo de nuevas estrategias de control antimicrobiano y eliminación de biofilms. Entidad financiadora: MINECO- CTQ2017-88948-P. IQAC, 1-1-2018 - 31-12-2020. Lourdes Pérez and M.T. García. 145.200€

Contracts

Optimización de parámetros para la fabricación de espuma de Polidocanol. Contract with a Spanish company of Medical devices. 2018. IP: Ramon Pons

Biophysics of Lipids and Interphases (BLI)



The scientific proposals of BLI group consider biophysical, biochemical, physical-chemical and technological aspects applied to certain biological substrates with strong lipid involvement and focused on applications for the improvement of health. Our research is based on the study of colloidal systems in which lipids and other amphiphiles have a major role, liposomes, micelles, bicelles and bicosomes. We also are focused on the study of complex biological tissues and membranes such as skin and more recently mucous membranes and tissue of the central nervous system. In addition, we have addressed the knowledge and adaptation of high resolution technologies to apply them properly in the study of both colloidal systems and biological tissues. During the last years we have started a task focused on business development, participating in the foundation of the start-up company Bicosome S.L. with the aim of bringing knowledge and scientific results to the industrial field.

In general, our scientific objectives are the following:

- Study of the phase behavior of lipid aggregates.
- Design, preparation, physical-chemical characterization of nanostructured lipid systems.
- Use of nanostructured lipid systems for biomedical applications: membrane models, skin, mucosa, blood brain barrier.
- Study of the microstructure, composition and functions of the skin tissue.
- Use of lipid systems to improve angiogenic therapies.
- Application of synchrotron radiation in the study of biological materials: peptides and proteins, membrane models, skin, among others.

Our studies allows us to propose research lines that are based on basic research topics oriented to the health field with a tendency to technological innovation and looking for industrial potential.

Staff

Group leader:

Olga López Serrano

Postdocs:

Mercedes Cócera Núñez

Estitxu Fernández Pinto

Predocs:

Verónica Moner del Moral

Kirian Talló Domínguez

Daniela Vergara

Undergraduate students:

Sophia Kioulaphides

Sarah Dohadwala

José Luis Maquilón

Wissam M'Rabet Driss Boulden

Research projects

Investigation of angiogenic therapies based on tissular factor (RTC-2016-4957-1), IP: Olga Lopez, 105.812 Eurs, Retos –Colaboración, Ministerio de Economía y Competitividad. 2016-2019.

Advanced lipid nanostructures to overcome blood-brain-barrier, IP: Olga Lopez, 15.000 Eurs, "La Caixa" Foundation Research Strategy. 2018-2020.

Elucidating self-assembly organization of a new lipid hydrogel using SAXS/WAXS: effect of pH, temperature and ionic strength (2019023392). CSIC, Synchrotron ALBA, Total amount: 6 shift. 2019.

Contracts

Optimization of bicosomes containing active principles from microalgae. Contract with a Spanish biotechnological company in the framework of the Dimaskin European Project. 2018-2019. 21.000 €. IP: Olga López.

Characterization of lipid systems with astaxantine and omega 3 fatty acids and their interaction with skin. Contract with a Spanish biotechnological company in the framework of the Vopsa 2.0 European Project. 2018-2019. 14.000€. IP: Olga López

Cosmetic and Textile Innovations (CTI)



The main scientific activity of this group focuses on the study of cosmetic and textile application of vehicles, able to encapsulate active principles. These lipid structures, such as liposomes, microspheres, etc., modulate the penetration of the actives in the different substrates. The effectiveness of the topical application on skin or hair to improve the hydration and skin barrier function, lipid peroxidation, etc. is evaluated. Percutaneous absorption profile of these formulations after being applied directly to the skin or through biofunctional textiles are also being studied.

The basic knowledge of hydrophilic-lipophilic balance of lipid-proteinaceous keratin systems, such as wool, human hair and stratum corneum of human skin is also being explored. This knowledge is essential to design formulations for industrial application in the textile, cosmetic and dermatopharmaceutical fields.

Development of sustainable processes seeking the substitution of products harmful to health and the environment with other harmless and ecologically sustainable products in obtaining new materials, DWOR (water and oil repellents) FR (flame retardants), etc..

Characterization of the structure and properties of textile materials and new materials, in particular thermal, mechanical properties, viscoelastic behavior and relaxation is also a main objective of our group.

Staff

Group leader:

Prof. M^a Luisa Coderch Negra

Research staff:

Dr. Albert M Manich Bou

Postdocs:

Dr. Cristina Alonso Merino

Dr. Clara Barba Albanell

Predocs:

Victor Carrer Vives

Marc Oliver Nicolau

Asma Fraj

Abir Zouari

Technicians:

Dr. Meritxell Martí Gelabert

Isabel Yuste Hernández

Joan Lloria Tolrà

Undergraduate students

Blanca Suarez

Andrea Prieto

Sandra Llamas

Master students:

Beatriz Guzmán Monreal

Research projects

Mitigation of environmental impact caused by Flame Retardant textile finishing chemicals. LIFE-FLAREX. Life 16 ENV/ES/000374 E.U. June 2017-June 2020. L. Coderch. 94.835€ (EU Contribution 56.901€)

Tejidos Biofuncionales con fines cosmético-dermatológicos. CTQ2018-094014-B-I00. MICIU. January 2019 - December 2021. L. Coderch. 145.200€

Sustainable Processes and Materials Characterization



The analysis of future trends in leather production emphasizes the introduction of cleaner leather processing technologies. One of the expected results includes avoiding the presence in the leather of substances from the Restricted Substances Lists (RSL) due to its proven impact on human health and ecosystems as well as its use in leather processing. Due to its carcinogenic character, formaldehyde is one of these substances and its presence in leather should be avoided or kept below allowable limits

From February 2019, after retirement of the Group Leader Dr. Agustí Marsal, the remaining members of the Group have been incorporated to the Cosmetic and textile innovations.

Staff

Group Leader

Agustí Marsal Monge

Research Staff

Albert Maria Manich Bou

Postdocs

Sara Cuadros Domènech

Technicians

Joan Lloria Tolrà

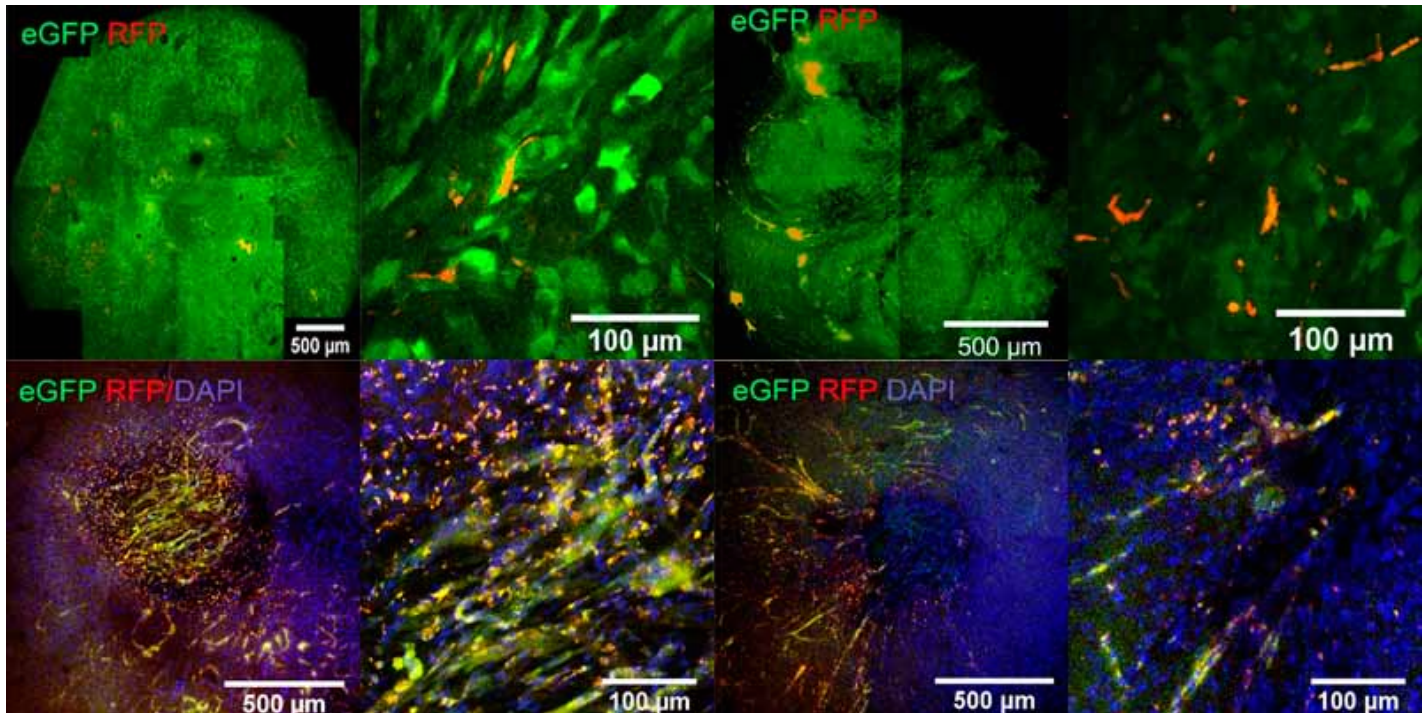
Research project

Mitigation of environmental impact caused by DWOR textile finishing chemicals studying their non-toxic alternatives (MIDWOR). LIFE14 ENV/ES/000670. AM Manich. 01/10/2015-30/09/2018. 64.992€

Obtención y ennoblecimiento de cáñamo para substratos textiles. MAT 2016-79352-R. C Cayuela. 30/12/2016 - 29/12/2020. 90.750€

Mitigation of environmental impact caused by Flame Retardant textile finishing chemicals (LIFE-FLAREX). LIFE16 ENV/ES/000374. L Coderch. 01/07/2017-30/06/2020. 56.901€

Cell Therapy



The Cell Therapy group was interested in two related applied-research fields: regenerative medicine and tumor therapy. In the first case, the objective was the analysis of cell behavior in biomaterials used as scaffolds for tissue repair. In the second case, the objective was to develop antitumor therapies using stem cells as vehicles for the local delivery of therapeutic agents and the study of therapeutic-cell tumor interactions. However, both, the procedures and models developed also allowed more general analysis of tumor response to chemical and biological agents.

For these studies the group used mesenchymal stromal cells from adipose tissue. This special stem cell type capable of producing multiple chemokines and growth factors is a very promising therapy agent, not only due to its elevated capacity for multi-lineage differentiation (tissue repair applications) and tumor homing (therapy), but also for its abundance and easy generation from human adipose tissue.

This group was active until the end of 2018, when the group's leader, Dr. Jerónimo Blanco (Ad Honorem), retired.

Staff

Group Leader

Jerónimo Blanco Fernández

Postdocs

Nuria Rubio Vidal

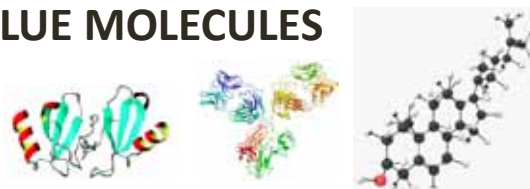
Marta Guerra Rebollo

Cristina Garrido López

TECHNOLOGICAL PLATFORMS

SMALL MOLECULES AND BIOMOLECULES PRODUCTION

- SYNTHESIS OF HIGH ADDED VALUE MOLECULES
- SYNTHESIS OF PEPTIDES UNIT
- CUSTOM ANTIBODY SERVICE



INSTRUMENTAL ANALYSIS AND CHARACTERIZATION OF MOLECULES AND MATERIALS

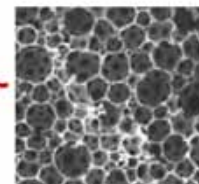
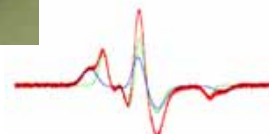
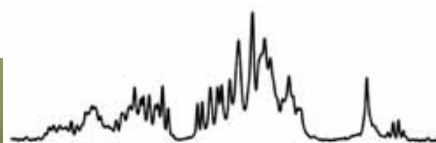
● SPECTROSCOPY

NMR

EPR

SAXS/WAXS

FTIR-UV



● MASS SPECTROMETRY

● MICROANALYSIS

● THERMAL ANALYSIS AND CALORIMETRY

● CHARACTERIZATION OF COLOIDAL DISPERSIONS

BIOMEDICAL AND ENVIRONMENTAL ASSESSMENT

- DERMOCOSMETIC ASSESSMENT
- OMICS & MS-IMAGING
- BIODEGRADATION & ECOTOXICITY
- CELL CULTURE FACILITY (CID)
- ANIMAL FACILITY (CID)



SMALL MOLECULES AND BIOMOLECULES PRODUCTION

This platform is dedicated to the production of small molecules, peptides and antibodies through 3 different facilities:

- Synthesis of High Added Value Molecules
- Custom Antibody Service (CAbS)
- Synthesis of Peptides Unit

Synthesis of High Added Value Molecules

SIMchem is a service created in 2009 to provide chemical and synthetic support to R+D+i activities in industry, university and public organizations. It is aimed at filling the gap between custom synthesis performed by companies and the synthetic research groups in academy. The service is intended to provide 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 synthetic and analytical expertise of the group members.

Services available

- **Synthetic projects and services**

SIMChem offers chemical services to the chemical and pharmaceutical sectors through projects personalized and adapted to any requirement, including development projects and route design. Projects can be defined in a time or target basis.

The fully equipped laboratories designed for chemical synthesis, the skilled staff, and access to spectroscopic and chromatographic techniques required for the purification and characterization of the products guarantee a satisfactory result.

- **Analytical projects and services**

Accurate chemical analyses are crucial for the successful development of R+D projects and for the correct characterization of products. Most of the instruments available can be used in a self-service manner or with personalized support. Furthermore, the analytical personnel together with the broad instrumentation allows an efficient development of analytical projects under request. The analytical techniques available include: HPLC (analytical and preparative scale); HPLC-MS/MS; GC and GC-MS, with a large assortment of HPLC columns (direct/reverse phase, ionic exchange, preparative, chiral and UPLC columns) and detectors.

- **Photopharmacology projects and services**

The photopharmacology laboratory allows to carry out the photocharacterization of compounds, studies about pharmacodynamic and pharmacokinetic properties, in vitro functional and binding assays, fluorescence, absorbance, alfa-screen and luminiscence measurements, among others. This laboratory is divided into two separated areas to perform experiments under light or dark conditions without interferences.

Staff

Amadeu Llebaria Soldevila (Scientific Director)

Carme Serra Comas (Technical Director)

Lourdes Muñoz Rubio (Specialist Technician)

Teresa Sarrias Solà (Technician)

Custom Antibody Service (CAbS)

Short description: The Custom Antibody Service (CAbS), is a service located at the Institute of Advanced Chemistry of Catalonia IQAC- CSIC (group NB4D) that belongs to CIBER-BBN. CAbS is part of NANBIOSIS ICTS (infrastructure of production and characterization of nanomaterials, biomaterials and biomedical systems). 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. Detailed description of the services and features provided by CAbS:

Services available

A) Monoclonal antibody development: Custom monoclonal antibody development from mice or rats. We can adapt our protocols for the user special needs. This includes immunization protocols and screening conditions. The service includes:

1. Discussion of the project
2. Immunization: We immunize BALB/c mice or Wistar rat. The animal with the best immune response receives a final immunization to boost the antibody producing cells.
3. Cell fusion, screening and cloning: The spleen cells are isolated for direct fusion with immortal myeloma cell lines. After fusion, screening of the hybridoma supernatants will be performed by ELISA. We perform subcloning with the limited-dilution method, which ensures that the clone is truly monoclonal and improves the long-term stability. Positive clones are grown and screened for stability and antigen specificity. Screening against multiple antigens (positive and negative screening) is available. The best clones are isolated and cryoconserved.

B) Polyclonal antibody development: Polyclonal antibodies are raised in rabbits, mice and rats. The service includes:

1. Discussion of the details of the project
2. Immunization protocol: As accorded by the customer.
3. Isolation of the antiserum and ELISA testing of serum.

C) Additional services:

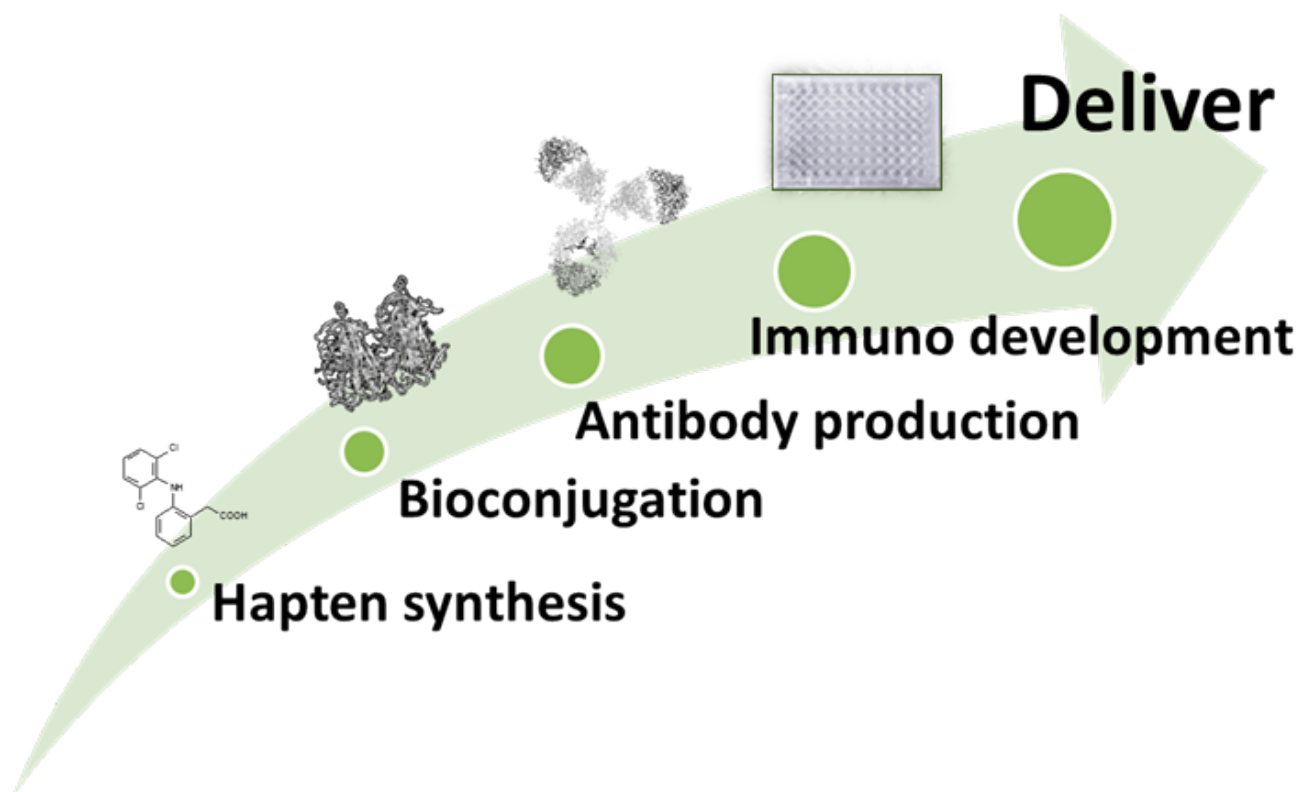
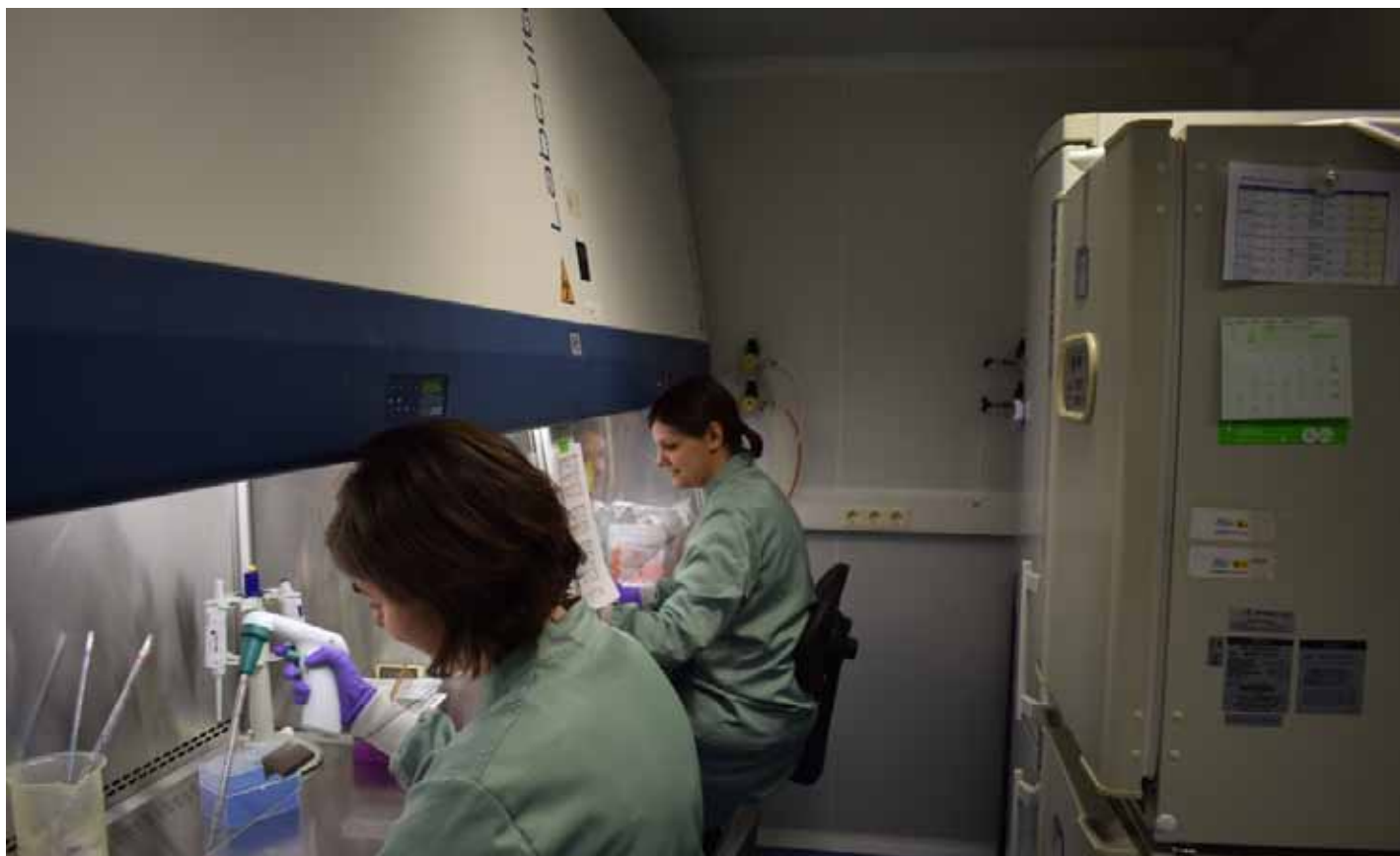
1. Preparation of bioconjugates: labelled antibodies, haptened proteins and enzymes, biotinylated and fluorescent probes, gold nanoparticle conjugates, etc.
2. Antibody production from hybridoma cell lines
3. Antibody purification from serum, and culture supernatants
4. Development of immunochemical methods: ELISA, immunoaffinity columns, etc.
5. Antibody characterization (isotyping).
6. Hybridoma cryopreservation.
7. Mycoplasma testing

Staff

M^a Pilar Marco Colás (Scientific director)
Nuria Pascual Duran (Scientific coordinator)

Technicians

Astrid Garcia Amenos
Melek Denizli
Fabiola Felipe Salmoral
Laia Joval Ramèntol



Synthesis of Peptides Unit

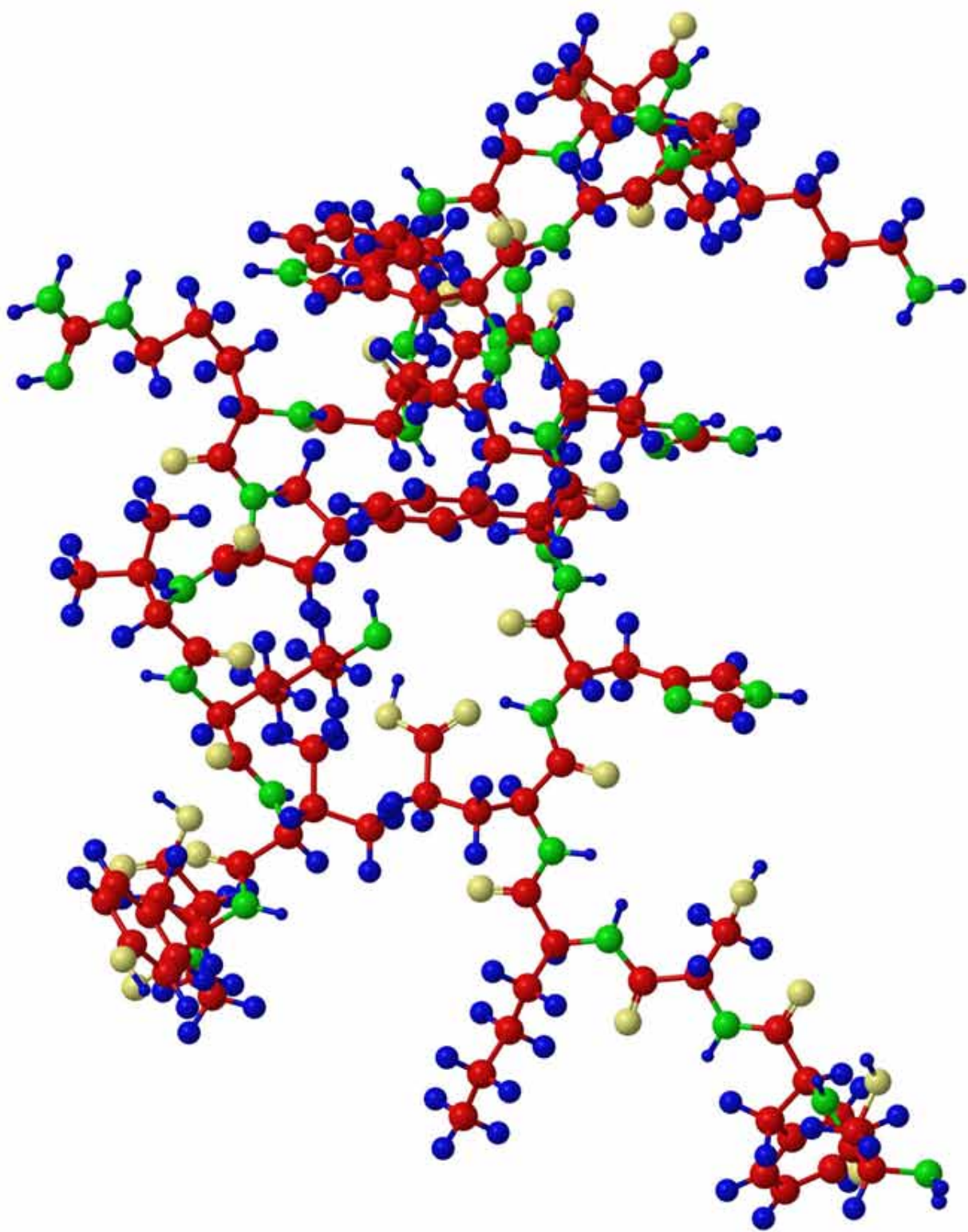
The Peptide Synthesis Unit provides services of synthesis of peptides, at different scales (mg to g) with different degrees of purity, fully characterized (HPLC and HPLC-MS) and was installed at the IQAC-CSIC at the beginning of 2019. The unit performs the synthesis of linear, branched (multivalent) and different types of cyclic peptides (disulfide, lactone, lactam, C-C bridges, stapled peptides). They also offer post-synthesis modification services as conjugation to proteins, fluorescent probes or other compounds. This Peptide Synthesis Unit (U3), is also part of the platform of Biomolecules production of NANBIOSIS-CIBERBBN, a Spanish ICTS dedicated to production and characterization of nanomaterials (<https://www.nanbiosis.es/portfolio/u3-synthesis-of-peptides-unit/>).

This unit is equipped with an automated peptide synthesis for large scale (grams) and analytical HPLC-PDA and HPLC-PDA-UV instruments for peptide characterization. The laboratory is fully equipped to perform manual solid -phase peptide synthesis and post-synthesis modifications. The unit has also access to preparative HPLC for peptide purification and lyophilization systems. This facility benefits from the wide experience of the group of Multivalent Systems for Nanomedicine (MS4N) on design and synthesis of different types of peptides and their modification to be introduced into nanaconjugates and other molecules.



Staff

Miriam Royo Expósito (Scientific & Technical Director)
Gerardo Alexis Acosta Crespo





INSTRUMENTAL ANALYSIS AND CHARACTERIZATION OF MOLECULES AND MATERIALS

This is a largest IQAC platform and it includes to most costly instruments of the Institute. It is devoted to the full characterization and quality control of molecules and materials, which is instrumental in our research programmes in order to guarantee that high quality chemicals are provided to the various users for different applications. The platform includes the following facilities:

- Spectroscopy
- Mass Spectrometry
- Thermal Analysis and Calorimetry
- Microanalysis
- Characterization of Colloidal Dispersions

Spectroscopy

The Spectroscopy Unit includes the following facilities:

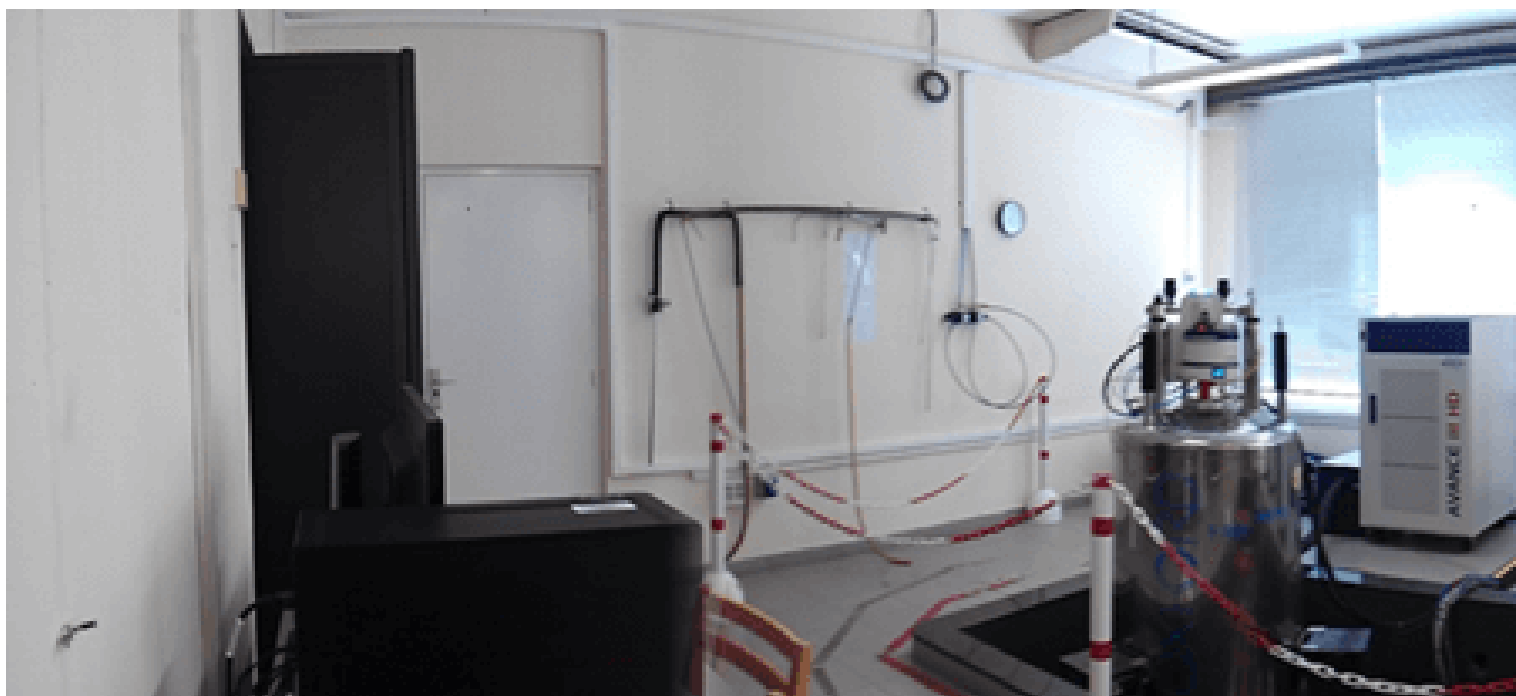
- Nuclear Magnetic Resonance (NMR)
- Electron Paramagnetic Resonance Spectroscopy (EPR)
- Small and Wide Angle X Ray Scattering Service (SAXS-WAXS)
- Small Instrumentation (UV-Vis, FT-IR)

Staff

Dr. Yolanda Pérez Ruiz, PhD (NMR Facility Manager)
Dr. Ramon Pons Pons (Scientific Supervisor, SAXS-WAXS)
Lluís Fajará Agudo (EPR Facility Manager)
Dr. Ricardo Molina Mansilla (Scientific Director, FTIR and UV-Vis)
Naiara Solozábal Mirón, MSc (NMR Facility Technician)
Jaume Caelles Balcells (SAXS-WAXS Technician)
Alberto Vilchez (EPR, FTIR and UV-Vis Technician)

Nuclear Magnetic Resonance (NMR)

Photo: IQAC Nuclear Magnetic Resonance Spectroscopy Facility. Author: Naiara Solozábal Mirón (IQAC)



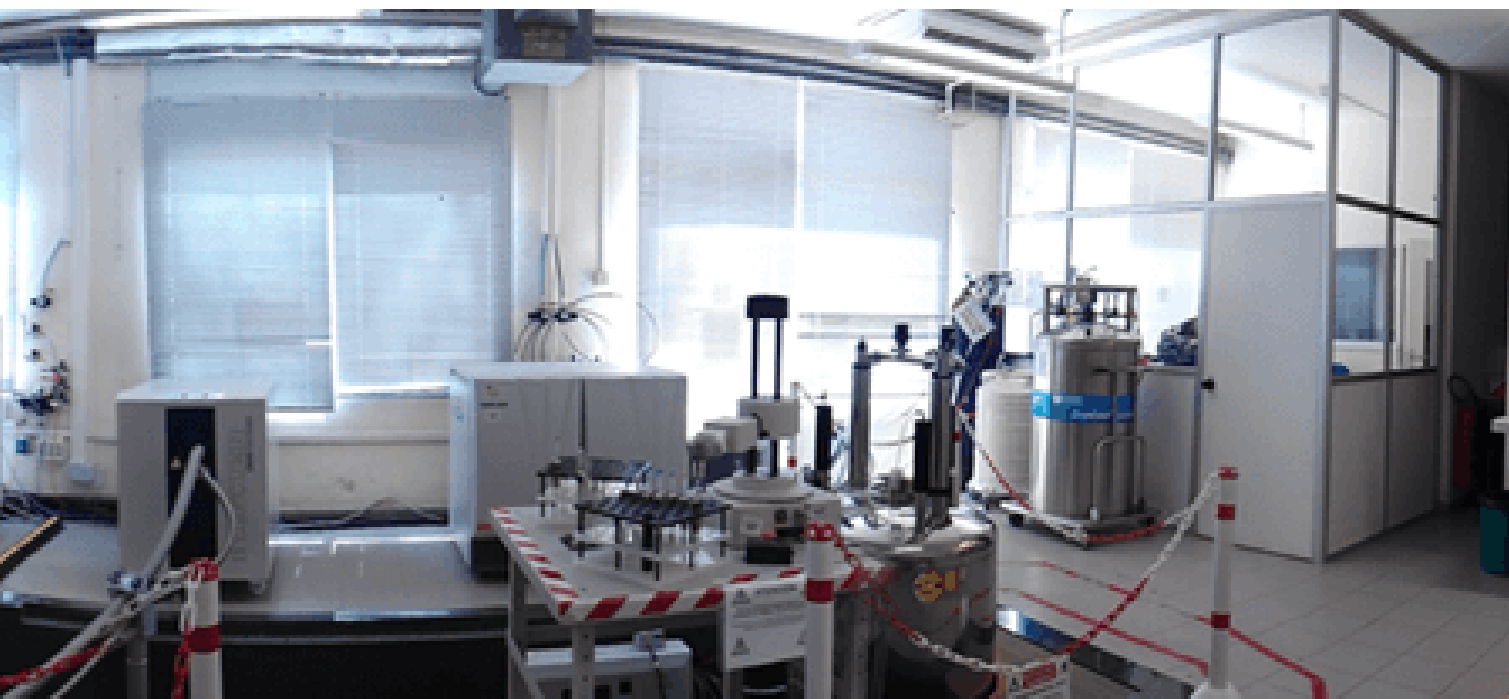
INSTRUMENTAL ANALYSIS AND CHARACTERIZATION OF MOLECULES AND MATERIALS

The Nuclear Magnetic Resonance Spectroscopy service is a research support facility for the IQAC, other universities and public research organisms, as well as for private companies. The NMR Facility provides access to the following state-of-the-art methodologies:

- Structure elucidation and quality control in synthetic chemistry by solution 1D/2D-NMR.
- NMR-based drug screening.
- NMR spectra of cells, cell extracts, and metabolomics-by-NMR.
- Diffusion experiments and DOSY.
- Double/Triple resonance experiments for peptides/small proteins.

The available equipment includes:

- Software licenses: NUS, Dynamics Center, AMIX and BBioRefCODE (metabonomics database; currently 350 metabolites).
- 2 NMR spectrometers
- 500 MHz (11.7 T) NMR Bruker spectrometer with a TCI-cryoprobe (originally Agilent, magnet from 2001, console upgraded and cryoprobe installation in december-2015). TCI cryoprobe Inverse Triple Resonance/Z PFG with three channels $^1\text{H}/^{13}\text{C}/^{15}\text{N}$, working temperature 5-45°C and ^1H sensitivity 5804:1/ ^{13}C sensitivity 932:1.
- 400 MHz (9.4 T) NMR Agilent spectrometer with a One-NMR probe (magnet from 2001, console upgraded in 2010). Room temperature two channel probe/Z PFG (^1H or ^{19}F)/X, tunable to X nuclei from ^{15}N (40,5 MHz) to ^{31}P (161,9 MHz), working temperature 25°C, ^1H sensitivity 480:1/ ^{13}C sensitivity 225:1.
- Auxiliary Equipment
 - UPSs for both spectrometers
 - Oil-free air compressor and air dryer
 - Small equipment for sample preparation: analytical balance, centrifuge, vortex ...
 - Data Server for NMR data transfer to users computers



Electron Paramagnetic Resonance Spectroscopy (EPR)

The Electron Paramagnetic Resonance Spectroscopy (EPR) or electron spin resonance (ESR) allows detecting and studying stable or transient paramagnetic species such as free radicals, some transition metal ions and defects in materials in a wide range of temperatures. This EPR crosses several disciplines including: chemistry, physics, biology, materials science and medical science. The free radicals are often short-lived, but still play crucial roles in many processes such as photosynthesis, oxidation, catalysis, and polymerization reactions. The electron paramagnetic resonance studies the interaction of a paramagnetic species with the electromagnetic radiation (microwave radiation) in the presence of an external magnetic field. It detects and measures the transition between energy levels of the two orientations of the spin-electron. The spectrometer records the net absorption energy of this transition. An EPR spectrum can provide the following information: Unequivocal detection of paramagnetic species, species identification, distinction between free radicals and paramagnetic transition metals, detection of free radicals of short half-life (spin trapping), quantified information on the 'geometric and electronic structure, etc... Spectra can be acquired from solid powder, tissues or solutions at temperatures between 4 K and above room temperature

Small and Wide Angle X Ray Scattering Service (SAXS-WAXS)

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

The following services are available:

- SAXS measurement with lineal collimation
- SAXS measurement with point collimation
- GISAXS measurements
- Use of 2D detector (CCD camera) in SAXS instrument

Small Instrumentation (UV-Vis, FT-IR)

The Infrared and ultraviolet-visible spectroscopy laboratory focuses in recent years on the qualitative and quantitative characterization of materials and chemical compounds. It is worth highlighting the use of infrared spectroscopy for the characterization of polymeric nanoparticles, coatings in textile materials, advanced polymeric films, liposomes or chemicals in solution and degradation kinetics of chemical or radical compounds. The laboratory is equipped with a middle infrared spectrophotometer (FTIR Avatar 360) with different accessories in order to perform analysis of liquids, films, textile materials and/or powdered substrates. In this way, transmission measurements of chemical and pharmaceutical products can be performed in KBr pellets or over NaCl crystals. The service is also equipped with attenuated total reflectance (ATR) accessories in order to analyze solid, powdered or films (diamond ATR, vertical and horizontal ZnSe ATR) and liquids (horizontal ATR tray). On the other hand the service is equipped with and UV-Visible Cary 400 spectrophotometer (175-900 nm) in order to perform characterization, quantitative analysis and reactions kinetics or chemical compounds.



Mass Spectrometry

The IQAC Mass Spectrometry Service was created to support IQAC research groups as well as other CSIC institutes, University, Public Organizations and Industry. The service is focused in the analysis of a wide range of molecules and materials by means of two Instruments, which offer the following capabilities:

- Acquity ultra-high performance liquid chromatography system (Waters) connected to a Time of Flight (LCT Premier XE) Detector controlled with Micromass MassLynx software. Mass accuracy at a resolving power of 10,000 and reproducibility are maintained by using an independent reference spray via the LockSpray interference. It has the capability to switch of positive/negative source ionization on a per-injection basis.

The instrument allows the analysis of small organic molecules (natural products, synthetic compounds, metabolites or peptides) by High Resolution Mass Spectrometry with previous components separation (or not) with ultra-high performance liquid chromatography. It is an instrument that has ability to detect analytes with full spectral acquisition. Analytical application areas include: Metabolite identification (metabolomics), impurity profiling in chemical synthesis, trace level component analysis in food or environmental samples, peptide/protein applications requiring full spectral sensitivity or natural product identification among others.

- Autoflex III Smartbeam Matrix Assisted Laser Desorption Ionization Mass Spectrometer (Brucker). The instrument was updated with the modules for MALDI Imaging.

This equipment allows the analysis of biomolecules (proteins, peptides, oligonucleotides, sugars, ...) and large organic molecules (such as polymers, dendrimers, polyphenols and other macromolecules). Some of the analytical advantages of MALDI TOF MS are its speed (time to results) and application flexibility, also the analyses can be performed with very low sample volume requirements and with the presence of other contents as salts and buffers. One of the main applications of MALDI-TOF MS is protein or peptide characterization providing primary protein sequences of intact protein targets in just minutes. With a variety of available ionization matrices and the option for analysis in both positive and negative ion modes, MALDI-TOF MS and MS/MS workflows offer critical advantages in the quality control of peptides, oligonucleotides and many classes of polymers. The MALDI Imaging technique allows for 2-dimensional spatial resolution of proteins and small molecules in tissues.

Both Instruments, together with NMR, are used in the “OMICS and MS-Imaging” facility



Staff

Josefina Casas Brugulat (Scientific Director)
Carme Quero López (Technical Director)
Eva Dalmau Alsina (Technician)

Thermal Analysis and Calorimetry (ATC)

The Thermal Analysis and Calorimetry (ATC) laboratory offers its services to IQAC groups, other CSIC institutes and university research groups, as well as R + D departments of the chemical-pharmaceutical, plastic, cosmetic and food industries. The service is mainly used for quality control, optimization of lyophilisation processes, storage temperature, drying isotherms, compatibilities active-exipient principle, polymorphism, obtaining isotherms of sorption-desorption, determination of the glass transition (T_g), compositional analysis of fibres, dilatometry studies, thermoporometry, coefficients of thermal expansion and studies of useful average life of materials.

The services are offered through the following equipment:

- Differential Scanning Calorimetry, DSC and microDSC
- Thermogravimetric Analysis, TGA
- Thermomechanical Analysis, TMA
- Dynamic vapour sorption, DVS

Staff

Dr. Albert M Manich Bou (Scientific supervisor)
Dr. Sonia Pérez Rentero (Technical supervisor)

Microanalysis

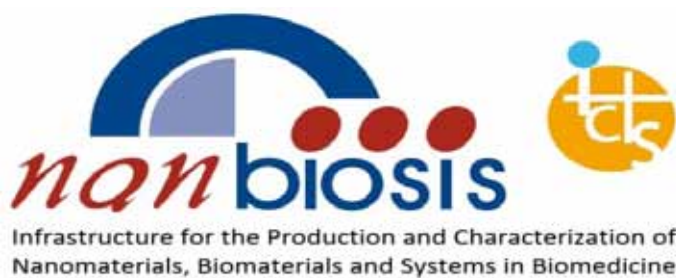
The Microanalysis laboratory provides micro-determination of total carbon, hydrogen, nitrogen, sulphur (C, H, N, S) and halogens present in a wide range of organic and inorganic compounds. This facility has the appropriate instruments for accurate sample analysis. Main instruments include:

- Elemental Microanalyzer (A5) model Flash 1112, for C,H,N determination.
- Elemental Microanalyzer (A7) model Flash 2000, for C,H,N,S determination.
- Mettler Microscale (B3 and B4) models MT5 and MX5.
- Metrohm Titrando model 808 for Cl,Br,I and F determination.

Staff

Maria Teresa Vila Terrades (Technical Director)
Nuria Barrera De Paz (Technician)

Characterization of Colloidal Dispersions



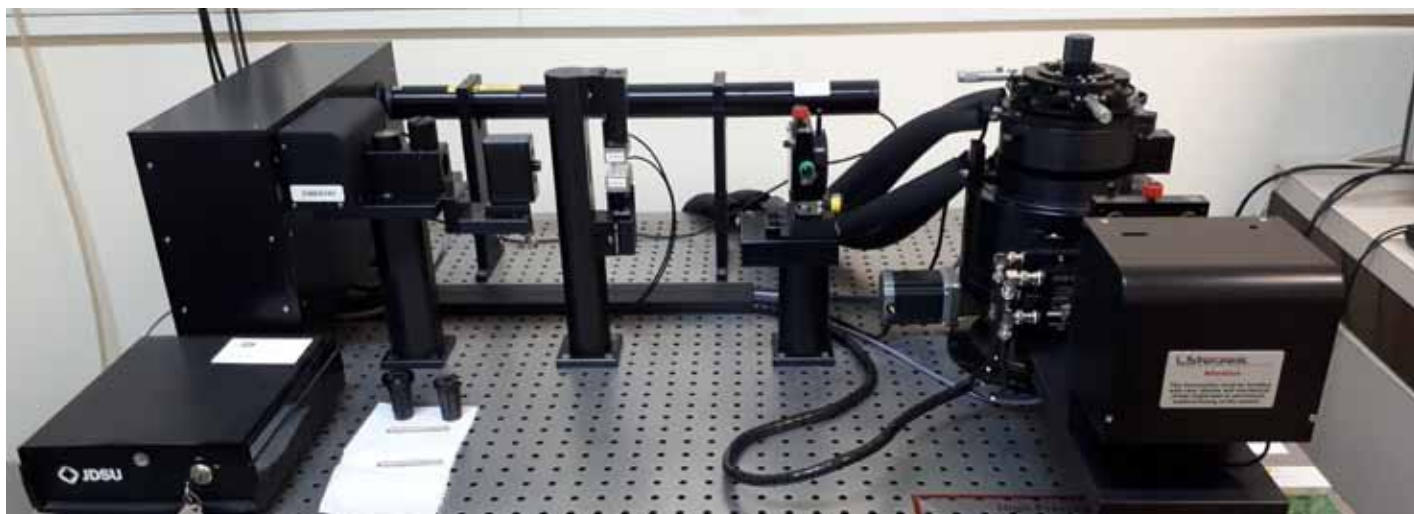
This service is dedicated to the characterization of nano-structured liquids (e.g. micelles, vesicles, liquid crystals, microemulsions, nano-emulsions etc.) and solid dispersions (e.g. organic inorganic or hybrid nanoparticle suspensions). The characterization includes the determination of size, morphology, phase transitions, surface, interfacial and rheological properties.

The service has been awarded a quality certificate by ACCIÓ (Generalitat de Catalunya), and it is currently upgrading the quality management system to fully comply with ISO 9001 rules, aiming to receive the certificate.

Services Available

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

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



INSTRUMENTAL ANALYSIS AND CHARACTERIZATION OF MOLECULES AND MATERIALS

- **Rheology**

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



- **Turbidimetry**



Time and position-resolved turbidimetry by back-light scattering for the characterization of dispersion stability.

- **High resolution optical microscopy with spectral analysis**

Imaging of nanosize objects (e.g. nanoparticles, nano-emulsions) and spectral mapping.



Other techniques:

- Laser Light Diffraction
- Differential Refractometry
- Tensiometry
- Optical Microscopy
- Densimetry
- Electrophoretic mobility and surface charge (Zeta Potential)
- Osmometry
- Fluorimetry
- Pore and surface area analyzer
- Benchtop Scanning Electron Microscopy

Staff

Scientific Supervisor:

Jordi Esquena Moret

Carlos Rodríguez Abreu

Technical Director:

Susana Vílchez Maldonado

Technician:

José Antonio Durán González

BIOMEDICAL AND ENVIRONMENTAL ASSESSMENT

This platform offers the evaluation of molecules and materials on different biological and environmental systems. It includes the following facilities:

- Dermocosmetic Assessment
- OMICS and MS-imaging
- Biodegradability and Toxicity
- Cell Culture (CID)
- Animal Facility (CID)

Dermocosmetic Assessment

The DERMOCOSMETIC ASSESSMENT Service (DC) was constituted in 2002 and it is now divided in three sections: Skin Absorption, Skin Efficacy and Hair Efficacy. Since May 2012, the Service of Dermocosmetic Assessment (DC) is accredited with a Quality System of Management in accordance with the UNE-EN ISO 9001:2008 certified by AENOR with the reference ER-0430/2012. Besides, it works under Good Laboratory Practices (GLP) from 2019 for Percutaneous Absorption Tests. It is important to remark that this is the first Service in the CSIC with this certification.

Services Available

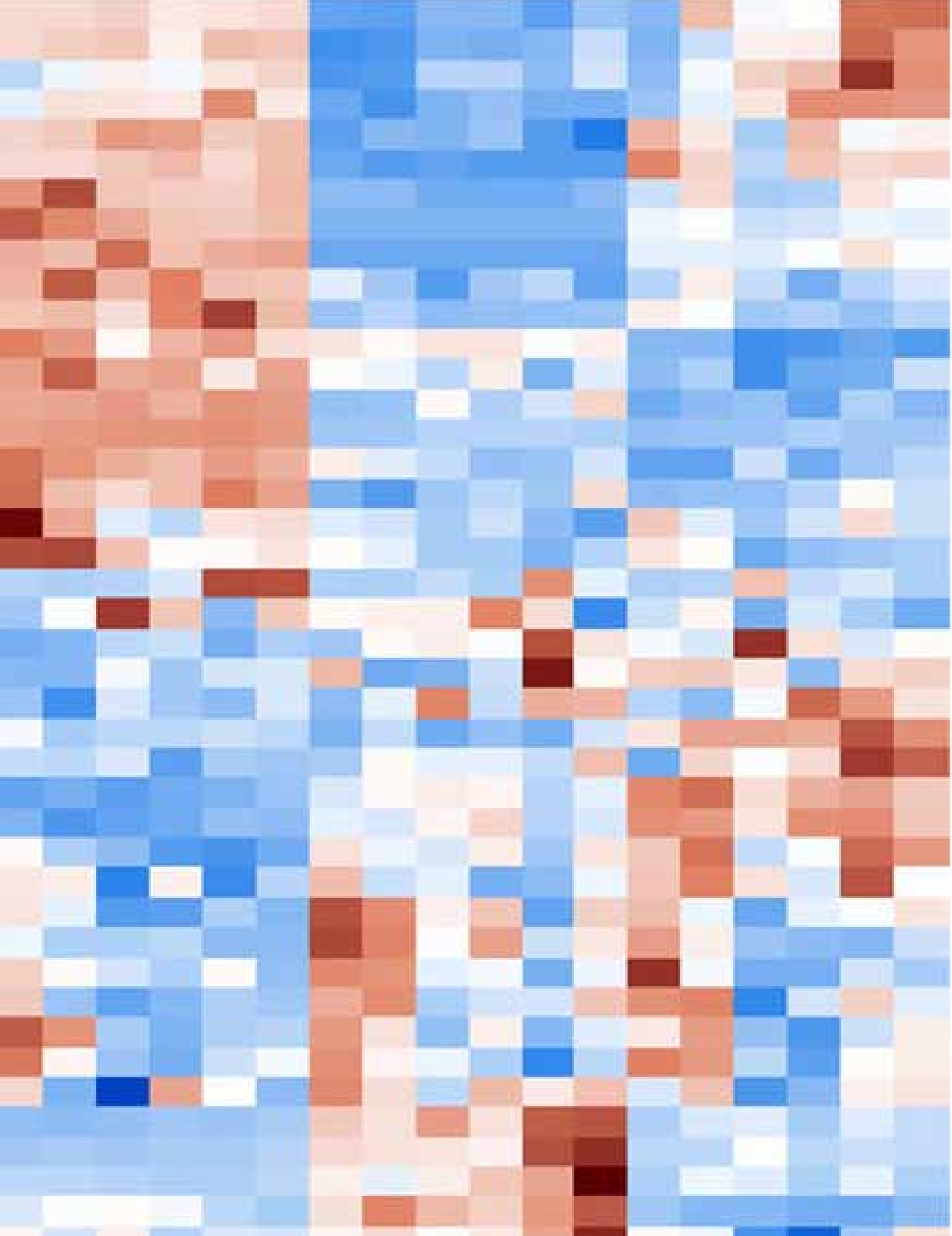
The skin absorption is specialized in determining the absorption profile through the skin of any compound when it is topically applied, using mainly an in vitro experimental methodology adopted by the OECD. Meanwhile, the skin efficacy is specialized in evaluating the efficacy of formulations applied to the skin and nails. The methodologies applied are based, preferably, on the use of biophysical techniques. Furthermore, the hair efficacy works evaluating in vitro the efficacy of cosmetic products in human hair. The service developed is focused on the needs of the industry (pharmacy, cosmetic, chemical and textile) and also on its own research and that of other groups requiring its scientific expertise support.



Staff

Scientific Director:
Prof. M. Luisa Coderch Negra

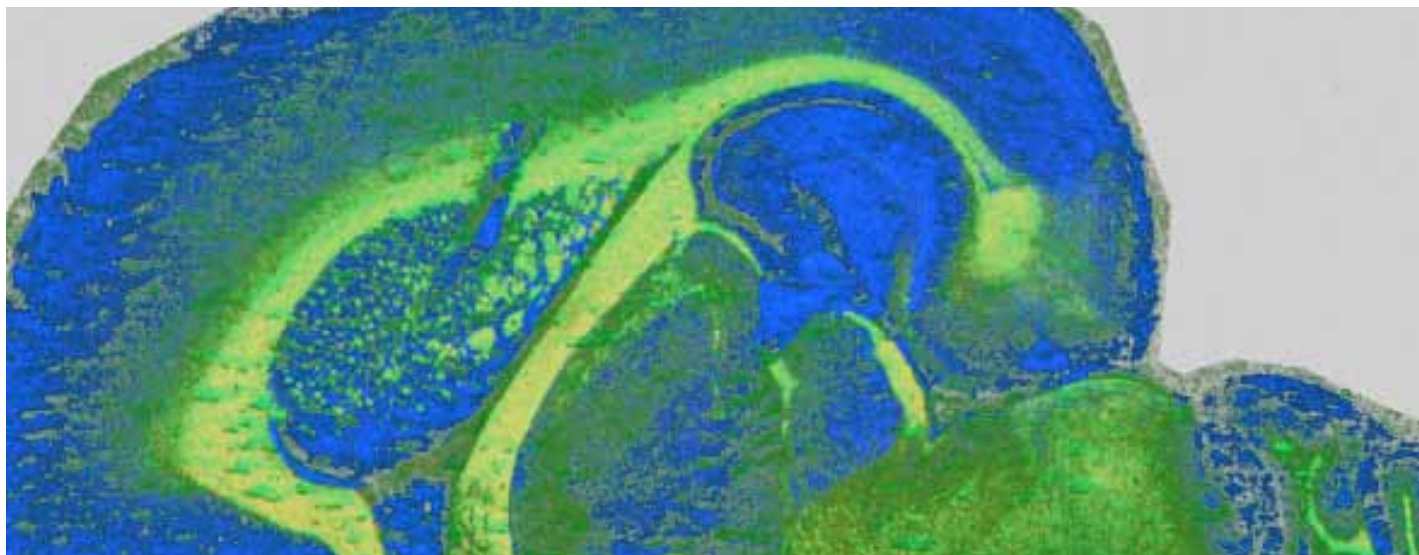
Technicians:
Dr. Cristina Alonso Merino
Dr. Clara Barba Albanell
Dr. Meritxell Martí Gelabert
Isabel Yuste Hernández

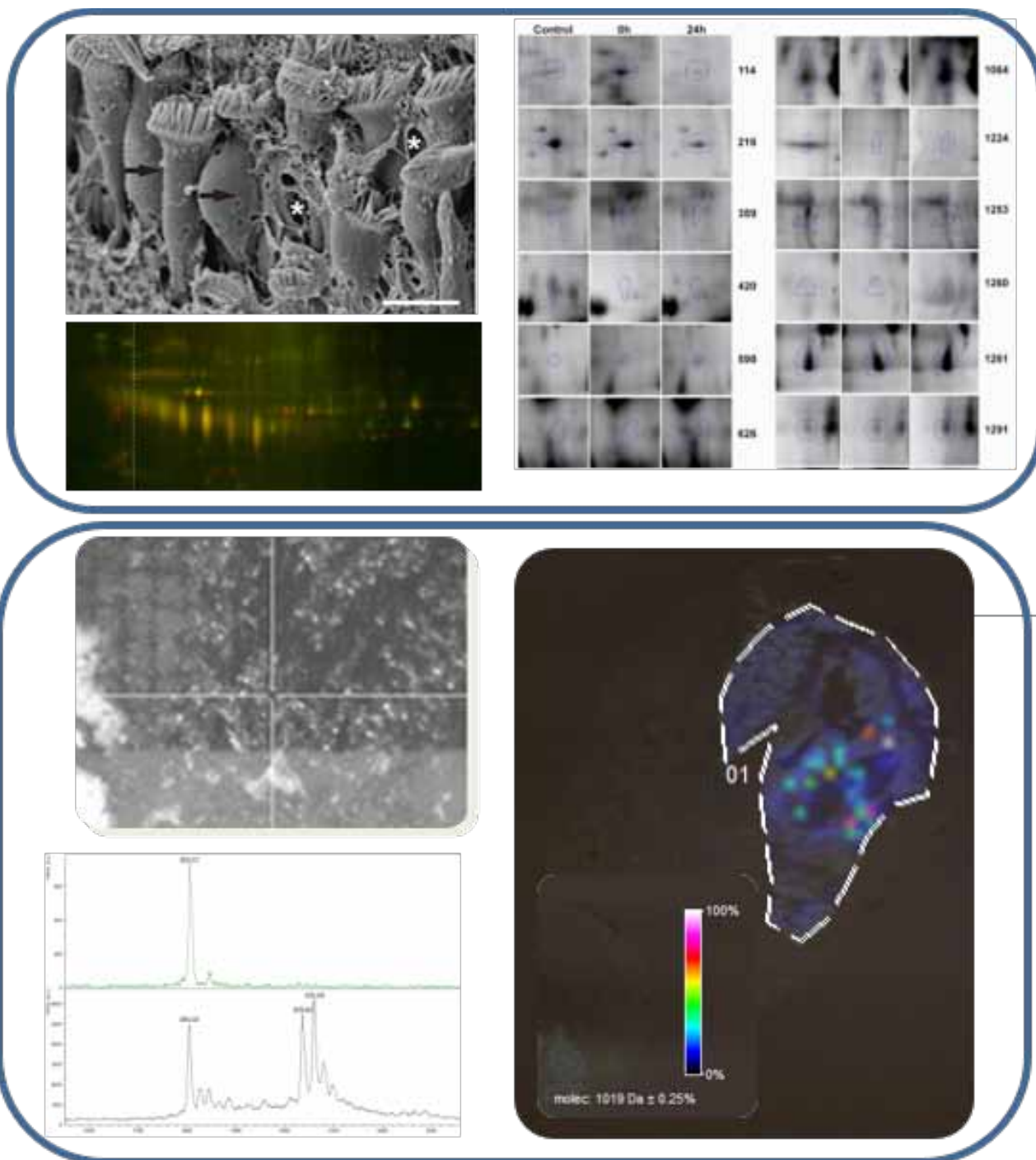


Omics and MS-Imaging

This service offers the characterization of metabolites (metabolomics), lipidomes (lipidomics) and proteomes (proteomics) in a wide range of samples, as well as the distribution of molecules of interest in tissues (MS-Imaging). Analyses are carried out by highly specialized staff using both RMN and Mass Spectrometry. The Service provides training and scientific advice in sample preparation methods and development of methods and protocols.

- The Lipidomics service conducts comprehensive analysis of cellular lipids that encompass endocannabinoids, acylcarnitines, glycerolipids, glycerophospholipids and sphingolipids. The service includes sample preparation, lipid identification by mass spectrometry, LC-MS lipid profiling, LC-MS lipid quantification,. Biological matrices encompass mammalian cells, organs, tumors, plasma, yeast, viral particles, Zebra fish and Daphnia. 670 lipid species, from 19 lipid families are routinely analyzed.
- The Proteomics Service is focused on the analysis of biomolecules (proteins, peptides, protein modifications, oligonucleotides, sugars,...) and large organic molecules (such as polymers, dendrimers, polyphenols and other macromolecules) by MALDI-TOF/TOF mass spectrometry. The Service offers separation, quantification, identification and characterization of peptides and proteins in biological and biomedical systems using two-dimensional electrophoresis and mass spectrometry techniques.
- The facility also offers MALDI Imaging. This technique allows direct measurement of different types of biomolecules, as well as drugs and metabolites distribution in tissues. The great advantage of MALDI Imaging is that the distribution of the detected compounds can be visualized as images, which can be integrated with other imaging modalities. This method is label-free and allows multiplex analysis of several molecules in the same tissue section simultaneously. In this technique, a thin slice of tissue is placed onto a MALDI target plate and coated with a matrix. The plate is then placed into a mass spectrometer and data is acquired under a fine laser beam. The result is a 2-dimensional optical image of the tissue slice that shows that mass spectral peaks of interest.





Staff

Josefina Casas Brugulat (Scientific Director, Lipidomics)
 Carme Quero López (Technical Director Proteomics and MS-Imaging)
 Yolanda Pérez Ruiz (NMR Facility manager, NMR Metabolmics)
 Eva Dalmau Alsina. Technician
 Alexandre García Barrera. Technician

Biodegradation and Aquatic Toxicity

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 costumers from industry, public administration, universities, and research organisms. Suitable technology and an expert and qualified staff guarantee the availability of results.



Staff

M. Teresa García Ramón (Scientific Director)
Isabel Ribosa Fornoví (Technical director)
Ana de la Fuente Polo (Technician)
Marta Andrés Nieto (Technician)

Services Available

Biodegradation tests

- Aerobic biodegradability.
 - Ready biodegradability tests:
 - CO₂ Headspace test, OECD301-ISO 14593
 - Closed Bottle test, OECD 301D
 - Modified Screening Test, OECD 301E);
 - Inherent biodegradability tests
 - Zahn-Wellens Test. OECD 302B
- Anaerobic biodegradability
 - Anaerobic biodegradability
 - Biogas production test. OECD 311

Effects on biotic systems

- Daphnia magna immobilization test (OECD 202)
- Bioluminescent bacteria test (Microtox)
- Activated sludge inhibition respiration test (OECD 209)
- Inhibition of biogas production from anaerobically sewage sludge (OECD 224).



Cell Culture

The Cell Culture Service (SCC) is a research support unit that belongs to CID and offers either in-house research groups from IQAC and IDAEA or external laboratories the equipment and appropriate facilities to carry out in vitro culture and maintenance of human and animal cell lines in order to perform bioassays in several aspects of the biomedical and toxicological sciences.

The Service provide biosafety level 2 (BSL-2) facilities, suitable for work involving agents of moderate potential hazard to personnel and the environment, and all work is performed using approved BSL-2 guidelines.



Staff

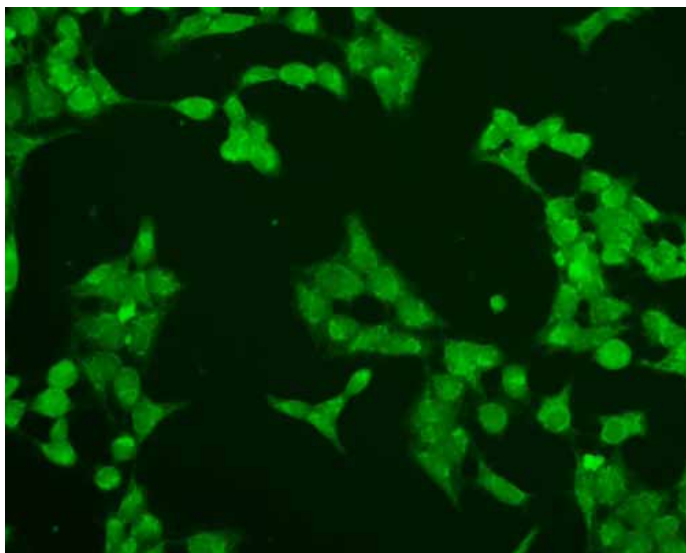
Supervising Director
Gemma Fabriàs Domingo

Technical director and Contacting person
Ignacio Pérez Pomeda

BIOMEDICAL AND ENVIRONMENTAL ASSESSMENT

The facility is equipped with the following instruments and devices:

- 4 Laminar flow cabinets (Class I).
- 1 Biological safety cabinet (Class II).
- 7 CO₂ incubators set up for mammalian cells.
- 2 Incubators set up for non-mammalian cells.
- 2 Liquid nitrogen tanks for cell cryopreservation.
- 4 Refrigerators and freezers.
- 1 Phase contrast inverted microscope.
- 1 Fluorescence microscope equipped with a digital camera
- 2 Thermostatic water baths.
- 1 Tabletop refrigerated centrifuge.
- 1 Countess automatic cell counter.
- 1 Guava EasyCyte flow cytometer



Animal Facility

The Animal Facility, also belonging to CID, is a common infrastructure for the two institutes hosted in the center: IQAC (Institute of Advanced Chemistry of Catalonia) and IDAEA (Institute of Environmental Assessment and Water Research). It also provides service to the IBMB (Institute of Molecular Biology of Barcelona) housed in the Parc Científic de Barcelona.

Services available

In addition to the management, facility maintenance and care of the animals, the service provides scientific expertise, technical advice and collaboration in procedures. It is responsible for the simultaneous tasks of facilitating research and assuring animal welfare according to current regulation.

The facility houses mammals for research in biology, chemistry and biomedicine (rats, mice and rabbits) as well as aquatic animals (zebrafish) for research in environmental chemistry and aquatic toxicology.

It also owns an Antibody Production Platform devoted to the production of polyclonal antibodies in rabbits, rats and mice, both for internal and external users from public research centers and private companies.

Staff

Head of service:

Eva Prats Miravittlas

Technician:

Alejandro Padilla García

Animal care manager:

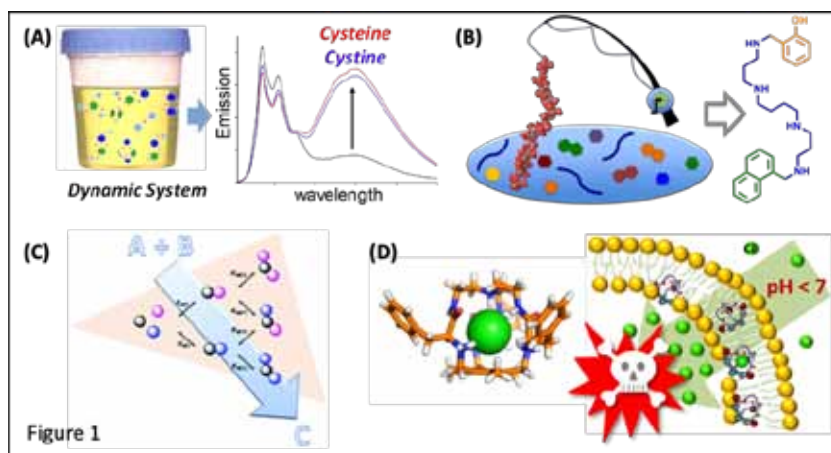
Juan Manuel Rodríguez Palacios



RESEARCH HIGHLIGHTS

BIOLOGICAL
CHEMISTRY
DEPARTMENT
Supramolecular
Chemistry

During this biennial period, our most remarkable research results can be classified in the three main research lines of the group. Within the study of dynamic covalent systems, we have advanced in two main directions using different covalent bonds for connecting the corresponding building blocks. Following our work with disulfide-based dynamic covalent mixtures of pseudopeptidic thiols, we designed a system able to produce a fluorescent signal upon the presence of cysteine and its oxidized dimer, cystine. This allowed to selectively detect these biothiols in aqueous media, including human urine, as a potential diagnostic tool for cystinuria disease (Figure 1A). These results have been patented (PCT/ES2019/070226) and published in a top multidisciplinary chemistry journal (Angew. Chem. Int. Ed. 2018, 57, 8421-8424), highlighted in the inner cover of the issue. On the other hand, we have also used C=N covalent bonds for the dynamic screening of potential ligands against a biologically relevant glycosaminoglycan, heparin (Figure 1B). The amplified member of the library showed a strong binding to heparin using different techniques (fluorescence, NMR, ITC and modelling) and efficiently inhibited the anticoagulant activity of heparin in an in vitro enzymatic test. These results were also published in a top-rated journal (Angew. Chem. Int. Ed. 2018, 57, 11973-11977) and selected as hot paper by the editorial team. The application of the dynamic system concept to chemical problems has been also demonstrated in the field of catalysis, by the optimization of a metal templated stereoselective catalyst from a mixture of bipyridine ligands bearing organocatalytic functions that, upon assembling, highly



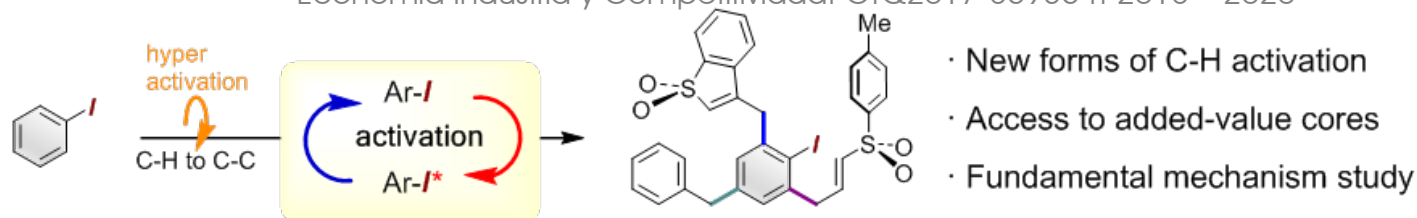
improved the performance in terms of rate and stereoselectivity (Figure 1C). The deep study of the dynamic system allowed the full understanding of the observed catalytic properties (Chem. Commun. 2019, 55, 7970-7973). Finally, we have also contributed in the design and synthesis of optimized receptors for biologically relevant species. We prepared small pseudopeptidic cages that selectively bind chloride anion when protonated, also promoting the chloride transport through lipid bilayers.

Their anionophoric properties improved at acidic pH, suggesting an H⁺/Cl⁻ symport mechanism. NMR studies in micelles demonstrated that the cages bind chloride within the lipid phase, showing higher affinity and faster exchange rate at acidic pH. This increases cytotoxicity towards lung adenocarcinoma cells at the pH of the microenvironment of a solid tumor (Figure 1D). The results have been recently published in a very prestigious scientific journal (Angew. Chem. Int. Ed. 2019, 58, 12465-12468).

BIOLOGICAL
CHEMISTRY
DEPARTMENT
Synthetic
Methodology
and
New Building Blocks

Main group chemistry: from high energy intermediates to rapid building block assembly

The group's proposal BISI Bonds (full title: Main group chemistry: from high energy intermediates to rapid building block assembly) received a 3-year grant (2018-2020) through a competitive call from the Ministerio de Economía, Industria y Competitividad. The project is co-directed by Dr. Alexandr Shafir (IQAC) and by Dr. Ana Belén Cuenca (IQS-URL), and aims to develop a series of highly-efficient atom- and energy-economical synthetic methods by combining the chemistries of the main-group elements, in particular that of Boron, Silicon and Iodine. In addition to providing the fundamental knowledge regarding the properties of these species, the project has already produced a series of original methods for making carbon-carbon bonds, including the highly efficient synthesis of propargylated aromatics via the C-H coupling (Chem. Eur. J. 2018) or the mechanistically intriguing para-selective C-H benzylation (Angew. Chem. Int. Ed. 2019). These new synthetic tools have a high potential to aid in the medicinal chemistry discovery by rapidly scanning wide swaths of chemical space. IP: Alexandr Shafir (IQAC) and Ana Belén Cuenca (IQS-URL). Ministerio de Economía Industria y Competitividad: CTQ2017-86936-P. 2018 – 2020



BIOLOGICAL
CHEMISTRY
DEPARTMENT
Theoretical and
Computational
Chemistry

Methyl hydrotrioxide last between 0.2 to 1.8 hours in the atmosphere.

Methyl hydrotrioxide is an intermediate in the atmospheric oxidation of methane and, consequently, its oxidation by hydroxyl radical plays an important role in the chemistry of the atmosphere. Our research predict this reaction to be fast, producing methoxy radical in more than 94%, and its lifetime is predicted to range from of 1.8 hours at 225 K, raising up to 3.9 hours at 275 K and decreasing to 0.2 hours at 310 K. (Phys.Chem. Chem.Phys., 2018, 20, 27406-27417)

The atmospheric chemistry of SO₂ is an important source of OH radicals in the atmosphere and may play a role in the formation of sulfuric acid.

Sulfur dioxide (SO₂) is known to be the precursor of sulfuric acid, a major component of acid rain and a key contributor to aerosol nucleation. We have discovered that photochemistry of SO₂ at the surface of water droplets is also an efficient precursor of OH and HOSO radicals. The reaction proceeds through light absorption to an excited singlet followed by intersystem crossing to a reactive triplet state, which readily reacts with water through a proton coupled electron transfer mechanism producing HOSO and OH radicals. Moreover, using first-principles simulations, we show that HOSO displays a strong acidity (pK_a = -1) comparable with nitric acid, and it is fully dissociated at the air-water interface. Accordingly, HOSO might play an important role in acid rain formation in the atmosphere. (J. Am. Chem. Soc., 2018, 140, 12341–12344; Phys.Chem.Chem. Phys., 2019, 21, 9779,9784; J. Am. Chem. Soc. 2019, 141, 16564-16568)

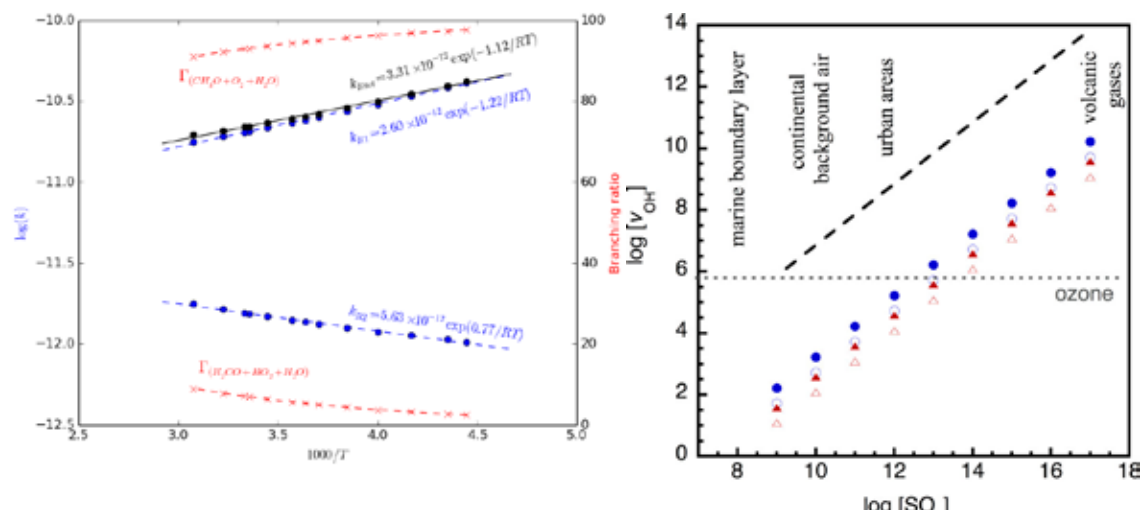


Figure 1: The left side shows the calculated rate constant and branching ratios for the oxidation of Methyl hydrotrioxide by hydroxyl radical. The right side shows the estimated OH production rates (molecule·cm⁻³·s⁻¹) as a function of SO₂ concentration in gas phase (molecule·cm⁻³). Triangles and circles correspond to gas phase calculations assuming 20% and 100% of RH, respectively. The dashed line is the production rate at the air-water interface

Unconventional hydrogen bonds stabilize polyglutamine helical tracts

Computational modelling helps us understand the biophysics of several human diseases. A family of diseases called polyglutamine diseases, which includes Huntington disease, are caused by anomalously long polyglutamine tracts in different proteins. These polyglutamine tracts appear in (presumably) disordered regions of the protein, that is, regions which do not fold into structured conformations.

conformations.

Previous NMR and circular dichroism results had shown that the polyglutamines in the androgen receptor adopt a helical structure. Patterns of helical structure determine protein-protein interactions, and influence liquid-liquid phase separation. They are relevant for understanding the functioning of proteins and therefore for their biomedical consequences when this functioning is altered.

If polyglutamines were considered to form disordered regions, what causes

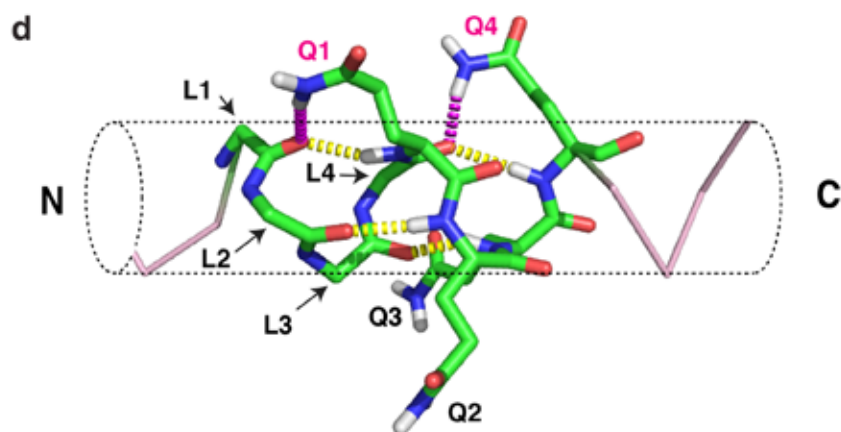


Figure 2: side-chain to main-chain hydrogen bonds (purple) help stabilize α -helical canonical hydrogen bonds (yellow). Leucine (L) side chain shield the former from water and give polyglutamines a high helical content.

their helical propensity? We found that the flanking regions of the polyglutamine tract strongly determine its helicity, and we looked for the physical or chemical elements promoting the helices.

Based on the integration of molecular dynamics, NMR chemical shifts and quantum chemical calculations, we suggested that glutamine side-chain to main-chain hydrogen bonds strengthen the helix and that these hydrogen-bonds are protected by the side-chains of the flanking regions.

Overall, this work (Nat. Commun., 2019, 10, 2034) shows how molecular explanations can help understand structural biology effects with biomedical consequences.

BIOLOGICAL CHEMISTRY DEPARTMENT P l a s m a C h e m i s t r y

Development of atmospheric plasma configuration for advances technologies

Different configurations of atmospheric plasmas have been developed in the plasma chemistry group for specific treatments (Figure 1). Dielectric barrier discharge (DBD) has been used for surface treatment of polymers, seeds, elimination of chemical compounds in waste water and in situ polymerization of monomer solutions in liquids. Jet plasma configuration and surface plasma configurations have also been obtained for advanced technologies.



DBD plasma



Jet Plasma



Surface Plasma

Figure 1. Plasma configurations for advances technologies.

Plasma in agriculture

DBD plasma treatments increase water uptake velocity and independent of the irrigation conditions plasma treated wheat seeds reach the initial water content required to initiate germination faster. Although the overall germination capacity of treated seeds depends on the type of seed and irrigation, the germination rate for conditions of scarce availability of water increased (Figure 2).

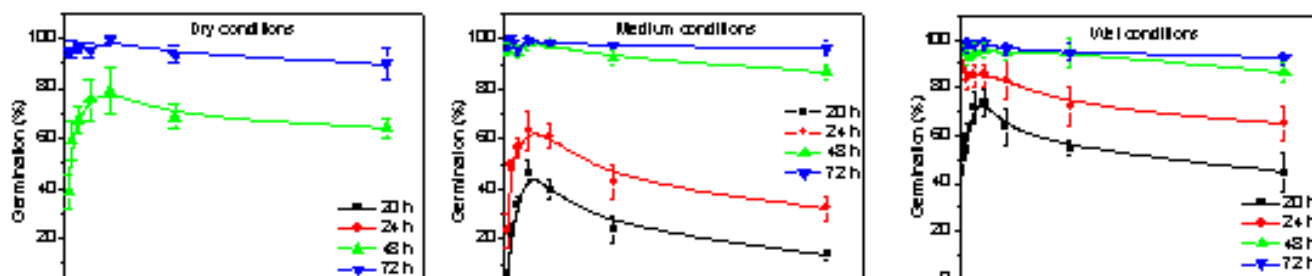


Figure 2. Germination of plasma treated wheat seeds in different irrigation conditions for different periods (20-72h).

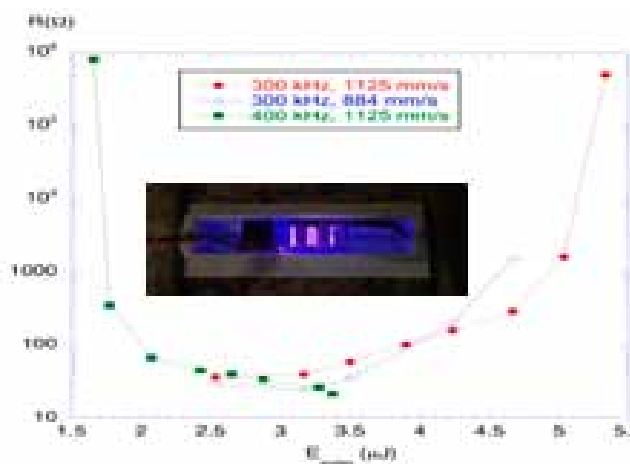


Figure 3. Evolution of the electrical resistance as a function of the energy per pulse.

Laser processing: metallic circuits onto transparent substrates for plasma sources

Metal electrodes (Ag) on glass surfaces deposited by means on Laser Ablation Backwriting (LAB) has been obtained in order to generate surface plasmas. Electrical resistance of the deposited metal circuits depends drastically on the laser experimental parameters (Figure 3).

BIOLOGICAL
CHEMISTRY
DEPARTMENT
Medicinal
Chemistry

Research activities of the group are focused on drug discovery and chemical biology, aimed at obtaining novel biologically active compounds and their application in new therapies, as well as the development of new pharmacological research tools. Current main lines of research include:

Photopharmacology - Reversible photoswitches

The administration of a photocontrolled ligand in combination with illumination that is patterned in space and time can provide a novel degree of control and regulation of receptor activity. This method would allow focusing the action of the ligand, controlling the location and the temporal extension of its effects. When applied in vivo, the use of photoregulation can reduce side effects by targeting receptors located in specific tissues, establishing personalized drug schedules to patient needs.

In particular, azobenzene photoisomerization can control biological functions. We have obtained phenylazopyridines with light-dependent activity as negative allosteric modulators (NAM) of metabotropic glutamate receptor subtype 5 (mGlu5), that result in atypical pharmacological profiles, both in vitro and in vivo, in studies of zebrafish larva motility and the regulation of the antinociceptive effects in mice. Thus, local administration of a photoswitchable compound combined with irradiation with light in the peripheral tissues of rodents or in the brain results in a



precise illumination-dependent analgesic effect.

Also, azobenzene photoswitchable allosteric modulators of mGlu4 allow the control of endogenous mGlu4 activity with light and reversible inhibition of persistent pain symptoms by receptor photocontrol in the brain of freely behaving animals.

These compounds can be used to define novel and more precise therapeutic treatments and to study in vivo the physiological roles of the receptors.

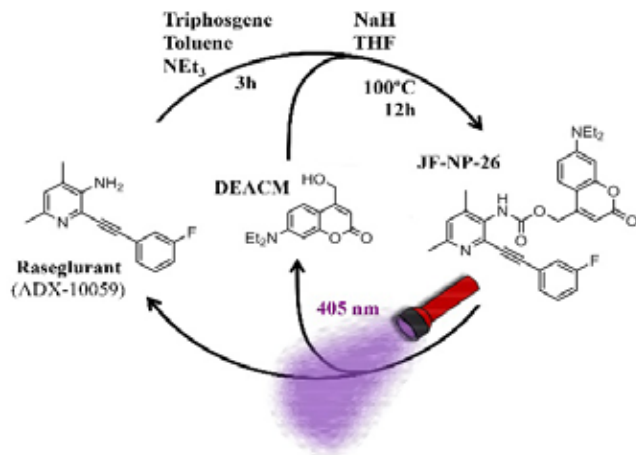
Photopharmacology - Photolabile caged compounds

Another approach to control the activity of therapeutic compounds by means of light is through the use of photolabile compounds. These are caged drugs, inactive while caged, that result in the controlled release of the active compound

when irradiated with light.

JF-NP-26 is a coumarin-caged derivative of raseglurant, a mGlu5 receptor negative allosteric modulator. Light illumination of JF-NP-26 induces a photochemical reaction releasing the active drug, which effectively controls mGlu5 receptor activity both in ectopic expressing systems and in striatal primary neurons.

After systemic administration of JF-NP-26 in mice, local light-emitting diode (LED)-based illumination, either of the thalamus or the peripheral tissues, induces light-dependent analgesia both in neuropathic and

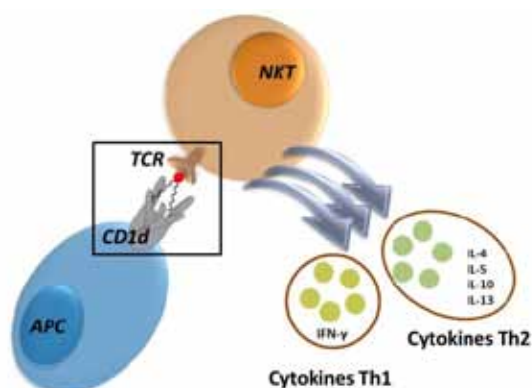


in acute/tonic inflammatory pain models.

This is the first example of photocontrol of analgesia in vivo using a caged mGlu5 receptor negative allosteric modulator

Immunotherapy - Non-glycosidic analogues of α -GalCer as NKT cell activators

Invariant natural killer T cells (iNKT), a unique subpopulation of T cells with immunomodulatory properties involved in a broad range of immune responses, are stimulated by glycolipid antigens, particularly by alpha-galactosylceramide (α -GalCer).



α -GalCer shows an exceptional potency on iNKT cell stimulation which is associated to different side effects. In addition, it simultaneously induces the expression of both Th1 and Th2 cytokines, which have opposite biological functions. Thus, new compounds are needed to achieve selective modulation of cytokine release.

A new family of non-glycosidic analogues of α -GalCer has been developed. They show strong activity in vitro to stimulate iNKT cell proliferation and highly efficient and potent selective cytokine release.

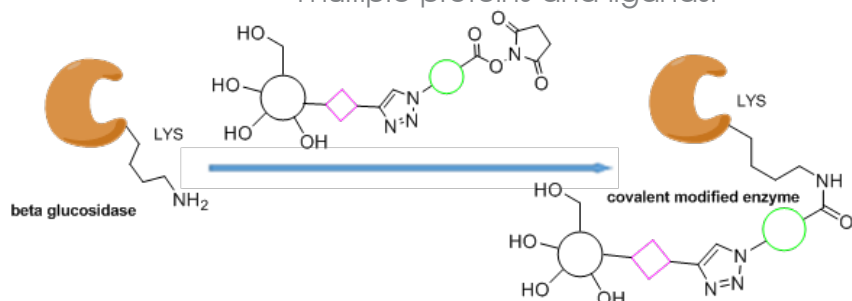
These compounds can have application in cancer immunotherapy, for cooperative stimulation of the patient immune system, and as vaccine adjuvants in autoimmune diseases or infections. A patent application has been filed in November 2017.

Selective protein labelling

We have developed a protein labelling method that consists in the selective and kinetically controlled conjugation on lysine residues exposed on the surface of the protein near the binding site of the ligand.

This approach is based on bioorthogonal Cu-catalyzed click-chemical reactions, in which a fast triazole synthesis from chemically stable azide and alkyne components results in an N- or S- diversely substituted imino or thiosugar ligand library. The protein affinity of the sugar-like ligand with a short lived NHS-ester group directs the chemical reaction on a terminal amino group of a specific lysine in the native protein.

This results in a practical chemical method for the selective covalent labelling of wild type proteins with high affinity without requiring previous genetic or chemical modification of the protein. Its modularity allows the application to multiple proteins and ligands.

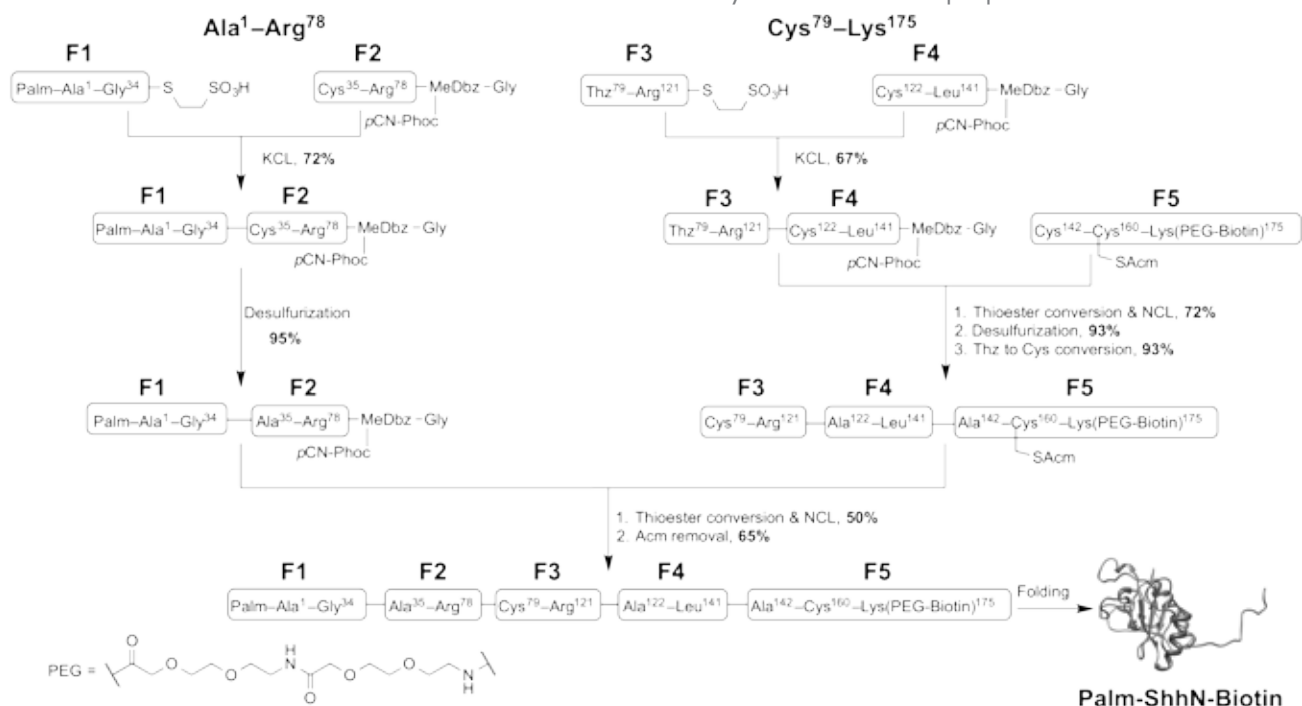


BIOLOGICAL
CHEMISTRY
DEPARTMENT
C h e m i c a l
B i o l o g y

The Chemical Biology research group has obtained relevant results in different research lines focused on the development of new methods for protein chemistry and the synthesis of new tools for studying autophagy and protein-lipid interactions.

Synthesis of N-terminal palmitoylated protein Sonic Hedgehog, a morphogen ligand of the Hedgehog signaling pathway
(*Angew Chem Int Ed Engl* 2018, 57 (49), 16120-16125.)

We have developed a simple procedure for C-terminal activation of peptides in solution and applied in native chemical ligation and protein synthesis. This method involves a mild thioesterification based on the conversion of an aryloxy-o-methylaminoanilide to thioester under aqueous conditions and in situ ligation with an N-terminal cysteine peptide. The versatility was shown in pH-controlled sequential ligations and in the synthesis of the palmitoylated N-terminal domain of human Sonic Hedgehog, a morphogen protein that binds the transmembrane receptor Patched and activates the Hedgehog signaling pathway, which is involved in embryonic development and in the proliferation of multiple tumors. This approach extended the chemical toolset of chemical protein synthesis based on o-aminoanilide and o-methylaminoanilide peptides.



A hydroxylamine probe for profiling S-acylated fatty acids on proteins
(*Chem Commun (Camb)* 2019, 55 (75), 11183-11186.)

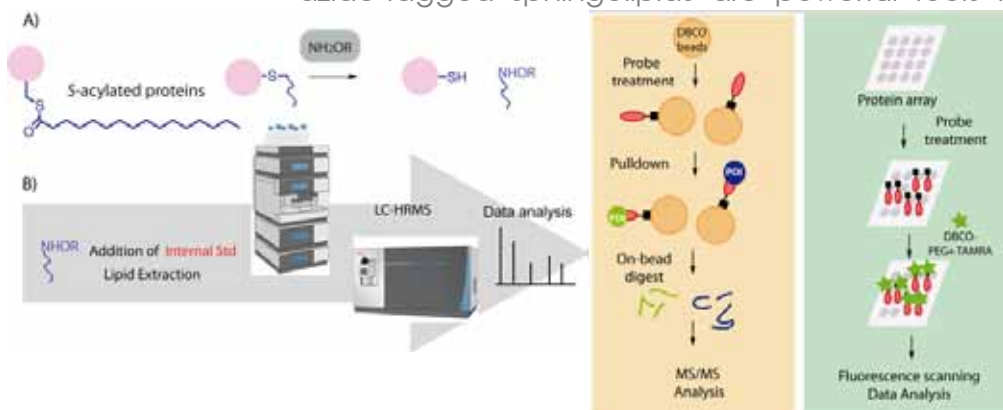
The covalent attachment of lipids to proteins is a key regulatory mechanism of protein function and localization. One of the most studied protein lipidation processes is the reversible palmitoylation of cysteine residues. Although there is increasing evidence that S-acylation is not restricted to palmitate, the diversity of this protein modification has not been fully explored. We have described a hydroxylamine-based chemical probe that combined with MS-based analysis

allows the rapid detection and quantification of fatty acids linked to proteins. We have used this approach to profile the S-acylome and to show that the oncogene N-Ras is heterogeneously acylated with two different fatty acids, palmitate and palmitoleate.

Identification of novel lipid-protein interactions.

(Schulte-Zweckel, J.; Schneidewind, T.; Abad, J. L.; Brockmeyer, A.; Janning, P.; Triola, G., *Chem Commun (Camb)* 2018, 54 (97), 13742-13745.)

Ceramide plays key roles in autophagy, inflammation and apoptosis. However, little is known about the molecular mechanisms regulating its function and only a handful of cellular effectors are known for this lipid. We have shown that azide-tagged sphingolipids are powerful tools to identify ceramide targets.

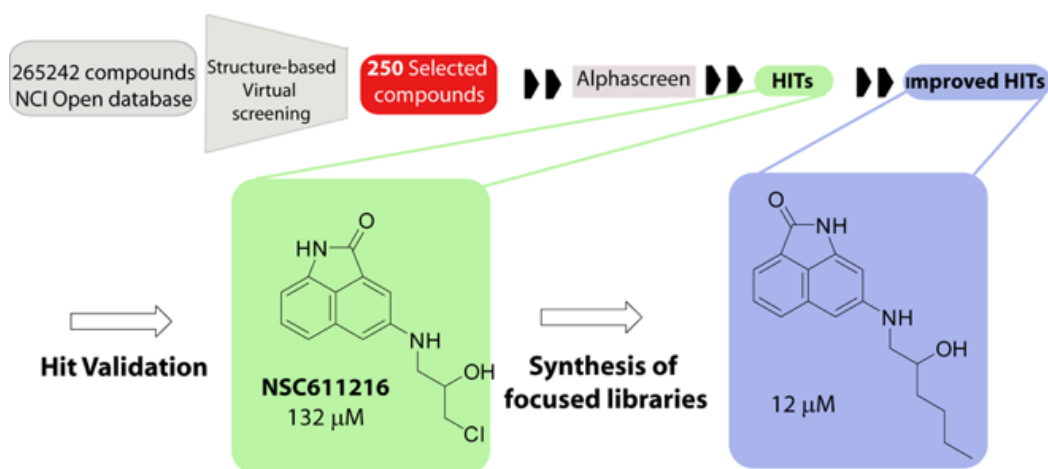


The combination of a protein array analysis and a mass spectrometry-based proteomic profiling successfully detects known ceramide-binding proteins and identifies others not yet reported, several of which we validated using a variety of techniques.

Identification of Atg4B inhibitors via a structure-based virtual screening and a novel AlphaScreen assay

Quintana, M.; Bilbao, A.; Comas-Barcelo, J.; Bujons, J.; Triola, G., *Eur. J. Med. Chem.*, 2019, 178, 648-666.

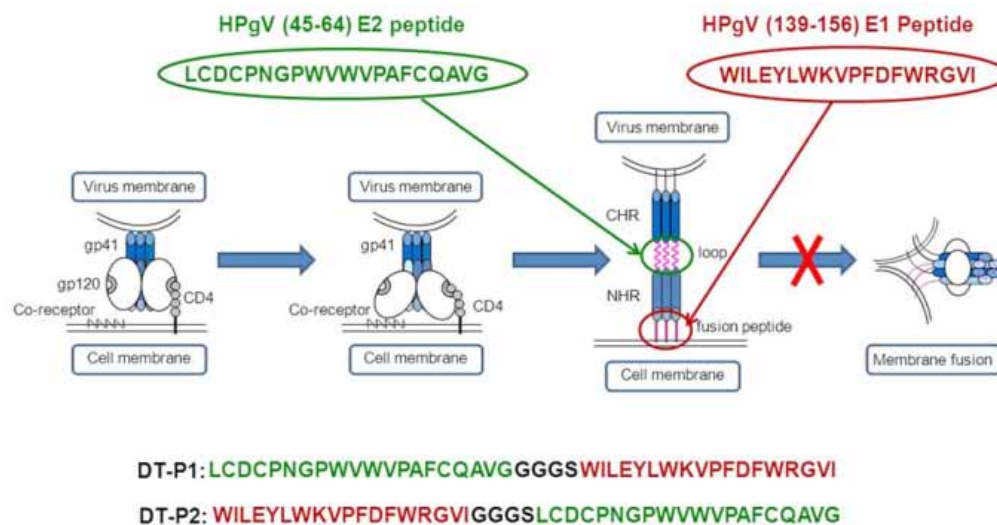
Targeting autophagy is a promising therapeutic strategy for cancer treatment. As a result, the identification of novel autophagy inhibitors is an emerging field of research. We have described the development of a novel AlphaScreen HTS assay that combined with a structure-based high-throughput virtual screening have enabled the identification of benzo[cd]indol-2(1H)-one as a novel scaffold that targets Atg4B. In addition, inhibition of autophagy was also investigated in cells by measuring LC3-II and p62 protein levels.



BIOLOGICAL
CHEMISTRY
DEPARTMENT
Synthesis and
Biomedical
Applications
of Peptides

Peptide assembly on the membrane determines the HIV-1 inhibitory activity of dual-targeting fusion inhibitor peptides

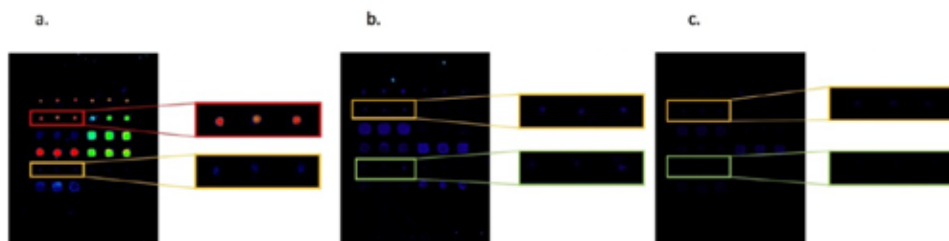
We described the design of dual-targeting peptides composed of peptide domains of the E2 and E1 envelope proteins from Human Pegivirus with the aim of targeting simultaneously both the loop region and the fusion peptide domains of HIV-1 gp41. Two different dual-targeting peptides, where the E1 peptide is on the N- or the C-terminus respectively, were chemically synthesized and their antiviral activities evaluated with HIV pseudotyped viruses from different clades. The overall results point out to the necessity that fusion inhibitor peptides that specifically interfere with the N-terminal region of gp41 are embedded within the membrane in order to interact properly with their viral target.



A Multiplex Assay based on Chimeric Citrullinated Peptides for the Diagnosis of Rheumatoid Arthritis

Anti-citrullinated peptide/protein antibodies (ACPAs) are the most specific serological biomarkers for RA that have both diagnostic and prognostic value and are related with a more aggressive joint disease in RA. However, a single biomarker cannot differentiate the different RA subtypes. We have developed a multiplex assay based of chimeric citrullinated peptides derived of filaggrin, fibrin, vimentin and enolase human proteins. The relative frequency of ACPA positive for the combination of the eight chimeric peptide antigens, that yielded positive to 3 or more peptides in the RA cohort was 61.4%; on the contrary the healthy BD and PsA cohorts showed 0%. Within anti-CCP3-negative patients, ACPA reactivity detected by the chimeric peptides-based multiplex was only detected in one

serum sample. Peptides with other posttranslational modifications could potentially be included in the multiplex assay to improve the sensitivity/specificity balance.



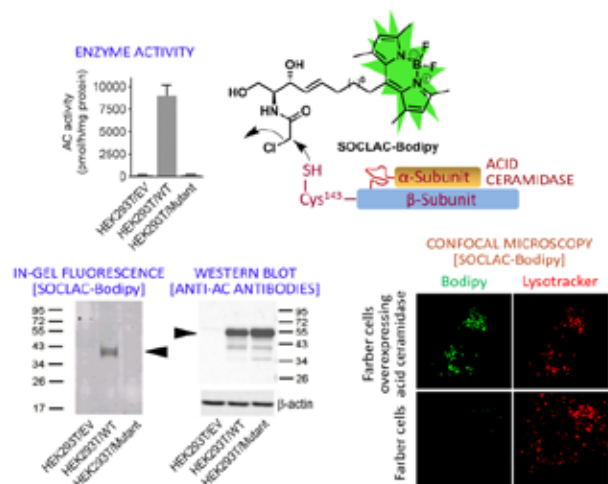
BIOLOGICAL
CHEMISTRY
DEPARTMENT
Research
Unit on
BioActive
Molecules
(RUBAM)

Activity-Based Imaging of Acid Ceramidase in Living Cells

(J Am Chem Soc, 141, 7736-7742, 2019)

Acid ceramidase (AC) hydrolyzes ceramides into sphingoid bases and fatty acids. The enzyme is overexpressed in several types of cancer and in Alzheimer's disease, and its genetic defect causes different incurable rare disorders, such as Farber disease and spinal muscular atrophy with progressive myoclonic epilepsy. The availability of a method for the specific visualization of catalytically active AC in intracellular compartments is crucial for diagnosis and follow-up

of therapeutic strategies in diseases linked to altered AC activity. In this work, we report on activity-based probes (ABP) for the detection of functional AC. The novel ABPs were found to irreversibly inhibit AC with very high potency (two-digit nM range) by reaction of their halomethyl unit with the enzyme active site Cys143. The probes proved useful for in-gel AC detection at submicromolar concentrations and short incubation times and it successfully stained endogenous levels of active enzyme. Moreover, no AC labeling occurred after protein denaturation, showing that the correct protein folding is a labeling requirement (as it is for activity). Importantly, one of the probes (Bodipy-SOCLAC) represents a major advantage in that it allowed the unprecedented lysosomal staining of active, but not inactive, AC in intact cells. In contrast, antibodies react with both inactive and active AC, being not able to distinguish both enzyme forms. These overall results are of biomedical relevance to visualize the location and monitor the trafficking of active AC, as well as for the analysis of novel pharmacological chaperones for the treatment of Farber disease and spinal muscular atrophy with progressive myoclonic epilepsy.

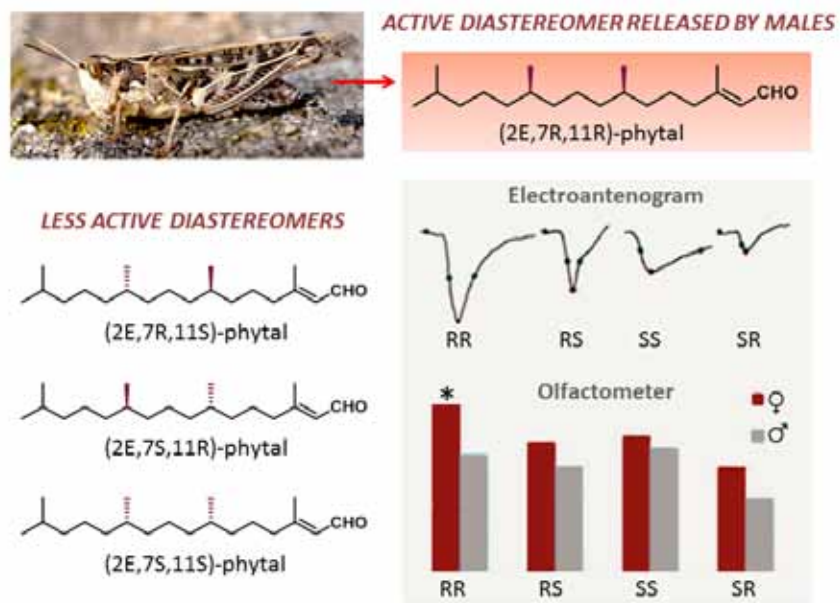


Detection of acid ceramidase (AC) with SOCLAC-Bodipy. In the in vitro AC labeling, HEK 293T cells were transfected with WT AC, the inactive C143S mutant or the empty vector (EV). Enzyme activity was determined with a fluorogenic substrate. Cell lysates were incubated with the probe and the reaction mixtures were resolved on SDS-PAGE before in-gel fluorescence analysis. For Western Blot analysis, proteins were transferred to a PVDF membrane and immunodetected with an anti-AC antibody. Arrows indicate AC. AC labeling in living cells was examined by confocal fluorescence microscopy after treatment with the probe. Here we show the results obtained with Farber cells carrying an inactivating mutation and the same cells transduced to overexpress AC. The expected lysosomal staining is observed in cells with active enzyme, but not with the inactive mutant.

Enantioselective Synthesis and Activity of All Diastereoisomers of (E)-Phytal, a Pheromone Component of the Moroccan Locust, *Dociostaurus maroccanus*

(J. Agric. Food Chem., 67, 72-80, 2019)

The Moroccan locust, *Dociostaurus maroccanus* (Orthoptera: Acrididae), is a polyphagous pest capable of inflicting large losses in agriculture under favorable environmental and climatic conditions. Currently, control of the pest relies solely on the application of conventional insecticides that have negative effects on the environment and human safety. In the search for a more rational, environmentally acceptable approach for locust control, we have previously reported that (Z/E)-phytal is a male-produced candidate sex pheromone of this acridid. This molecule, with two stereogenic centers at C-7 and C-11, has four different diastereomers along with the Z/E stereochemistry of the double bond at C-2. In this paper, we present the enantioselective synthesis of the four diastereomers of (E)-phytal and their electrophysiological and behavioral



activity on males and females. Our results demonstrate that the (R,R)-phytal is the most active diastereomer in both assays, significantly attracting females in a double-choice Y olfactometer, and confirming the previous chromatographic assignment as component of the sex pheromone of the Moroccan locust.

BIOLOGICAL CHEMISTRY DEPARTMENT Nutraceuticals and Free Radicals

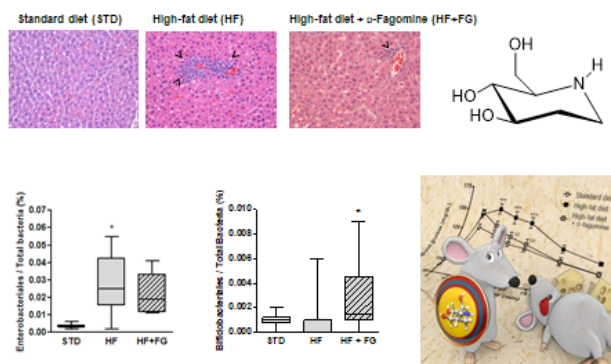
Fat, sugar and pre-diabetic factors

Insulin resistance (IR) and impaired glucose tolerance (IGT) are the first manifestations of diet-induced metabolic alterations leading to Type 2 diabetes, while hypertension is the deadliest risk factor of cardiovascular disease. We examined the roles of dietary fat and fructose in the development of IR, IGT, and hypertension in male Wistar-Kyoto (WKY) rats in a 24-week study. Fat affects IR and IGT earlier than fructose through low-grade systemic inflammation evidenced by liver inflammatory infiltration without triggering hypertension. Increased populations of gut Enterobacteriales and Escherichia coli may contribute to systemic inflammation. Unlike fat, fructose induces increased levels of diacylglycerols (lipid mediators of IR) in the liver, urine F2-isoprostanes (markers of systemic oxidative stress), and uric acid, and hypertension. Dietary fat and fructose trigger IR and IGT in clearly differentiated ways in WKY rats: early low-grade inflammation and late direct lipid toxicity, respectively; gut microbiota plays a role mainly in fat-induced IR, and hypertension is independent of inflammation-mediated IR.

Ramos-Romero, S., et al. (2018). "Mechanistically different effects of fat and sugar on insulin resistance, hypertension, and gut microbiota in rats." *American Journal of Physiology-Endocrinology and Metabolism* 314(6): E552-E563.

The iminosugar D-Fagomine counteracts fat-induced pre-diabetes

D-Fagomine delays the development of a fat-induced pre-diabetes in Wistar-Kyoto rats by reducing low-grade inflammation. The variables measured were fasting blood glucose and insulin levels; glucose tolerance; diacylglycerols as intracellular mediators of insulin resistance in adipose tissue (AT), liver, and muscle; inflammation markers (plasma IL-6 and leptin, and liver and AT histology markers); eicosanoids from arachidonic acid as lipid mediators of inflammation; and the populations of Bacteroidetes, Firmicutes, Enterobacteriales, and



Bifidobacteriales in feces. It was found that D-fagomine reduces fat-induced IGT, inflammation markers, and mediators (hepatic microgranulomas and lobular inflammation, plasma IL-6, prostaglandin E2, and leukotriene B4) while attenuating the changes in the populations of Enterobacteriales. We suggest that the anti-inflammatory effect of D-fagomine may be linked to a reduction in fat-induced overpopulation of minor gut bacteria such as *Escherichia coli*. Ramos-Romero, S., et al. (2018). "Functional effects of the buckwheat iminosugar D-fagomine on rats with diet-induced prediabetes." *Molecular nutrition & food research* 62(16): e1800373-e1800373.

BIOLOGICAL CHEMISTRY DEPARTMENT

Unit of Glycoconjugate Chemistry

The aim of the Unit is to study biochemical or medicinal chemistry issues by using chemical methodologies. Most frequently used tools are peptide and carbohydrate chemistry, halogenation reactions, aqueous organometallic catalysis and proteomic techniques. Traditional fields of interest are enzyme catalysis, pain and immunity related mechanisms (glycobiology), and drug discovery projects to search for transthyretin amyloidosis inhibitors and recently, for Alzheimer's Disease (AD) interfering compounds. These activities are carried out in multidisciplinary projects involving computer scientists, biochemical, biological, pharmacological, conformational (NMR), crystallographic and nuclear chemistry groups at national and international level.



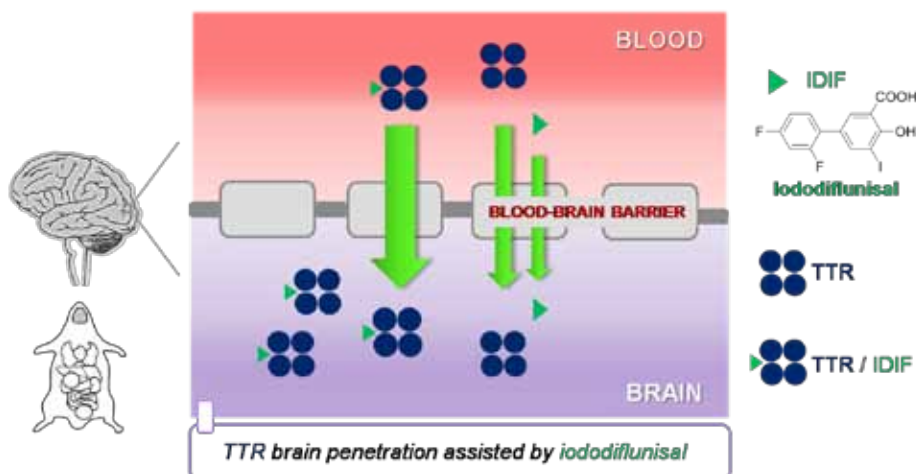
Drug discovery of small-molecule chaperones of the interaction of transthyretin and Abeta peptides as drug candidates for Alzheimer's disease.

These studies are an extension of the drug discovery effort initiated in year 2000 to find drug candidates for a group of rare diseases associated to transthyretin (TTR) which is a thyroid hormone transporter protein. These systemic amyloid diseases are always triggered by single point hereditary or spontaneous mutations on the protein. We searched for small-molecule compounds that stabilize the TTR tetrameric structure, preventing its dissociation and further misfolding and aggregation of its monomers into amyloid fibrils and deposits.

We found that a particular set of TTR stabilizing compounds favor the formation of TTR-A β interactions when studied in vitro. These results have prompted us to study the activity of one of such compounds, namely Iododiflunisal (IDIF), when administered in an AD animal model.

Previous in vivo studies have shown that IDIF orally administered to the AD mouse model A β PPswe/PS1A246E/TTR+/- (AD/TTR+/-) decreases brain A β levels and deposition and improves cognitive functions, suggesting that TTR acts as a carrier in brain A β efflux at the BBB. This work continued throughout

a project of Fundació La Marató de TV3 (year 2015). The DRUG DISCOVERY project aimed at the characterization of the molecular events involved in these physiological events and to identify small-molecule drugs with similar activity profiles by applying drug repurposing methodologies. The consortia integrated five multidisciplinary research teams with tracked expertise in different disciplines and with a translational vision. The project gathered experts in computational chemistry, medicinal chemistry/radiochemistry, structural and cell biology, molecular neurobiology of AD and molecular imaging.



By structural and computational studies we have found that Abeta(12–28) is the main recognition element of the Abeta peptide in the interaction with TTR. The NMR results, assisted by molecular modeling protocols, have provided the first structural model for the TTR-Abeta interaction, as well as for the ternary complex formed in the presence of IDIF. In vivo intravenously administered IDIF can modulate BBB-crossing

capacity of TTR, while the formation of the TTR-IDIF complex enhances the BBB penetration capacity of both TTR and IDIF. By combining cutting-edge basic and translational research, we aim at identifying one SMC candidate to undergo clinical trials as disease-modifying drug for AD.

SURFACTANTS
AND
NANO BIO
TECHNOLOGY
DEPARTMENT
N u c l e i c
A c i d s
C h e m i s t r y

Synthesis of nanodrugs for the treatment of metastasis

An important result was obtained in a long-term collaboration with the group of Dr. Ramon Mangués (Hospital de Sant Pau) and the group of Drs. Antonio Villaverde and Esther Vázquez (UAB) under the umbrella of CIBER-BBN. A nanodrug against colorectal cancer metastasis was demonstrated to be functional in mice models. The new nanomedicine consisted in an engineered protein with high affinity to cancer stem cells functionalized with small oligomers of 5-fluorouracil derivatives. The nanodrug is able to bind specifically to target metastatic cells and internalize. After internalization the 5-fluorouracil derivatives are released to destroy the cancer cell as a Trojan horse.

Optimization of aptamers and siRNA derivatives

Chemical modification of nucleic acids is an important issue in order to obtain new potential drugs with enhanced nuclease stability and higher affinity to their targets. In collaboration with the group of Alberto Pais (University of Coimbra, Portugal) and Laura Lechuga (ICN2) we were able to design new thrombin binding aptamers modified with short peptides with enhanced binding properties. A detailed structural analysis revealed close contacts between the target thrombin and the short modifying peptide.

The discovery of the RNA interference (RNAi) pathway and the identification of the small interfering RNA (siRNA) molecules as RNAi triggers have paved the way to the development of new medicines. Recently two siRNAs have been approved for clinical use and very soon a novel siRNA may be approved for the control of cholesterol in blood. Due to the high relevance of RNA interference we conducted a systematic study by introducing chemical modifications at siRNA 3'-overhang using both computational and experimental techniques. This study allows us to find simple modifications to obtain modified siRNA more efficient for gene silencing.

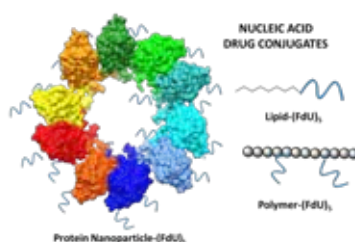
Use of DNA origami to fight drug resistance to cancer drugs

Fluoropyrimidines, such as 5-fluorouracil (5-FU) and related prodrugs are considered one of the most-successful agents in the treatment of colorectal cancer, yet poor specificity and tumor cell resistance remain major limiting bottlenecks. We exploited the ability of two DNA nanostructures, DNA tetrahedron (Td) and rectangle DNA origami, to incorporate 5-fluoro-2'-deoxyuridine (FdUn) oligomers. Both DNA nanostructures attained comparable cytotoxic effect yet Td displays higher antiproliferative action. The study suggests that self-assembled DNA nanoparticles are privileged carriers for delivering fluoropyrimidines, opening new avenues to the development of promising therapeutics for cancer treatment.

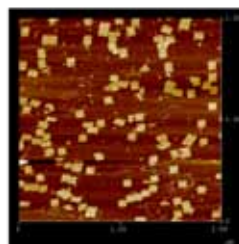
siRNA optimization



Molecularly defined Nanodrugs



DNA origami

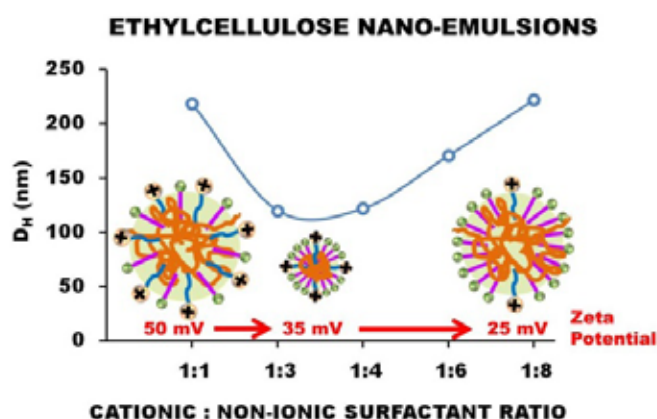


Graphical abstract of the main results obtained by the Nucleic Acids Chemistry group. Synthesis of nanodrugs for the treatment of metastasis. Optimization of siRNA derivatives. Use of DNA origami to fight drug resistance to cancer drugs.

**SURFACTANTS
AND
NANO BIO
TECHNOLOGY
DEPARTMENT
Colloidal
and
Interfacial
Chemistry**

Size and surface charge of ethylcellulose nanoparticles can be modulated through the use of nano-emulsion templates.

Ethylcellulose-loaded nano-emulsions have been obtained by the low-energy phase inversion composition (PIC) method in a system containing a volatile oil dispersed in water by a cationic-nonionic surfactant mixture. The droplet sizes of the nano-emulsions obtained are typically below 200 nm and the zeta potential values are in the range between +10 mV and +50 mV. It is shown that the size and the surface charge of the nano-emulsion droplets can be modulated in a controlled manner by changing composition variables such as the oil-to-surfactant ratio, the cationic to non-ionic surfactant ratio and the ethylcellulose (EC) and water content.



Changes in the droplet size and the surface charge of the nano-emulsions take place following defined trends which are maintained upon EC nanoparticle formation by solvent evaporation.

Calderó et al. Modulating size and surface charge of ethylcellulose nanoparticles through the use of cationic nano-emulsion templates. Carbohydrate Polymers 225 (2019) 115201 <https://doi.org/10.1016/j.carbpol.2019.115201> ; <https://digital.csic.es/handle/10261/192456>

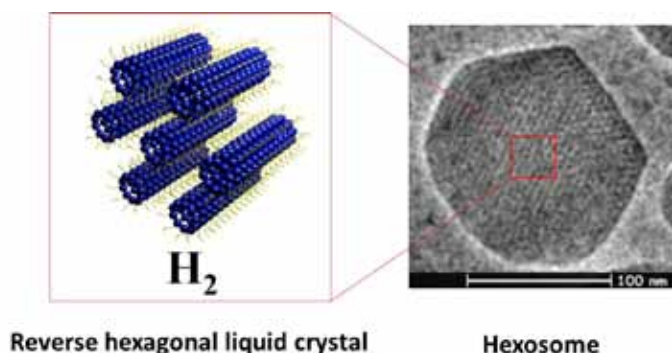
Soft and structured nanoparticles are formulated using a technical grade, biocompatible diglycerol surfactant.

A biocompatible, technical grade diglycerol surfactant forms a reverse hexagonal (H₂) liquid crystal at room temperature upon hydration. A simple method is developed to disperse that liquid crystal into soft structured nanoparticles (hexosomes) with encapsulated active molecules that consists in (1) producing, using ultrasound, a nano-emulsion with surfactant+organic volatile solvent in droplets stabilized by an amphiphilic block copolymer (2) evaporating the solvent to produce hexosomes. The size of the hexosomes and the required ultrasonication time are markedly reduced by using the auxiliary solvent. Dynamic light scattering shows that the size of the hexosomes decreases as the concentration of stabilizer copolymer or encapsulated active

molecule increase. In vitro experiments showed that the release of the active molecule from the hexosomes is pH-dependent, which has interesting implications in potential oral administration.

Magaña et al. Formulating stable hexosome dispersions with a technical grade diglycerol based surfactant. Journal of Colloid and Interface Science 550 (2019) 73–80

<https://doi.org/10.1016/j.jcis.2019.04.084>;
<https://digital.csic.es/handle/10261/184861>



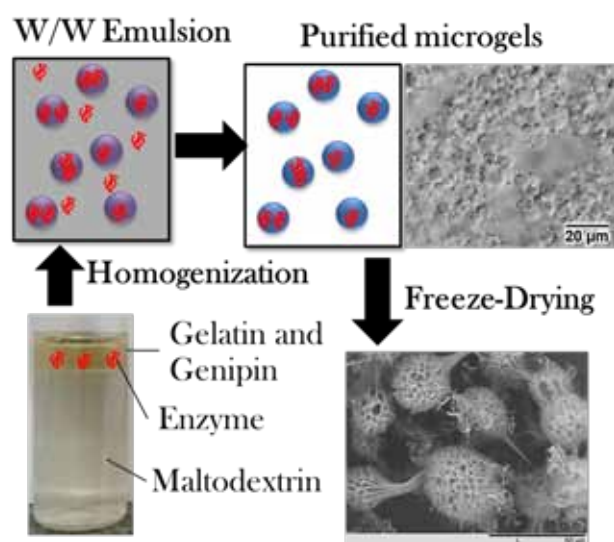
SURFACTANTS AND NANO BIO TECHNOLOGY DEPARTMENT Surface Chemistry

ENCAPSULATION OF LACTASE IN GENIPIN-CROSSLINKED GELATIN MICROGELS, OBTAINED IN WATER-IN-WATER (W/W) EMULSIONS.

Lactose intolerant people cannot consume milk dairy products, unless lactose has been previously removed, due to absence of the enzyme lactase (β -Galactosidase). Immobilization of β -Gal has a great interest in industrial production of lactose-free milk, as direct addition of β -Gal into dairy products is inefficient. We studied the formation of gelatin microgels in gelatin-in-maltodextrin water-in-water emulsions. Gelation of the dispersed gelatin droplets was induced by cooling and crosslinking with genipin, which is a natural crosslinking

reagent. The enzyme lactase was incorporated into the microgels, optimizing encapsulation yield and activity recovery. Microgel particles, loaded with the enzyme, could be freeze-dried, and the enzyme remained active after a complete cycle of freeze-drying and rehydration. The stability of the enzyme at 37 °C under gastric and neutral pH conditions was tested and led to the conclusion that the crosslinked microgels could be suitable for food-industry, where β -Gal carriers are of interest for hydrolyzing lactose in milk products.

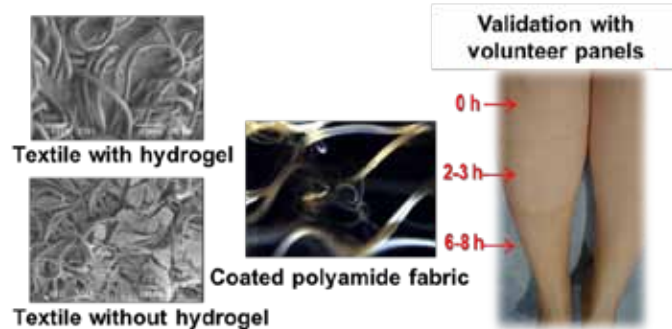
Y. Beldengrün et al, Langmuir, 34 (2018), 9731-9743.



POLYAMIDE FABRICS, COATED WITH DIHYDROXYACETONE-LOADED CHITOSAN HYDROGELS, FOR COSMETO-TEXTILE APPLICATIONS.

Cosmeto-textiles can allow the administration of molecules when in contact with the skin, and then are increasingly developed by cosmetic industries. We designed an innovative approach for cosmeto-textile products, based on the impregnation of textile fibers with chitosan hydrogels, which have been loaded with active components. As an illustrative example, an active with tanning effects (dihydroxyacetone, DHA) was incorporated into polyamide fabrics coated with chitosan hydrogels crosslinked with genipin. These coated textile materials were characterized and the release of DHA was evaluated. Finally, the performance

of fabrics as cosmeto-textiles, with a tanning effect, was evaluated by skin-colorimetry, measured with an evaluation panel of 10 people in collaboration with AITEX technological center. The results clearly proved that DHA-loaded textiles had a tanning effect. Thus, we concluded that the incorporation of DHA-loaded chitosan hydrogels into polyamide fabrics represents a friendly and appropriate strategy to obtain a cosmeto-textile product.

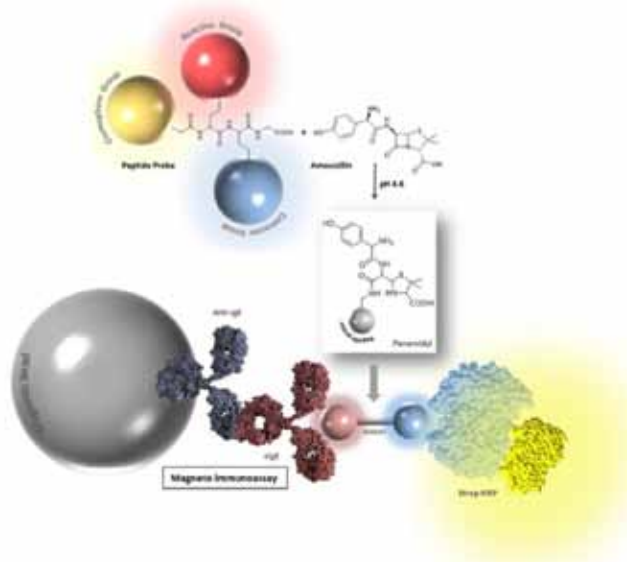


I. Solé et al, Journal of Industrial Textiles, 9 (2019), 1-17.

SURFACTANTS
AND
NANOBIOTECHNOLOGY
DEPARTMENT
N a n o b i o
t e c h n o l o g y
f o r
D i a g n o s t i c s
(N b 4 D)

Immediate hypersensitivity to penicillins. Identification of a new antigenic determinant

The study of adverse drug reactions (ADRs) constitutes a challenge in the area of Medicine. Drugs generate a large number of the total registered hypersensitivity reactions, where penicillins are responsible for more than half of them. In vitro tests in the market are not efficient enough since they lack in sensitivity and specificity. This is the reason why in vivo tests are carried out, with the subsequent danger to the patient's life. It is essential to discover new β -lactam antigenic determinants to develop more effective detection systems and thus, obtain better explanations of the allergic mechanisms related to these drugs. We propose a strategy based on the use of "peptide probes", small labeled and chemical active peptides which have been structurally modified for reacting with the β -lactam moiety at different conditions. The probes also contain a biotin group for application in an immunoassay format. Three different amoxicillin adducts have been obtained, purified and characterized by HPLC-MS and NMR techniques. These results have helped us to elucidate and propose a new antigenic determinant for β -lactams, named the "penamidyl" epitope. All the adducts have been validated and evaluated with sera from different penicillin allergic patients by means of a Magneto-ELISA, immunochemical technique that has allowed us to detect specific IgEs in a very high percentage of the serum samples. An immunoassay has been developed, validated and applied as a diagnostic tool for the detection of specific IgEs in the sera of penicillin allergic patients using a new antigenic determinant.



Enzyme-linked immunosorbent assays for therapeutic drug monitoring coumarin oral anticoagulants in plasma

The development of high-throughput immunochemical assays to assist on precision medicine for patients treated with coumarin oral anticoagulants (OA) is reported. The assays are able to quantitate Warfarin (W) and/or Acenocoumarol (ACL) directly in plasma samples without any previous sample pretreatment. The detectabilities (W, 3.52 ± 2.25 nM and ACL, 1.56 ± 0.64 nM) and the working ranges achieved (W, 1.19 ± 0.73 to 12.05 ± 2.99 nM and ACL 0.63 ± 0.20

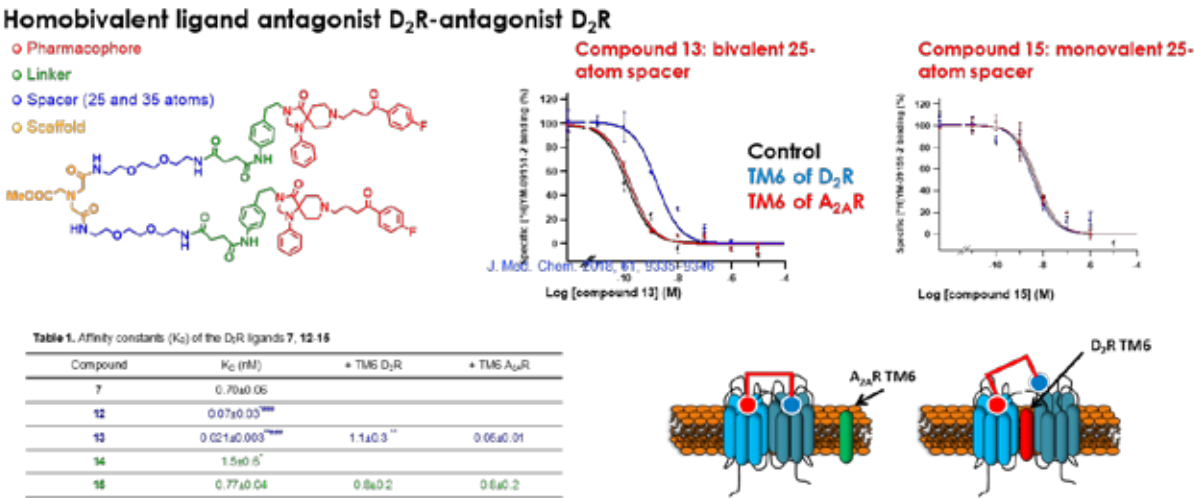
to 10.19 ± 6.69 nM) are within the therapeutic levels usually found in patients treated with these drugs. The assays are specific with only cross-recognition of 4'-NH₂-ACL on the ACL ELISA, which is one of the main metabolites of this drug. Moreover, accuracy studies performed with blind spiked samples show very good correlation between the spiked and the measured concentrations. Finally, a small clinical pilot study has been performed analyzing 96 plasma samples from treated and untreated patients, showing that the assay is able to quantitate ACL. The results obtained allow envisaging the possibility to use these assays for pharmacokinetic studies, dosage assessment or therapeutic drug monitoring.

Since 2018, Nb4D participates, in collaboration with the Fundació Hospital Universitari Vall d'Hebron – Institut de Recerca (VHIR) in the project “Ús de molècules de senyalització del Quòrum Sensing com a eines pel diagnòstic d'infeccions bacterianes”, granted by the Patronat de la Fundació de la Marató de TV3 of 2017.

The final aim of this project is to develop fast and accurate diagnosis methods for the detection of two important pathogenic microorganisms (Pseudomonas aeruginosa and Staphylococcus aureus) through immunochemical studies of their Quorum Sensing (QS) system. In addition, the setting up of these technologies will help on understanding the mechanisms involved in the pathogenesis caused by these two bacteria. The above mentioned pathogens are between the most commonly isolated microorganisms in healthcare associated and community acquired infections among other important diseases.

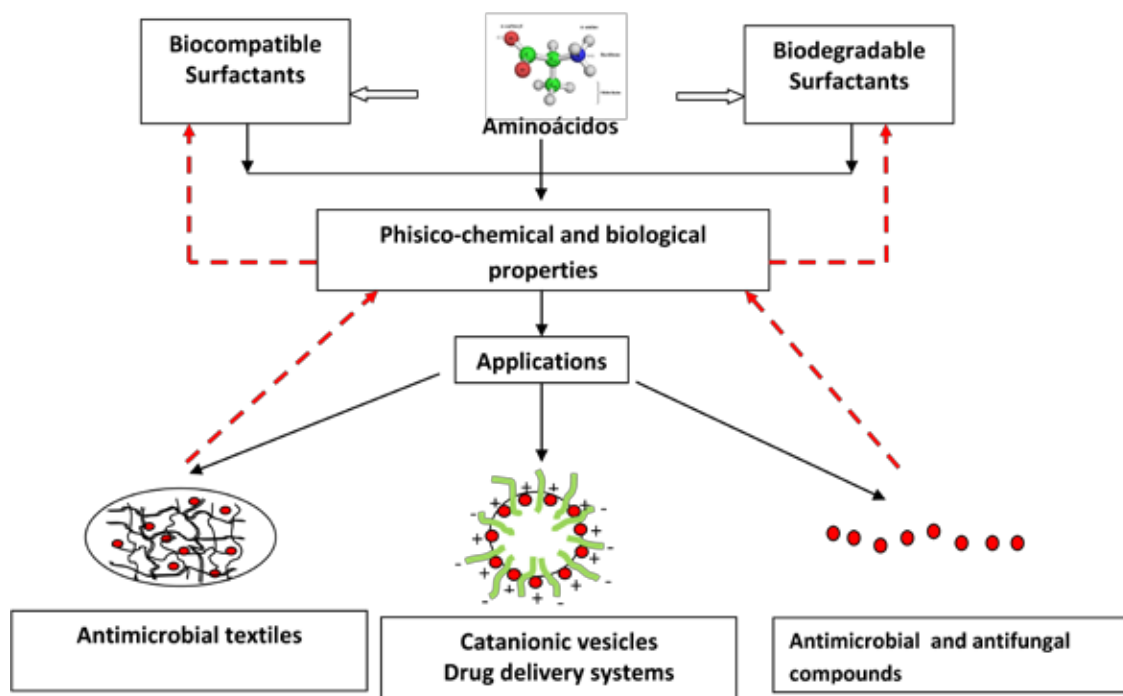
SURFACTANTS
AND
NANOBIOTECHNOLOGY
DEPARTMENT
Multivalent
Systems for
Nanomedicine
(MS4N)

MS4N group has developed a strategy that allows us to generate high affinity bivalent ligands and corroborate unequivocally their simultaneous mode of action. As a proof of concept they have designed and synthesized a bivalent ligand for D₂R-D₂R homodimers with picomolar affinity in native tissue. Using “disturbing transmembrane peptides” that disturbs the dimerization the simultaneous interaction of the bivalent ligand has been confirmed. This strategy is applied to to explore bivalent ligands as novel therapeutics for motor dysfunctions.



**SURFACTANTS
AND
NANO BIO
TECHNOLOGY
DEPARTMENT**
Biocompatible
Surfactants
and Ionic
Liquids
(BSILs)

- Design and development of amino acid-based surfactants and ionic liquids from renewable raw materials with high antimicrobial activity, low cell toxicity and, low environmental impact. The compounds are prepared following the requirements of Green Chemistry, using renewable, energy efficient and water-based synthetic approaches. Optimization of structural parameters in order to obtain biodegradable and biocompatible cationic amphiphiles with selectivity against bacterial membranes.
- Development of new strategies based on biocompatible surfactants and ionic liquids that can prevent and control bacterial growth and biofilm formation.
- Formulation of new nanostructured systems, i.e., eco-friendly catanionic vesicles in order to maximize the efficiency of antimicrobial surfactants.
- Design of formulations able to give antimicrobial properties to medical textiles. Development of simple strategies to adhere these compounds to textiles in order to prevent the growth of bacteria and biofilms.
- Study of the self-aggregation properties of both the pure surfactants in aqueous medium as well as the different formulations prepared with the biocompatible amphiphiles.
- Evaluation of antimicrobial and antibiofilm activity of pure compounds, catanionic formulations and modified textiles against different Gram-negative, Gram-positive and fungi.
- Study of the potential toxicity of these compounds and formulations to asses' human risk by in vitro assays.
- Study of the potential environmental impact of the new surfactants and ionic liquids by evaluating their biodegradability and eco-toxicity.



SURFACTANTS
AND
NANOBIOTECHNOLOGY
DEPARTMENT
Physical
Chemistry of
Surfactant
Systems

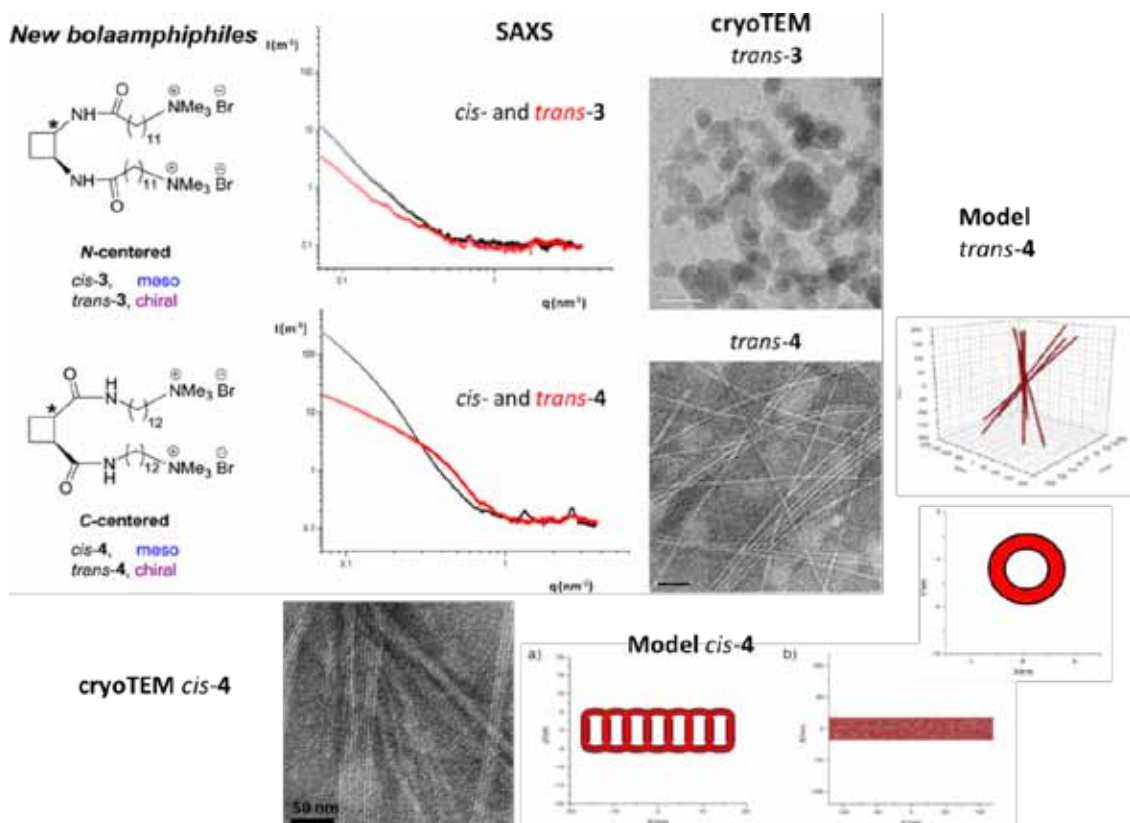
Figure 1. N-centered and C-centered bolaamphiphiles derived either from diamino or diacid cyclobutane in their meso and chiral forms self-assemble in water either in nondistinct structures (compatible with bilayer fragments) or in filaments (cylinders) depending on the intra- or intermolecular hydrogen bonding patterns. (Langmuir, 34, 11424-11432, 2018).

Some of the researches have been directed to the study of new amphiphiles, both derived from natural amino acids as well as artificial ones built using the cyclobutane scaffold. In particular, stereoisomerism and hydrogen binding capability strongly influences the shape of the structures formed by self-assembly of such molecules. Tridimensional modeling of the structures together with visualization with cryo-TEM allows to obtaining details of the structures through the fitting of SAXS spectra.

New gemini histidine surfactants have low cmc values and reduced the surface tension of water solutions at very low concentrations. SAXS measurements indicate that at low concentrations in aqueous solutions these compounds form triaxial core shell ellipsoids.

Much effort has also been directed to the determination of the situation of additives at liposome bilayers. The specific location of drugs in liposomes allows to rationalize the availability of drugs carried by liposomes.

Through the use of new low-cost high-performance computing capabilities the group has renovated the efforts directed to making user friendly tools for the interpretation x-ray scattering of nanostructures and other low crystallinity systems such as low crystallinity proteins.



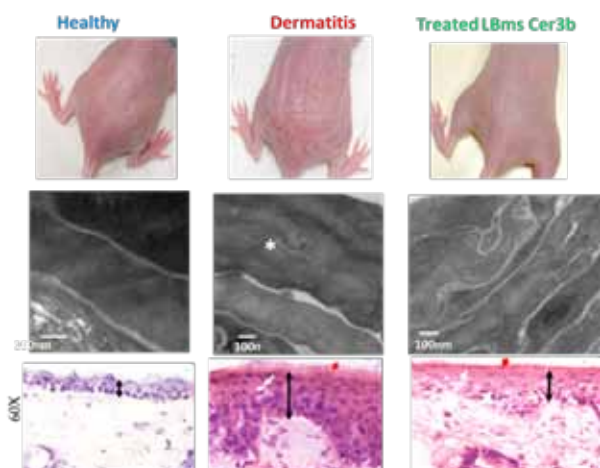
**SURFACTANTS
AND
NANO BIO
TECHNOLOGY
DEPARTMENT
Biophysics
of Lipids and
Interphases
(BLI)**

Lamellar body mimetic system for skin treatment

Epidermal lamellar bodies are responsible to form the barrier function of the skin. Our research group has developed a nanostructured lipid system that mimicks the epidermal lamellar bodies in morphology, composition and function. This mimetic system penetrates and is retained into the skin, improving the lipid matrix and the barrier function in healthy and damaged skin. In a dermatitis mouse model, the treatment with our system reduced inflammation and improved the typical skin lesions of dermatitis condition.

Vesicular nanostructures composed of oleic acid and phosphatidylcholine: Effect of experimental parameters.

Phospholipids and fatty acids are the main building blocks of biological membranes. Oleic acid is a mono-unsaturated omega-9 fatty acid commonly found in many natural sources. Its characteristic kinked structure grants this molecule with a great number of biological properties. To better understand the role that this kind of fatty acids play into phospholipid membranes, nanostructured systems formed with hydrogenated soy phosphatidylcholine and oleic acid has been studied using cryo-electron microscopy, dynamic light scattering and differential scanning calorimetry. Differences concerning size, morphology and phase behavior are found when these systems are prepared at different conditions of pH and composition. Broadly, alkaline mediums and high proportions of oleic acid reduce the size of the structures and increase the fluidity of the membranes.

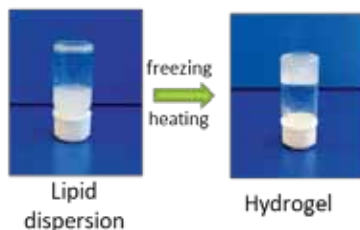


Images of skin surface, microstructure (using TEM) and biopsies from healthy, dermatitis and dermatitis after treatment with lamellar body mimetic system containing ceramides (LBms Cer3b) show the effect of the system on dermatitis condition.

The ease of preparation of these lipid systems, and the response to pH suggests a future use of these systems as model membranes or delivery systems.

Hydrogel composed of phospholipids and free fatty acids with potential biomedical applications.

0.5% Oleic acid + 4.5% HSPC + 95% Water



A hydrogel formed with phospholipids and fatty acids would be of great interest in the medical field due to the biological relevance that these molecules have in living organisms. However, the tendency of phospholipid mixtures to form vesicular or micellar aggregates at high water content hinders the formation of this type of hydrogel. We have prepared a highly hydrated hydrogel (95% water) with hydrogenated phosphatidylcholine and oleic acid. The preparation method involved a freeze-heating cycle of the aqueous lipid mixture, favouring the

supramolecular aggregation of these molecules into a microscopic spongy morphology. Confocal fluorescence imaging showed that the microstructure of the hydrogel is made from the aggregation of giant multilamellar vesicles (5–20 μm diameter) while transmission electron microscopy revealed the existence of nanosized unilamellar vesicles (150 nm diameter) coexisting with lipid lamellae.

Despite this type of aggregation, X-ray scattering experiments performed on the hydrogel show almost no correlation between lipid membranes. In terms of rheological properties, the material shows a prevalent elastic behaviour and low structural strength, a consequence of non-covalent interactions. With such properties and composition, this structured but easily deformable material might become a useful tool for biomedical applications.

SURFACTANTS AND NANOBIOTECHNOLOGY DEPARTMENT Cosmetic and Textile Innovations

Cosmetic and textile Innovations group works in the interphase of textiles and human skin, one of its research lines is based in the study the textile flame retardants toxicity via dermal path

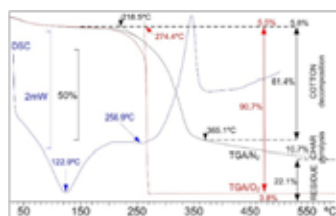
LIFE-FLAREX is a project with the aim of contribute to the mitigation of the environmental and health impacts caused by toxic compounds resulting from bromide-, formaldehyde- and antimony- containing FR textile finishing products on European ecosystems, by analyzing the best available textile finishing products and implementing those innovative technologies for FR applications. The project will demonstrate that the alternative FR products are economically and environmentally viable and do not represent a concerning health risk to humans or animals.

This LIFE Environmental Policy and Governance project, groups four textile clusters from Spain, Italy and Czech Republic (AEI TÈXTILS, ATEVAL, CLUTEX and CS-POINTEX) which represent the industrial textile sector of their countries and also, joins two technological centers from Spain and Belgium (LEITAT and CENTEXBEL) and a Spanish research center (IQAC) that belongs to the Spanish Research Council (CSIC). IP: L. Coderch, M. Martí, A. Manuch.

TEXTILES

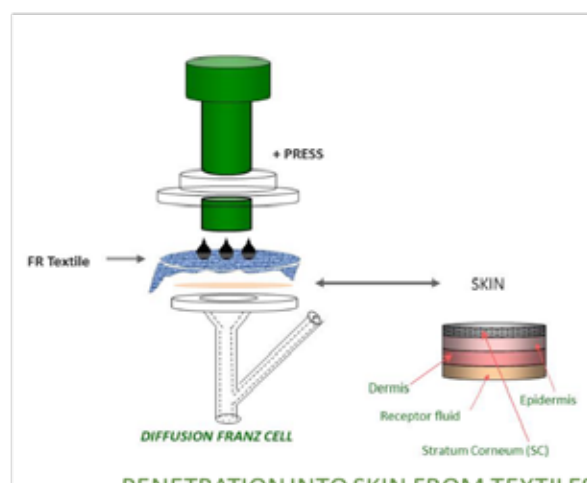


CHEMICAL PRODUCTS COSMETIC PRODUCTS



**TGA/DSC CHARACTERIZATION
TEXTILE FLAME RETARDANTS**

HUMAN SKIN



**PENETRATION INTO SKIN FROM TEXTILES
TOXICOLOGIC ASSESS**



TEACHING ACTIVITIES

Training courses

- R. Eritja. 2018 and 2019. Ph.D. course: "Genetic and Molecular Bases of Biotechnology" (GMBB, Biotechnology) U. of Barcelona.
- R. Eritja. 2018 and 2019. "Biomolecular Biosciences" 4^o course of the Nanoscience and Nanotechnology Grade, Faculty of Sciences, Autonomous University of Barcelona (UAB).
- R. Eritja. "A Corbella Summer School on Organic Synthesis". Gargnano, Italy. 10-14 June 2018. Title of the conference: Controlled organization of matter by DNA origami. Applications in life sciences.
- Emulsiones. Course for a company, 23/07/2018-25/07/2018.
- Tecnologías Avanzadas de Encapsulación, Consorci Universitat Internacional Menéndez Pelayo de Barcelona (CUIMPB) - Centre Ernest Lluch. Centre QCI, Barcelona, 01/10/2018-04/10/2018.
- Tecnologías de Nano y Microencapsulación, Consorci Universitat Internacional Menéndez Pelayo de Barcelona (CUIMPB) - Centre Ernest Lluch. Centre QCI, Barcelona, 15/10/2019-18/10/2019.
- Emulsiones. Course for the Company HIPRA (Amer, Girona), 23/07/2018-25/07/2018. Jordi Esquena, Susana Vilchez and Jonathan Miras (Surface Chemistry Group) and Carlos Rodríguez and Gabriela Calderó (Colloidal and Interfacial Chemistry Group).
- Curso básico Los tensioactivos y sus aplicaciones, Comité Español de la Detergencia, Tensioactivos y Afines (CED), Barcelona 10/04/2018; Valencia 05/06/2018; Sevilla 12/06/2018; Valencia 04/06/2019. Susana Vilchez and Jonathan Miras.
- Tecnologías Avanzadas de Encapsulación, Consorci Universitat Internacional Menéndez Pelayo de Barcelona (CUIMPB) - Centre Ernest Lluch. Centre QCI, Barcelona, 01/10/2018-04/10/2018. Jordi Esquena, Susana Vilchez and Jonathan Miras (Surface Chemistry Group) and Carlos Rodríguez and Gabriela Calderó (Colloidal and Interfacial Chemistry Group).
- Tecnologías de Nano y Microencapsulación, Consorci Universitat Internacional Menéndez Pelayo de Barcelona (CUIMPB) - Centre Ernest Lluch. Centre QCI, Barcelona, 15/10/2019-18/10/2019. Jordi Esquena, Susana Vilchez and Jonathan Miras (Surface Chemistry Group) and Carlos Rodríguez and Gabriela Calderó (Colloidal and Interfacial Chemistry Group).
- Practical Sessions of the "Master in Cosmética y Dermofarmacia" of "Centro de Estudios Superiores de la Industria Farmacéutica, CESIF". Organized every year (29/05-26/06/2018 and 29/05-26/06/2019). Coordinator Jordi Esquena.
- M. Martí gave the course on Textile Materials and their Care in CEICID (Centro De Estudios E Investigacion De Ciencias Domesticas) in Pamplona. October 2019.
- A. M. Manich participate in the course on Introduction of Statistical Experimental Desing at the IQAC/IDAEA- CSIC (Curso de Postgrado y Especialización)UIMP (Centre Ernest Lluc) from 19 to 23 of november 2018
- A. M. Manich participate in the course on Introduction of Statistical Experimental Desing at the UIMP (Centre Ernest Lluc) from 5 to 13 of june 2019
- A. M. Manich participate in the course on Introduction of Statistical Experimental Desing at the IQAC/IDAEA- CSIC (Curso de Postgrado y Especialización)UIMP (Centre Ernest Lluc) from 18 to 22 of november 2019

- I. Alfonso. Lecture: "DYNAMIC NMR & CHEMICAL EXCHANGE" at the XIII Manuel Rico NMR School, Jaca, Spain, June 2019.
- Master's course at the Universitat de Barcelona in "Molecular Biotechnology" 2013-2014; 2014-2015; 2015-2016; 2016-2017; 2017-2018, November 2018-2019 Lecture: Engineering of D-fructose-6-phosphate aldolase for exploitation in organic chemistry.
- Ramon Crehuet, "Python para científicos" March 2018, CSIC Training Plan(30 horas)
- Ramon Crehuet & Fermín Huarte (UB), teachers and organizers of the course "Python for Scientists" at the ICIQ, July 2018 (30 hours)
- Ramon Crehuet & Fermín Huarte (UB), teachers and organizers of the course "Python for Scientists" at the Universitat de Barcelona (post-graduate course), June 2019 (30 hours)
- Sara Ramos-Romero. Faculty of Biology. University of Barcelona. Assistant Professor (Profesora asociada, part time compatible with CSIC). Theory and Practice teaching, Physiology Section of Departament of Cellular Biology, Physiology and Immunology. September 2018 to September 2019
- M. José Bleda, "Estadística Aplicada I (Estadística básica)" April 2018 and May 2019, CSIC Training Plan (25 hours).
- M. José Bleda, "Introducción al software estadístico R. Aplicaciones en estadística básica" October 2018 and 2019, CSIC Training pPlan (25 horas).
- M. José Bleda, Albert Manich. "Introducción al diseño de experimentos" November 2018, CSIC Training Plan (25 hours).
- M.J. Bleda, A. Manich. (20 hours) "Introducción al diseño de experimentos". Consorci Universitat Internacional Menendez Pelayo Barcelona (CUIMPB) - Centre Ernest Lluch taught in the IQAC, Barcelona, June 2019.
- M. José Bleda, Albert Manich. "Investigación eficiente: herramientas estadísticas de diseño y análisis experimental" November 2019, CSIC Training Plan (25 hours).

Master courses

- "Surfactants" within the course "Pharmaceutical Nanotechnology", Máster en Nanociencia y Nanotecnología, Faculty of Pharmacy and Food Sciences, University of Barcelona, 2018, 2019.
- "Tensioactivos", within the course "Desarrollo y formulación de formas farmacéuticas" Máster en Investigación, Desarrollo y Control de Medicamentos (RDCM)", Faculty of Pharmacy and Food Sciences, University of Barcelona, 2018, 2019.
- Profesor del Máster "Nanociencia y Nanotecnología (NANO)", sobre "Formation, Characterization and Stability of Emulsions" (2 horas), Facultad de Farmacia, Universidad de Barcelona, 24/10/2018 and 30/10/2019. Jordi Esquena and Carlos Rodríguez
- Profesor del "Máster en Investigación, Desarrollo y Control de Medicamentos (RDCM)", sobre "Formation, Characterization and Stability of Emulsions" (2 horas), Facultad de Farmacia, Universidad de Barcelona, 25/10/2018 and 16/10/2019. Jordi Esquena and Carlos Rodríguez.
- I. Alfonso. Lecture "Supramolecular Chemistry" at the Master Interuniversitario en Química Sostenible, Universitat Jaume I, Castellón, Spain. 10 hours/year in 2018 and 2019.
- Ramon Crehuet, 2018. Teacher in the "Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry" Interuniversity Master (UB-UPC)
- Sara Ramos-Romero. Open University of Catalonia (Universitat Oberta de Catalunya). Consultant Professor. Supervisor of Master Theses in Nutrition and Health. September 2018 to september 2019
- Josep Lluís Torres. Faculty of Pharmacy, University of Barcelona. Invited Professor. Master Program in Molecular Biotechnology. October 2018, 2019

SCIENTIFIC RESULTS

SCI publications

BIOLOGICAL CHEMISTRY DEPARTMENT Supramolecular Chemistry

- Aguiló, E.; Moro, A. J.; Gavara, R.; Alfonso, I.; Pérez, Y.; Zaccaria, F.; Fonseca Guerra, C.; Malfois, M.; Baucells, C.; Ferrer, M.; Lima, J. C.; Rodríguez, L.; Reversible Self-Assembly of Water-Soluble Gold(I) Complexes, *Inorg. Chem.* 2018, 57, 1017-1028. Front Cover and ACS Editor's Choice. DOI: 10.1021/acs.inorgchem.7b02343.
- Puig-Castellví, F.; Bedia, C.; Alfonso, I.; Piña, B.; Tauler, R.; Deciphering the underlying metabolomic and lipidomic patterns linked to thermal acclimation in *Saccharomyces cerevisiae*; *J. Proteome Res.* 2018, 17, 2034-2044. DOI:10.1021/acs.jproteome.7b00921.
- Puig-Castellví, F.; Pérez, Y.; Piña, B.; Tauler, R.; Alfonso, I.; Compression of multidimensional NMR spectra allows a faster and more accurate analysis of complex samples, *Chem. Commun.* 2018, 54, 3090-3093, Inside Front Cover. DOI: 10.1039/c7cc09891j.
- Lafuente, M.; Solà, J.; Alfonso, I.; A dynamic chemical network for cystinuria diagnosis, *Angew. Chem. Int. Ed.* 2018, 57, 8421-8424, Inside Front Cover. DOI: 10.1002/anie.201802189.
- Corredor, M.; Carbajo, D.; Domingo, C.; Pérez, Y.; Bujons, J.; Messegue, A.; Alfonso, I.; Dynamic covalent identification of an efficient heparin ligand, *Angew. Chem. Int. Ed.* 2018, 57, 11973-11977, Hot Paper. DOI: 10.1002/anie.201806770.
- Puig-Castellví, F.; Pérez, Y.; Piña, B.; Tauler, R.; Alfonso, I.; Comparative analysis of ¹H NMR and ¹H-¹³C HSQC NMR metabolomics to understand the effects of medium composition in yeast growth, *Anal. Chem.* 2018, 90, 12422-12430. DOI: 10.1021/acs.analchem.8b01196.
- Faggi, E.; Luis, S. V.; Alfonso, I.; Sensing, transport and other potential biomedical applications of pseudopeptides, *Curr. Med Chem.* 2019, 26, 4065-4097. DOI: 10.2174/0929867325666180301091040.
- Lafuente, M.; Alfonso, I.; Solà, J.; Structurally selective assembly of a specific macrobicycle from a dynamic library of pseudopeptidic disulfides, *ChemSystemsChem* 2019, 1, 25-31. DOI: 10.1002/syst.201900002.
- Serra-Pont, A.; Alfonso, I.; Solà, J.; Jimeno, C.; An efficient dynamic asymmetric catalytic system within a zinc-templated network, *Chem. Commun.* 2019, 55, 7970-7973, DOI: 10.1039/c9cc03958a.
- Tapia, L.; Pérez, Y.; Bujons, J.; Bolte, M.; Casas, J.; Solà, J.; Quesada, R.; Alfonso, I.*; pH-dependent chloride transport by pseudopeptidic cages for the selective killing of cancer cells in acidic microenvironments, *Angew. Chem. Int. Ed.* 2019, 58, 12465-12468, DOI: 10.1002/anie.201905965.

- Roldán, R.; Hernández, K.; Joglar, J.; Bujons, J.; Parella, T.; Fessner, W.-D.; Clapés, P., Aldolase-Catalyzed Asymmetric Synthesis of N-Heterocycles by Addition of Simple Aliphatic Nucleophiles to Aminoaldehydes. *Adv. Synth. Catal.* 2019, 361 (11), 2673-2687.
- Marín-Valls, R.; Hernández, K.; Bolte, M.; Joglar, J.; Bujons, J.; Clapés, P., Chemoenzymatic Hydroxymethylation of Carboxylic Acids by Tandem Stereodivergent Biocatalytic Aldol Reaction and Chemical Decarboxylation. *ACS Catal.* 2019, 9 (8), 7568-7577.
- Česnik, M.; Sudar, M.; Roldan, R.; Hernandez, K.; Parella, T.; Clapés, P.; Charnock, S.; Vasić-Rački, Đ.; Findrik Blažević, Z., Model-based optimization of the enzymatic aldol addition of propanal to formaldehyde: A first step towards enzymatic synthesis of 3-hydroxybutyric acid. *Chem. Eng. Res. Des.* 2019, 150, 140-152.
- Zhou, T.; Vallooran, J. J.; Assenza, S.; Szekrenyi, A.; Clapés, P.; Mezzenga, R., Efficient Asymmetric Synthesis of Carbohydrates by Aldolase Nano-Confined in Lipidic Cubic Mesophases. *ACS Catal.* 2018, 8 (7), 5810-5815.
- Roldán, R.; Hernandez, K.; Joglar, J.; Bujons, J.; Parella, T.; Sánchez-Moreno, I.; Hélaine, V.; Lemaire, M.; Guérard-Hélaine, C.; Fessner, W.-D.; Clapés, P., Biocatalytic Aldol Addition of Simple Aliphatic Nucleophiles to Hydroxylaldehydes. *ACS Catal.* 2018, 8 (9), 8804-8809.
- Junker, S.; Roldan, R.; Joosten, H.-J.; Clapés, P.; Fessner, W.-D., Complete Switch of Reaction Specificity of an Aldolase by Directed Evolution In Vitro: Synthesis of Generic Aliphatic Aldol Products. *Angew. Chem. Int. Ed.* 2018, 57 (32), 10153-10157.
- Hurtado, C.; Domínguez, C.; Clapés, P.; Bayona, J. M., Determination of the β -glycosylate fraction of contaminants of emerging concern in lettuce (*Lactuca sativa* L.) grown under controlled conditions. *Anal. Bioanal. Chem.* 2018, 410 (23), 5715-5721.
- Hernández, K.; Szekrenyi, A.; Clapés, P., Nucleophile Promiscuity of Natural and Engineered Aldolases. *ChemBioChem* 2018, 19, 1353-1358.
- Hernández, K.; Joglar, J.; Bujons, J.; Parella, T.; Clapés, P., Nucleophile Promiscuity of Engineered Class II Pyruvate Aldolase YfaU from *E. Coli*. *Angew. Chem. Int. Ed.* 2018, 57 (14), 3583-3587.
- Kotronoulas, A.; Gomez-Gómez, A.; Fabregat, A.; Segura, J.; Yang, S.; Xing, Y.; Mutian, W.; Marcos, J.; Ventura, R.; Joglar, J.; Pozo, O.J., Alternative markers for the detection of testosterone misuse. Part I: transdermal administration. *Drug Test. Anal.* 2018, 10, 821-831.
- Kotronoulas, A.; Gomez-Gómez, A.; Fabregat, A.; Segura, J.; Yang, S.; Xing, Y.; Mutian, W.; Marcos, J.; Ventura, R.; Joglar, J.; Pozo, O.J., Alternative markers for the detection of testosterone misuse. Part II: intramuscular administration. *Drug Test. Anal.* 2018, 10, 849-859.
- Corredor, M.; Carbajo, D.; Domingo, C.; Perez, Y.; Bujons, J.; Messegue, A.; Alfonso, I., Dynamic Covalent Identification of an Efficient Heparin Ligand. *Angew Chem Int Ed Engl* 2018, 57 (37), 11973-11977.
- Quintana, M.; Bilbao, A.; Comas Barcelo, J.; Bujons, J.; Triola, G., Identification of benzo[cd]indol-2(1H)-ones as novel Atg4B inhibitors via a structure-based virtual screening and a novel AlphaScreen assay. *Eur.J.Med. Chem.* 2019, 178, 648-666.

BIOLOGICAL CHEMISTRY DEPARTMENT Synthetic Methodology and New Building Blocks

- Wei Wen Chen, Ana B. Cuenca, Alexandr Shafir. The Power of Iodane-Guided C-H Coupling: A Group Transfer Strategy in Which a Halogen Works for Its Money. Mini-Review. *Angew. Chem. Int. Ed.* 2019, ASAP, <https://doi.org/10.1002/anie.201908418>
- A. Bucci, S. S. Mondal, V. Martin-Diaconescu, A. Shafir, J. Lloret-Fillol. Cobalt Amide Imidate Imidazolate Frameworks as Highly Active Oxygen Evolution Model Materials. *ACS Appl. Energy Mater.* 2019, 2, 8930-8938.
- V. Corrales Sánchez, C. Nieto-Jiménez, J. A. Castro-Osma, F. de Andrés, P. J. Pacheco-Liñán, I. Bravo, N. Rodríguez Fariñas, E. Niza, E. Domínguez-Jurado, A. Lara-Sánchez, Á. Ríos, M. Gómez Juárez, J. C. Montero, A. Pandiella, A. Shafir, C. Alonso-Moreno, A. Ocaña. Screening and Preliminary Biochemical and Biological Studies of [RuCl(p-cymene)(N,N-bis(diphenylphosphino)-isopropylamine)][BF₄] in Breast Cancer Models. *ACS Omega* 2019, 4, 13005–13014.
- Y. A. Vlasenko, P. S. Postnikov, M. E. Trusova, A. Shafir, V. V. Zhdankin, A. Yoshimura, M. S. Yusubov. Synthesis of Five-Membered Iodine–Nitrogen Heterocycles from Benzimidazole-Based Iodonium Salts. *J. Org. Chem.* 2018, 83, 12056-12070.
- Y. Wu, S. Bouvet, S. Izquierdo, A. Shafir. Synthesis of Polysubstituted Iodoarenes Enabled by Iterative Iodine-Directed para and ortho C-H Functionalization. *Angew. Chem. Int. Ed.* 2019, 58, 2617-2621.

BIOLOGICAL CHEMISTRY DEPARTMENT Theoretical and Computational Chemistry

- Josep M. Anglada, Albert Solé. Tropospheric oxidation of methyl hydrotrioxide (CH₃OOOH) by hydroxyl radical *Phys. Chem. Chem. Phys.*, 2018, 20, 27406-27417. DOI: 10.1039/c8cp04486d
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- Ana Sanchís. Immunoassay and amperometric biosensor approaches for the detection of deltamethrin in seawater – 11th Ibero-American Congress on Sensors and XXIII Transfrontier Meeting on Sensors and Biosensors. 17th-21th September 2018. Barcelona, Spain
- Klaudia Kopper. Multiplexed amperometric determination of environmental pollutants in sea water – 11th Ibero-American Congress on Sensors and XXIII Transfrontier Meeting on Sensors and Biosensors. 17th-21th September 2018. Barcelona, Spain
- Daniel Pulido. Sexto Encuentro sobre Dendrimeros (Eden VI). Sevilla, 22-23 February 2018. "Multivalent Oligoethylen Glycol (OEG) dendritic platform as chemical tools to study GPCR oligomerization".
- Edgar Cristóbal. 6th Young Research Symposium. Madrid, 21 June 2019. "Synthesis of cholesteryl-PEGn-peptide conjugates with highly monodisperse PEG lengths"
- Ramon Pons*, Bernat Pi-Boleda, Alessandro Sorrenti, Marta Sans, Ona Illa, Vicenç Branchadell, Rosa M. Ortuño. Cyclobutane Scaffold in Bolaamphiphiles: Effect of Diastereoisomerism and Regiochemistry on Their Surface Activity Aggregate Structure. Oral. 32nd ECIS. Ljubljana (Eslovenia). 2/7-9-2018
- AM Manich. "Efecto del engrase y del acabado en la cinética de absorción y desorción de humedad de la piel" (por AM Manich, J Barenys, L Martínez, J Lloria, J Carilla, A Marsal). LXV Congreso Nacional de la Industria del Cuero. Barcelona. 24-25 May 2018. Oral presentation.
- AM Manich. "Análisis Térmico (DSC, TGA) de retardantes de llama textiles con menor impacto ambiental" (by AM Manich, C Alonso, S Pérez-Rentero, L Coderch, M Martí). XXXVII REUNIÓN BIENAL DE LA RSEQ (Simposio2: Calorimetría y Análisis Térmico en la Química actual), Donostia 26/05/2019. Oral presentation.
- S Pérez-Rentero. "Thermal analysis (DSC, TGA) of textile flame retardants with lower environmental impact" (by S Pérez-Rentero, C Alonso, L Coderch, M Martí, and AM Manich). Summer School and Workshop in Calorimetry and Thermal Analysis, Calorimetry and thermal methods in material sciences, Lyon, France, 16-21 June (2019). Oral presentation.
- AM Manich. "Evaluation of Healthy and Ecological friendly Flame Retardants for Textiles using Thermal Analysis" (by AM Manich, S Pérez-Rentero, C Alonso, L Coderch, M Martí). CEEC-TAC5 & MEDICTA2019 CONFERENCE, Rome, Italy, 27-30 August. Oral presentation.
- AMManich. "Thermal Analysis of Healthy and Ecological friendly Flame Retardants for Textiles" (by AM Manich, C Alonso, L Coderch, M Martí, S Pérez-Rentero). International Conference on Engineering ICEUBI2019, Covilhã, Portugal, 27-29 November 2019. Oral presentation.
- C. Jimeno. "Pyridine ligands for asymmetric organocatalysis". 7a Jornadas de la Red de Catálisis Asimétrica. Hondarribia, Spain. October 2018.
- I. Alfonso. "Dynamic covalent identification of an efficient heparin ligand". XXXVII Reunión Bienal de la RSEQ. San Sebastian, Spain. May 2019.
- Precise control of GPCR receptors with light and allosteric photoswitchable ligands in cells and living animals. A. Llebaria. 6th ECBS/LS-EUCHEMS Meeting, April 2019, Madrid
- Juan B. Blanco. "Chemical synthesis of the Hedgehog signaling pathway activating ligand Sonic Hedgehog". XXXVII Reunión Bienal de la Real Sociedad Española de Química. San Sebastián 26/05/2019 - 30/05/2019.
- Roser Marin-Valls, Karel Hernández, Jesús Joglar, Jordi Bujons, Pere Clapés. 3-Methyl-2-oxobutanoate hydroxymethyltransferase (KPHMT) catalyzed synthesis of 2-ketopantoate and homologues aldol addition Biotrans2019 Groningen (The Netherlands) <https://biotrans2019.com/>

- B. Miralles-Pérez, M. R. Nogués, V. Sánchez-Martos, N. Taltavull, M. Hereu, S. Ramos-Romero, J.L. Torres, G. Dasilva, I. Medina, M. Romeu, M. Effects of D-fagomine and omega-3 combination on hepatic oxidative stress in high-fat high-sucrose diet-fed rats. XII GEIRLI Meeting. Faculty of Pharmacy of the University of Barcelona. Barcelona, Spain. 4th July 2019.
- S. Ramos-Romero, M. Hereu, L. Atienza, S. Amézqueta, F. Casas, J. L. Torres. The buckwheat imino-sugar D-fagomine attenuates sucrose-induced steatosis and hypertension in rats. 13th European Nutrition Conference. Malnutrition in an Obese World: European Perspectives. Dublin, Ireland. 15-18 October 2019
- G. Dasilva, S. Lois, S. Muñoz, L. Méndez, N. Taltavull, M.R. Nogués, S. Ramos-Romero, J.L. Torres, I. Medina. The regulation of proresolving lipid mediator profiles in adipose tissue of rats with diet-induced prediabetes. 17th Euro Fed Lipid Congress and Expo. Sevilla, Spain. 20-23 October, 2019
- G. F. de la Fuente, L. A. Angurel, R. Molina, D. Muñoz-Rojas, V. Rico, F. Yubero, A. R. González-Elípe "Metal coatings on glass via Laser Ablation Backwriting" V Congreso Hispano-Luso de Cerámica y Vidrio y LVI Congreso Nacional de la SECV, Barcelona (8-10 October 2018).
- A. Llebaria. Glycosphingolipid and analogues as immunostimulants of NKT cells. 29th International Carbohydrate Symposium, July 2018, Lisboa (Portugal)
- A. Llebaria. Allosteric ligands to control metabotropic glutamate receptors with light. NeuroFrance Meeting 2019, May 2019, Marseille (France)
- A. Llebaria. Glycosphingolipid analogues as immunostimulants of NKT cells. EUROCARB2019, July 2019, Leiden (Netherlands)
- Quero, C. "Nuevos hallazgos dirigidos al desarrollo de un control integrado del perforador del corcho *Coroebus undatus* (Fabricius, 1787) (Coleoptera: Buprestidae). XI Congreso nacional de Entomología aplicada. Madrid, 4-8 november 2019. ORAL COMM
- Gemma Fabrias Domingo, "Ceramidases: Chemical Sensors and Inhibitors". Sphingolipid Biology: Sphingolipids in Physiology and Pathology. FEBS special meeting. Cascais. Portugal. 6/4/2019 - 10/4/2019. Invited communication

Invited talks

- R. Eritja, Oligonucleotide synthesis platform, CIBER-BBN Annual Conference, October 21-22, 2019, Tarragona, Spain.
- R. Eritja, Development of nanomedicines based on nucleic acids. Jorge, A.F., Alagia, A., Aviñó, A., Grijalvo, S., Fàbrega, C., Eritja, R. University of Navarra. April 8, 2019.
- R. Eritja, Historical perspective on oligonucleotide synthesis. First Spanish meeting on oligonucleotide therapeutics (SMOT1). Valencia (Spain), June 1st, 2018 Valencia (Spain).
- R. Eritja, Nuevas estrategias terapéuticas mediante la utilización de ácidos nucleicos. Dellafore, M., Jorge, A.F., Alagia, A., Aviñó, A., Grijalvo, S., Fàbrega, C., Iribarren, A. M., Montserrat, J., Eritja, R. XXII Simposio Nacional de Química Orgánica (XXII SINAQO 2019), November 5-8, 2019, Mendoza, Argentina
- R. Eritja, DNA nanostructures for delivery of therapeutic oligonucleotides. Fàbrega, C., Jorge, A.F., Aviñó, A., Pais, A., Grijalvo, S., Eritja, R. 2on Spanish meeting on oligonucleotide therapeutics (SMOT2). Valencia (Spain), November 28-29, 2019, Valencia (Spain).
- Rodríguez, C. "Surfactant-based formulation of emulsions and derived functional particles at various size scales" 22nd International Symposium on Surfactants in Solution. Oklahoma, USA. June 4-8th, 2018.
- Rodríguez, C.; Shrestha, L.K. Molecular dye self-assemblies as structure directing agents for the fabrication of organic and inorganic fibers at various size scales. 69th Meeting of the Division of Colloid and Surface Chemistry, Tsukuba, Japan, September 18-20th, 2018
- Rodríguez, C. Multiscale Fibrillar Materials from Molecular Ionic Assembly of Dyes. International Symposium of Renewable and Sustainable Materials. Taipei, Taiwan. August 8-10th, 2019.
- Rodríguez, C. Recent Advances in emulsion formulation. Cosmatorium, Barcelona, Spain, October 23-24th, 2019
- Rodríguez, C. Fabrication of Organic-Inorganic Hybrid Colloidal Particles from Emulsions. Okinawa Colloids Conference. Okinawa, Japan. November 3-8th, 2019.
- J. Esquena. Novel emulsion systems and their potential applications. 49 Jornadas Anuales del Comité Español de la Detergencia. Barcelona, Spain. 12/03/2019 - 13/03/2019
- M. Pilar Marco. Challenging diagnostic multiplexation threats through nanobiotechnological approaches. 16th Iberian Peptide Meeting & 4th ChemBio Group Meeting. 5th-7th February 2018. Barcelona, Spain
- M. Pilar Marco. Nanobiotechnological approaches for multiplexed bioanalysis. UNISENSOR Scientific Day, "Innovation In Point of Care Diagnostic". 15th March 2018. Liège, Belgium
- M. Pilar Marco. Immunochemical Diagnostic Strategies based on the Quorum Sensing System (QS-profile). CIBER-BBN 2018 Annual Conference. 12th-13th November 2018. Valladolid, Spain
- Miriam Royo. Multivalent Systems for Nanomedicine. XXIII Semana Científica Antonio González. La Laguna, 1-4 October 2019.
- I. Alfonso. Dynamic pseudopeptidic disulfides: from complexity to applications. I Gordon Conference on Systems Chemistry. Sunday River, Maine, USA. July 2018. Invited Lecture.
- I. Alfonso. The usefulness of Complexity in Molecular Recognition. VI Brazil-Spain Workshop on Organic Chemistry (BSWOC-2018). Oviedo, Spain. October 2018. Keynote Lecture.
- I. Alfonso. Supramolecular approaches to Chemical Biology. 19th Meeting of the Spanish Medicinal Chemistry Society. Vitoria, Spain. July 2019. Invited Lecture.
- I. Alfonso. Molecular recognition in complex chemical systems with biological relevance. Merging

GSO-JMJC-JED Days, Societ  Chimique de France. Montpellier, France. October 2019. Plenary Lecture.

- I. Alfonso. From Supramolecular Chemistry to Chemical Biology. IV QuimBioQuim, CiQUS. Santiago de Compostela, Spain. October 2019. Plenary Lecture.
- I. Alfonso. Supramolecular chemistry with pseudopeptides: from non-covalent interactions to biological applications. Institut de Recerca Biom dica de Barcelona. Barcelona, Spain. May 2018.
- I. Alfonso. Supramolecular and Biological Chemistry: Two sides of the same coin. Universitat de Barcelona. Barcelona, Spain. October 2018.
- Pere Clap s. Evoluci  dirigida: de Charles R. Darwin a Frances H. December 2018. Barcelona (Seu de la Societat Catalana de Qu mica)
- A. Angurel, R. Molina, V. Rico, F. Yubero, A. R. Gonz lez-Elipse, D. Mu oz-Rojas, C. Masse, V. , G. F. de la Fuente. Metal films by Laser Ablation Backwriting on Glass. Science and Applications of Thin Films, Conference & Exhibition (SATF 2018), Cesme, Izmir, Turkey (17-21 September 2018).
- Carlos Rodriguez Abreu. Liquid and liquid crystal dispersions for encapsulation and controlled delivery. Lecture. University of Lille, France, January 2018
- Carlos Rodriguez Abreu. Chromonic liquid crystals : Self assembly and 1D materials. Lecture. Yokohama National University, Japan, December 2018
- Carlos Rodriguez Abreu. Functional materials from emulsions and chromonic self-assemblies. Lecture. Tokyo University of Science, Japan, December 2018
- Carlos Rodriguez Abreu. Formulation of emulsions and their use as templates for the fabrication of colloidal materials at various size scales. Lecture. National Taiwan University of Science and Technology, Taiwan, September 2018
- Jordi Esquena. Hydrogel formation and encapsulation in Water-in-Water emulsions. Seminar. Aalto University, Helsinki, Finland. 11/04/2019.
- Jordi Esquena. Design, properties and applications of porous materials obtained in highly concentrated emulsions. Seminar. Aalto University, Helsinki, Finland. 12/04/2019.
- Olga L pez; Assessment of Skin Treatment with a Lamellar Body Mimicking Lipid System; Gordon Research Conference - Barrier Function of Mammalian Skin, Waterville Valley, New Hampshire, USA, 11th-16th August 2019
- Silvia Panarello, Xavier G mez-Santacana, Control of membrane receptors with photoswitchable allosteric modulators. European School of Medicinal Chemistry (ESMEC), July 2018, Urbino (Italy)
- Maria Ricart-Ortega, Fanny Malhaire, Xavier G mez Santacana, Jean-Philippe Pin, Cyril Goudet and Amadeu Llebaria. Evaluating the influence of applied light on trans and cis alloswitch-1 binding to the metabotropic glutamate receptor mGlu5. 7th annual Meeting GDR3545, GPCR-Physio-Med, October 2018, Strasbourg (France)
- Silvia Panarello, Yevgenii Grushevskyi, Martin J. Lohse and Amadeu Llebaria. Photoswitchable allosteric ligands to decipher spatial and temporal mGluR1 signaling. Second International Symposium on Photopharmacology, November 2018, Vic (Barcelona)
- S. Panarello, X. G mez-Santacana, C. Serra, F. Malhaire, L. Pr zeau, C. Goudet, J-P. Pin, A. Llebaria. Development of novel photoswitchable PAM for the metabotropic glutamate receptor subtype 1 (mGlu1). GPCR International Meeting GDR3545, October 2019, Montpellier (France)
- M. Ricart-Ortega, A.E. Berizzi, V. Pereira, F. Malhaire, X. G mez-Santacana, J. Font, J. Catena, L. Mu oz, C. Serra, X. Rovira, J.P. Pin, C. Goudet and A. Llebaria. Deciphering the influence of applied light on photoswitchable mGlu5 negative allosteric modulators binding. GPCR International Meeting GDR3545, October 2019, Montpellier (France)
-

- Pere Clapés. Evolució dirigida: de Charles R. Darwin a Frances H. Arnold. December 2018. Place Barcelona (Seu de la Societat Catalana de Química)
- Carmen Quero. Desenvolupament de noves estratègies per al control de plagues. Jornada sobre nous reptes en química: nanovesícules i control biològic de plagues. Universitat de Girona, Girona. 20/09/2018
- Carmen Quero. Noves estratègies per al control de plagues. Màster de Química Analítica de l'IQS. Institut Químic de Sarrià, Barcelona. 9/05/2019
- Carmen Quero. Desenvolupament de noves estratègies per al control de plagues. Medi Ambient i Societat: Pautes per a la Gestió Ambiental. Sala Prat de la Riba, Institut d'Estudis Catalans, Barcelona. 5/06/2018
- Ramon Crehuet. Stabilization of alpha-helices by side-chain to main hydrogen bonds. Can current force fields describe the hydrophobic shielding?. 10th Triennial Congress of the International Society for Theoretical Chemical Physics, Trømso, Norway, July 2019
- Ramon Crehuet. How does PCNA slide along DNA?, Linderstrøm-Lang Centre for Protein Science, University of Copenhagen, September 2018.
- Anton Cunillera. The application of iodane-directed C-H allylation as an entry point to structurally diverse organic cores, including the drug analogues. Oral presentation at the 6th Barluenga Conference in Oviedo. November 2019.

RESEARCH TRAINING

Doctoral theses

- **Yoran Beldengrün**

Water-in-Water emulsions for obtaining enzyme-loaded microgels and encapsulated emulsions.

Director: Jordi Esquena Moret
University of Barcelona,
20/07/2018

- **Francesc Puig Castellví**

Development and application of Nuclear Magnetic Resonance spectroscopy and chemometric methods for the analysis of the metabolome of *Saccharomyces cerevisiae* under different growing conditions

Director: Ignacio Alfonso and Romà Tauler
Universitat de Barcelona
10/07/2018

- **Verónica Moner del Moral**

Desarrollo de sistemas lipídicos miméticos a los cuerpos laminares epidérmicos como estrategia de tratamiento de distintas afectaciones cutáneas

Director: Olga López Serrano
University of Barcelona
Faculty of Farmacia
12/12/2018

- **Mercè Hereu Planellas**

Role of D-fagomine and omega-3 polyunsaturated fatty acids on gut microbiota and related metabolic changes in healthy rats and in a model of fat-induced pre-diabetes

Directors: Sara Ramos Romero, Marta Romeu Ferran
Universitat de Barcelona
"Cum laude"
18/07/2019

- **María Lafuente Fabra.**

Study and applications of dynamic chemical networks of pseudopeptidic compounds

Directors: Jordi Solà and Ignacio Alfonso.
Universitat de Barcelona
18/07/2018

- **Mireia Quintana Agustí**

Screening and biological evaluation of novel anticancer agents and lipid profiling of autophagy-related proteins

Director: Gemma Triola
Faculty of Pharmacy
University of Barcelona
29/09/2019

- **Ana Bilbao Girona**

Síntesis de inhibidores de Atg4B y desarrollo de nuevos métodos de bioconjugación basados en derivados del ácido escuárico

Directors: Gemma Triola, Juan B. Blanco
Faculty of Pharmacy
University of Barcelona
29/10/2019

- **Aroa Domínguez Cuadrado.**

Estudios dirigidos a la ecología química de insectos plaga mediante semioquímicos

Programme of Biology.
Directors: Carmen Quero and Angel Guerrero.
Universitat de Barcelona
09/03/2018

- **Ana Sanchís Villariz**

New immunochemical approaches for multiplexed diagnostics.

Directors: M. Pilar Marco, J. P. Salvador
Universidad de Barcelona (UB)
25/07/2018

- **Anna Serra Pont**

Sistemes organocatalítics dinàmics autoassemblats en un metall

Directors: Jordi Solà and Ciril Jimeno.
Universitat de Barcelona
29/10/2018

- **Roser Borràs Tudurí**

Non-glycosidic analogues of alpha-galactosylceramide: design, synthesis and biological activity.

Director: Amadeu Llebaria

Universitat de Barcelona

06/06/2018

- **Anderson Ramos da Silva**

Nuevos tensioactivos catiónicos basados en ramnolípidos y aminoácidos: propiedades fisicoquímicas y biológicas

Directors: Lourdes Pérez and Angeles Manresa
Universitat de Barcelona

Facultat de Farmàcia, Biotecnologia

22/11/2019

CUM LAUDE

Master theses

- **Adrià Pérez Calm**

Synthesis and characterization of perylene-based building blocks for the fabrication of optically-active nanostructured materials.

Directors: Jordi Esquena Moret and Carlos Rodríguez Abreu

University of Barcelona

15/7/2019

- **Maxime Fruh**

Preparation and Characterisation of Self-Assembled Dye Fibers

Director: Carlos Rodríguez Abreu

University of Barcelona

2019

- **Clara Garcia Vallicrosa**

Incorporation of antibacterial activity into commercial soft contact lenses through chemical modification at the nanoscale level.

Director: Jordi Esquena Moret

University of Barcelona, 16/07/2018

- **Pablo Terroba Seara**

Design and synthesis of assembled peptide amphiphiles based on a peptide with anti-HIV-1 activity derived from the E1 protein of GB virus C

Director: Isabel Haro Villar

Master in Chemical and Process Engineering

Università di Bologna

2019

- **Carmen Hervés Carrete**

Phase behavior and formulation of structured drops in triphasic Systems.

Directors: Jordi Esquena Moret and Carlos Rodríguez-Abreu

University of Barcelona, 17/07/2018

- **Carles Martínez Juvés**

Synthesis of ligands for GPCR labelling with fluorescent probes.

Director: Amadeu Llebaria

Universitat de Barcelona

July 2019

- **Inés Teruel Llinares**

New phenylalanine immunoreagents for phenylketonuria monitoring.

M. Pilar Marco and Montserrat Rodríguez

Universidad de Barcelona (UB)

11/07/2018

- **Lupita Ivonne García Rojas**

Study of the predictive value of synthetic peptide sequences that contain specific post-translational modifications for the development of Rheumatoid Arthritis in Undifferentiated Arthritis patients

Director: Isabel Haro Villar

Translational Medicine. Facultat de Medicina

Universitat de Barcelona

2019

- **Arnau Rué Casamajó**

Evaluating the influence of applied light on trans and cis Optogluram binding to the metabotropic glutamate receptor mGlu4

Director: Amadeu Llebaria

July 2019

- **Ignasi Villarroya Arenas**

Cuantificación de residuos lipídicos en proteínas modificadas

Director: Gemma Triola

Faculty of Chemistry

University of Barcelona

13/09/2018

- **Cristina Duran Rebenaque**

Obtención de dendrímeros y de nanopartículas derivatizadas con péptidos penetradores celulares

Director: Isabel Haro

Màster en Recerca, Desenvolupament i Control de Medicaments Facultat de Farmàcia

Universitat de Barcelona

2019

- **Alexander Vazquez Pardo**

PROTACs; an encouraging strategy for degrading lipid metabolism molecules

Director: Josefina Casas

Master Biomedicine

Universitat Barcelona

2019

- **Jon Gil Martínez**

Pharmacological chaperones: Therapy for Niemann-Pick Disease Types A and B

Director: Josefina Casas

Master Biomedicine

Universitat Barcelona

2019

- **Teresa Paradell Gil**

Catanaionic system from gemini arginine based-surfactants

Director: Lourdes Pérez

Barcelona University

2017-2018

- **Laura Bassas Serra**

New fluorogenic substrates as potential selective probes of ceramidases

Directors: José Luís Abad and Antonio Delgado

Master in Organic Chemistry

Universitat Barcelona

2018.

- **Guillem Pons Barcons**

Development of the first activity-based probe for sphingosine 1-phosphate lyase (SPL)

Director: Josefina Casas

Master Translational Medicine

Universitat Barcelona

2018.

- **Sofía Iglesias Valle**

New luminogenic probes for sphingosine-1-phosphate lyase

Directors: José Luís Abad and Antonio Delgado

Master in Organic Chemistry

Universitat Barcelona

2018.

- **Oriol Esquivias**

The sliding mechanisms of PCNA over DNA: a computational approach

Universitat Autònoma de Barcelona

Director: Ramon Crehuet

10/7/2018

- **Marina Gual Fornés**

Cationic surfactants containing arginine and phenylalanine in the polar head: aggregation properties and antimicrobial activity

Director: Lourdes Pérez

Barcelona University

2018-2019

- **Inés Terrones Fernández**

Gemini surfactants from arginine with multiple cationic charges on the polar head: Physico-chemical and biological properties

Director: Lourdes Pérez

Barcelona University

2018-2019

- **Roger Barrull Pérez**

Effects of D-fagomine, inulin and resistant starch in rats with high-fat diet induced prediabetes: a comparative study

Master in Integrative Physiology. Dept. Physiology.

Directors: Sara Ramos Romero, Mercè Hereu,

Josep Lluís Torres

Universitat de Barcelona

June 2019

- **Beatriz Guzmán Monreal**

Artificial membranes as a model for percuraneous absorption

Director: M. Luisa Coderch Negra

2018

- **Paula Victoria Tyszko Gonzales**

Physico-chemical and biological study of cat-anionic mixtures of biocompatible surfactants with cholesterol

Director: Lourdes Pérez

Barcelona University

2018-2019

- **Cristina Busquets Roca**

Effects of polyphenol-rich grape pomace on the gut microbiota of patients with metabolic syndrome

Directors: Mercè Hereu, Sara Ramos

Universitat de Barcelona

September 2018

- **Pedro J. Buigues**

Generation of PolyQ tract ensembles by reweighting MD trajectories

Universitat Autònoma de Barcelona.

3/7/2018

- **Sebastian Robroeks**

Effect of dietary supplements on the gut microbiota of adult rats fed a high-fat diet

Master in Molecular Biotechnology

Directors: Sara Ramos Romero, Mercè Hereu,

Josep Lluís Torres

Universitat de Barcelona

September 2018

- **Teresa Paradell Gil**

Catanaionic system from gemini arginine based-surfactants

Director: Lourdes Pérez

Barcelona University

2017-2018,

- **Marina Gual Fornes**

Cationic surfactants containing arginine and phenylalanine in the polar head: aggregation properties and antimicrobial activity

Director: Lourdes Pérez

Barcelona University

2018-2019

- **Ines Terrones Fernández**

Gemini surfactants from arginine with multiple cationic charges on the polar head: Physico-chemical and biological properties

Director: Lourdes Pérez

Barcelona University

2018-2019

- **Albert Carcereny Sánchez**

Antifungal and antibiofilm activity of amino acid based surfactants

Director: Aurora Pinazo

Barcelona University

2019-2020

Final degree projects

- **Laia Oviedo López**

Synthesis of oligonucleotides carrying reactive groups for protein conjugation

Directors: R. Eritja, A. Lobo

2019

- **Marc Guasch Albanieue**

Synthesis of oligonucleotide-lipid conjugates

Directors: R. Eritja, C. Fàbrega

2019

- **Laura Reyes Fraile**

Non-canonical structures of DNA and RNA and their interaction with drugs
Directors: R. Eritja, A. Aviñó
2019

- **Santiago Herrera Restrepo**

Formation of chromonic liquid crystals from dyes and their confinement in water-in-oil and water-in-water emulsions.
Director: Carlos Rodríguez-Abreu
University of Barcelona
2019

- **Joan Barceló Mir**

Estudis de moduladors d'autofagia com a nous agents antitumoral
Director: Gemma Triola
Universitat de Barcelona
2018

- **Amin Boulahfa Lamdaghri**

Synthesis of a new class of cellular transporters
Director: Juan B. Blanco
Universidad de Barcelona,
2019

- **Pol Puigseslloses i Sánchez**

Synthesis and characterization of silicone-coated magnetic nanoparticles
Director: Carlos Rodríguez-Abreu
University of Barcelona
2018

- **Nestor Murciano Durán**

Gelled nano-emulsions for food and pharmaceutical Applications
Director: Carlos Rodríguez-Abreu
University of Barcelona
2018

- **Santiago Pons Allés**

Chromonic liquid crystals as precursors of polymer nanofibers
Director: Carlos Rodríguez-Abreu
University of Barcelona
2018

- **Alba Lalueza Sánchez**

Modulation of seed germination by plasma surface treatments
Director: Ricardo Molina
Facultad de Química
Universidad de Barcelona,
26/06/2019

- **Clara Jaén**

Formation and characterization of multiple W/W/W emulsions.
Director: Jordi Esquena Moret
University of Barcelona,
28/06/2018

- **Néstor Salinas**

Design, formation and characterization of biocompatible water-in-water (W/W) emulsions and encapsulation of these emulsions.
Directors: Sergio Madurga Díez, Jordi Esquena Moret, Jonathan Miras Hernández
University of Barcelona
25/01/2018

- **Joan Garriga Guitart**

Ús d'anticossos específics contra un factor de virulència de la bactèria pseudomonas aeruginosa, com a eines terapèutiques.
Directors: Lluïsa Vilaplana, M. Pilar Marco
10/2019
Qualification: Excellent

- **Jordi Grau Escolano**

Desenvolupament d'assaigs elisa per detectar i quantificar l'àcid quinolínic i la noradrenalina.
Directors: Lluïsa Vilaplana, Montserrat Rodríguez and M. Pilar Marco
Qualification: 8.9
13/07/2018

- **Zeno Fazio**

Pseudopeptidic molecules for chloride recognition and transport
Directors: Laura Rodríguez (UB) and Ignacio Alfonso
Universitat de Barcelona
January 2018

- **Natalia Nadal Alemany**

Human Serum Albumin as platform to perform asymmetric organocatalysis
Director: Ciril Jimeno
IQS-Universitat Ramon Llull
June 2018

- **Juan José Herrando**

Pseudopeptidic molecules for the recognition of biologically interesting ions
Director: Laura Rodríguez (UB) and Ignacio Alfonso
Universitat de Barcelona
January 2019

- **Araceli de Aquino Samper**

Towards asymmetric catalysis by using tripodal pseudopeptidic cages
Directors: Laura Rodríguez (UB), Jordi Solà and Ciril Jimeno
Universitat de Barcelona
June 2019

- **Blanca Plana Robles**

Disseny i síntesi de peptíds amfifílics derivats de la proteïna E1 del GBV-C com a potencials inhibidors del VIH-1
Director: M. José Gómara
Universitat de Barcelona. Facultat de Biologia
2019

- **Martí Recort Fornals**

Study of novel supramolecular structures based on peptide amphiphiles derived of a sequence with anti-HIV-1 activity
Directors: Isabel Haro and M. José Gómara
Universitat de Barcelona. Facultat de Química
2018

- **Elias Romero Cavagnaro**

Design and synthesis of assembled peptide amphiphiles with possible application in the preexposure prophylaxis (PrEP) of HIV-1 infection
Directors: Isabel Haro and M. José Gómara
Universitat de Barcelona. Facultat de Química
2019

- **Gisela Trenchs Mir**

Light activated drugs for protein activity remote control
Director: Amadeu Llebaria
June 2019

- **Andrea Llaves López**

Citrul·linació i homocitrul·linació en el diagnòstic i pronòstic de l'artritis reumatoide
Director: Isabel Haro
Universitat de Barcelona. Facultat de Biologia
2018

- **Clara Tejada Illa**

Peptíds sintètics per l'estudi de la coinfecció GBV-C/VIH-1
Director: M. José Gómara
Universitat de Barcelona, Facultat de Biologia
2018

- **Marta Remolà Grabulós**

Peptíds sintètics citrul·linats i homocitrul·linats en la diagnosi d'Artritis Reumatoide
Director: Isabel Haro
Universitat de Barcelona. Facultat de Biologia
2019

- **Marc Sibil Giralt**

Synthetic peptides as entry inhibitors of HIV-1
Directors: Isabel Haro and M. José Gómara
Universitat de Barcelona. Facultat de Química
2018

- **Pau Farrerons Calbet**

Synthesis of vimentin derived citrullinated peptides and study of peptide-peptide interaction by fluorescence
Directors: Isabel Haro and M. José Gómara
Universitat de Barcelona. Facultat de Química
2019

- **Ester Martí Selva**

La Jaspina B, un inductor de la metuosi
Director: Josefina Casas
Degree in Biochemistry
Universitat Barcelona
2018

- **Francesc Estrany Castillo**

Mecanisme d'acció de la Jaspina B com a inductor de mort cel·lular per metuosi

Director: Josefina Casas

Degree in Biochemistry

Universitat Barcelona

2019

- **Miriam González Pérez**

Chaperonas farmacológicas, terapia para la enfermedad de Niemann-Pick A/B

Director: Josefina Casas

Degree in Biochemistry

Universitat Barcelona

2018

- **Anna Gómez Ballester**

Sensibilització a la percepció de feromona en *Grapholita molesta* (Lepidoptera: Tortricidae)

Director: Carmen Quero

Degree in Biology

Universitat Barcelona

2018

- **Gema Gorjón de Pablo**

Moduladors químics del metabolisme d'esfingolípids en càncer

Director: Antonio Delgado

Degree in Pharmacy

Universitat Barcelona

2018

- **Natalia Ángela Escobar**

Uso de nanopartículas aplicado en la terapia antineoplásica

Supervisor: Antonio Delgado. Degree in Pharmacy

Universitat Barcelona

2019

- **Adriana Muñoz Nebot**

Phosphosphingolipid analogs as potential modulators of the enzymatic activity

Director: Antonio Delgado

Degree in Pharmacy

Universitat Barcelona

2018

- **Ignacio Corral Raxach**

La Miltefosina, perifosina i edelfosina com a possibles xaperones farmacològiques pel tractament de la malaltia de Niemann-Pick A y B

Director: Josefina Casas

Degree in Biochemistry

Universitat Barcelona

2019

- **Adriana Alí Cladellas**

Short-chain fatty acids determination in biological samples from rats fed different high-fat diets.

Graduation Project

Directors: Sara Ramos and Susana Amézqueta

Universitat de Barcelona

June 2019

- **Albert López de Moragas**

The ortho allyl group as a Trojan horse for diversity-oriented iodoarene synthesis

Director: Alexandr Shafir

June 2019, IQS.

- **Oriol Angurell**

Approaches towards photochemical reactivity using organoiodanes and organo(trifluoro)borates

Director: Alexandr Shafir

June 2019

- **Judit Ruiz Ibáñez**

Cationic surfactants containing arginine and tryptophan in the polar head: aggregation properties and antimicrobial activity

Director: Lourdes Pérez

Barcelona University

2018-2019

- **Yasmin Charik.**

TFG about optimization of the differential stripping technique

Director: M. Luisa Coderch Negra

2019

- **Ilaria Collini (Italy)**

Permeation kinetics of actives through lanolin-based artificial membranes
Director: M. Luisa Coderch Negra
2018

- **Maria Fernanda Esponda Fontoura.**

Antimicrobial activity of ampicillin-based ionic liquids
Director: M. Teresa García
Barcelona University
2018-2019

- **Núria Agustí Font**

Synthesis and evaluation of antimicrobial amino acid based ionic liquids
Director: M. Teresa García
Barcelona University
2018-2019

- **Maria Eugènia Agustí Carol**

Cationic mixtures prepared with histidine-based surfactants
Director: Lourdes Pérez
Barcelona University
2017-2018

- **Practicum, Erasmus, ...**

- **Raffaella Giordano**

Drug delivery systems for the treatment of colorectal cancer Erasmus + traineeship
01/04/2019 - 30/06/2019

- **Ana Paola García Lugo**

Manufacture of Pharmaceutical, Biotechnological and Related products
Director: M. Teresa García
IES Severo Ochoa. traineeship
2018

- **Sophia Kioulaphides**

Misti Spain Internship Agreement 2018
Preparation of lipid systems and their interaction with membrane models of endothelial cells
Director: Miriam Royo
2019

- **Sarah Dohadwala**

Misti Spain Internship Agreement 2019
Optimization and characterization of lipid system with different composition mimicking extracellular vesicles
Director: Miriam Royo
2019

- **Wei Wen Chen**

Group developing a new approach to the formation of ortho-allylated halogenated aromatic rings
Director: Alexandr Shafir
Institut Químic de Sarrià
Pharmaceutical Chemistry
Experimental Final Master work (TFM)
2019

- **Anna Argemí Gil**

"Assaig luminogènic per a la determinació de l'activitat S1P lliasa"
Director: Fina Casas.
Practicum. Degree in Chemistry
Universitat Ramon Llull
2019

- **Marta Díaz Baranda**

Group working on the chemistry of certain gem-bimetalloid species
Director: Alexandr Shfir
Institut Químic de Sarrià
Pharmaceutical Chemistry
Experimental Final Master work (TFM)
2019

- **Alex Guillamón Thiéry**

Efecto de la hipoxia y el frío en algunos grupos taxonómicos de la flora intestinal
Practicum
Director: Sara Ramos-Romero, Josep Lluís Torres
Institut Químic de Sarrià
October 2019

COMMUNICATION AND OUTREACH

Dissemination

Research on DNA. Science Week Conference. R. Eritja. 2018.

Què és la tensioactivitat i per a què serveix? J. Esquena. Setmana de la Ciència. IQAC, 16/11/2018.

Què és la tensioactivitat? J. Esquena. Matins de Recerca. IES Montserrat Roig, Barcelona, 26/09/2019.

Juguem amb sabó? Les claus de la tensioactivitat. J. Esquena, S. Vilchez, J. Miras, A. Pérez. Setmana de la Ciència. IQAC, Barcelona, 12/11/2019.

Las emulsiones, de aceite-en-agua a agua-en-agua, para mejorar nuestra calidad de vida, Cicle de Conferències Jornades Informatives de l'Escola del Treball, Barcelona, Jordi Esquena. 13/02/2019.

SMART4FABRY: New approaches for Lysosomal storage disorders. Edgar Crisóbal. BCNspiracy, Barcelona 9 November 2019.

Enfermedades raras: ¿Qué soluciones conocemos para curarlas?. Edgar Crisóbal. "Nit de la recerca". Barcelona, 27 September 2019.

Què fan els científics? Olga López. Science dissemination day at the elementary school Sant Pere in Monistrol de Montserrat. 16/05/2018.

Coloquio Químic i Salut a la Bial Ciutat i Ciència al Cosmocaixa, Olga López. 11 February 2019. From the lab to the market in the frame of 24th Week of Science 2019. Olga López. Barcelona. 2019.

Tensioactius: de bombolles a cristalls líquids (la importància de la Nanoestructura). Dilluns de Ciència: per què fer recerca en ... Química. Ramon Pons. <https://www.youtube.com/watch?v=a23gGVcJXHA>. 14 May 2018.

Participation in the activities organized within the International Day of Women and Girls in Science with a talk-colloquium in the elementary school "Cal Maillol" (Barcelona). Gemma Fabrias Domingo. 11/2/2019.

Introduction to Marie Curie's biography and to the movie "Marie Curie" (Marie Noelle, 2016). Chemistry and Celluloid Conference Cycle (Residence for Researches, CSIC, Barcelona). Gemma Fabrias Domingo. 4/10/2019.

Collaborated with Magma in the evaluation panel of Exporecerca Jove. Ramon Crehuet. 2018.

Dels rellotges a les proteïnes. De què serveix la recerca fonamental?. Dilluns de Ciència: per què fer recerca en ... Química. Ramon Crehuet. May 2018.

20th Symposium Neurodegenerative Diseases. Fundació Marató de TV3. Digital video/dissemination. Gemma Arsequell. 2019.

El servei de dispersió de raigs-X d'angle petit. Facility presentation at the II IQAC workshop, 7-6-2018, Ramon Pons.

Els elements químics i el seu rol en l'àrea de la Salut i de l'Aigua. M. Teresa García. 13a Festa de la Ciència. Barcelona, 26/10/2019

Workshops

Local organizing committee of the Workshop "Formulated Products: Enabling innovation through value chain and cross-sector collaboration", Barcelona. Organized by RISE Research Institutes of Sweden and AceForm4.0 Consortium 2018.

I-LINK Workshop, Institute for Advanced Chemistry of Catalonia, 2018.

Local organizing committee of the Workshop "Formulated Products: Enabling innovation through value chain and cross-sector collaboration", Barcelona. Organized by RISE Research Institutes of Sweden and AceForm4.0 Consortium. Chairperson: Isabel Mira (RISE); local committee: Carlos Rodríguez, Jordi Esquena. 28/05/2018 - 29/05/2018.

"Chemical ecology of insect crop pests" in Plant Science Summer School 2018. Université

d'Angers, Angers, France. Carmen Quero. 10/10/2018.

Thermal Analysis (in UPC Master on Technologies for Food Industry and Bioprocessin). S Pérez-Rentero and AM Manich. Barcelona, 19 April 2018

Thermal Analysis (in UPC Master on Technologies for Food Industry and Bioprocessin). S Pérez-Rentero and AM Manich. Barcelona, 16 May 2019.

Pere Clapés. Celebrem el Premi Nobel de Química 2018. Evolució dirigida: de Charles R. Darwin a Frances H. Arnold. Soc-Cat. Quim. Núm. 18 (2019).

"¿Que son los péptidos?: Algunas aplicaciones en biomedicina". Conferencia Semana de la Ciencia 2018. M. José Gómara.

Media

Papiroflexia del adn. R. Eritja. 2018. Digital Press release on Newsletter Genética Médica.

The first nano drug for selectively fighting metastatic cells. R. Eritja. 2018. Press release CSIC R+D. The first nano drug for selectively fighting metastatic cells.

Ciencia: Científicos españoles desarrollan el primer nanofármaco que frena la metástasis del cáncer de colon. R. Eritja. 2018. Programa de radio "La Linterna" Ciencia con Jorge Alcalde. Cadena COPE.

A study makes a significant contribution to progress in gene therapy efficiency by identifying the source of asymmetry in RNA · DNA hybrids. R. Eritja. 2019. Press release. IRB Barcelona.

Light! Impacto de la fotónica en el sector de la belleza, Estudio de la piel mediante microscopía de infrarrojo, Lucyana Barbosa-Barros, Estitxu Fernández, Mercedes Cócera, Gelsen Rodríguez, Manel Sabés, Olga López. Divulgative Journal. June 2018.

Tecnología Bicohair®: Enfoque dual para la protección externa e interna de la fibra capilar. M.L. Vázquez-González, G. Rodríguez, M. Cócera, E. Fernández, L.Barbosa-Barros, O. López. Magazine Industria cosmética. 2018.

Nuevo método de diagnóstico de la cistinuria mediante un examen de orina. Press release (CSIC). Ignacio Alfonso.

Press notes in general media about the cystinuria diagnostic test: Madri+d, EFEFuturo, Redacción Médica. Instituto Roche, La Vanguardia, DICYT, WebConsultas, ALCER, Vivir Mejor, Andalucía al día, AcceSalud, InfoSalus, WorldDiagnosticsNews, Catalunya Vanguardista, UNIVadis, Diario Médico, El Confidencial, April Ignacio Alfonso. 2018.

Identificada una molécula sencilla que inhibe el efecto del fármaco anticoagulante más común. Press release (CSIC) about heparin inhibitor. Ignacio Alfonso. 13/8/2018.

Press notes in general media about heparin inhibitor. RTVE, La Vanguardia, ElCorreo Gallego, InfoSalus, EcoDiario, Catalunya Vanguardista, Servimedia, Jano, Correo Farmacéutico, Web-Consultas, Prensa Latina (Cuba), Bolsamanía, Diario Siglo XXI, COPE, NovaCiencia, Química.es, Diario Médico, Madri+D, ID, NanoMed Spain, Infecto Forum, Asturias Mundial, Zona, médica. Ignacio Alfonso. August 2018.

Proponen usar 'jaulas' moleculares para destruir células cancerosas de forma selectiva. Press notes in general media about molecular for killing cancer cells: CSIC Delegació Catalunya, La Vanguardia, InfoSalus, Bolsamanía, Diario Siglo XXI, Estrella Digital, Asturias mundial, El Confidencial, Diario de Burgos, La Tribuna de Albacete, DICYT, COPE, Agencia Sinc, Biotech Spain, El Médico interactivo, EFE, IM médico hospitalario, Medicina 21, Catalunya vanguardista, El Confidencial, Diario Vasco, Intereconomía, El Día Segovia, , Diario de

Ávila, Onda Cero, InvDes, Telecinco, Navarra Información, Faro de Vigo, Cadena Ser, Salud a Diario, MedicinaTV, The World News, Diario de León, Madri+D, Aquí medios de comunicación, Ecuador Universitario, Jano, Navarra TV, Oncoweb, Noticias de la Ciencia. Ignacio Alfonso, July 2019,

Identifican compuestos químicos como posibles inductores de enfermedades inflamatorias intestinales. CSIC Delegació Catalunya, UAB, Biotech Spain, TV3, Carme Serra and Amadeu Llebaria. 18/5/2018.

El simposi de fotofarmacologia mostra a Vic les bases dels futurs fàrmacs regulats per llum. CSIC Delegació Catalunya, TV3, Biotech Spain, 2018.

Driving Innovation - Achievements and Impact of NEURON funding. ERA-NET NEURON Brochure. Amadeu Llebaria. June 2018.

Tecno certificatio. ACCIÓ acredita 9 entitats catalanes amb el segell TECNIO per impulsar la transferència tecnològica (Medicinal Chemistry & Synthesis-MCS) IQAC-CSIC. December 2018.

El grup MCS del CSIC ha estat acreditat com a nou Centre TECNIO. Parc de Recerca de la UAB. 14/11/2018.

D'aquí 10 anys: fotofarmacologia. RAC1. Interview with Amadeu Llebaria. 4/11/2018.

Participación en el programa "Lab24" del canal 24 horas de RTVE dedicado a los 50 años del CID. Isabel Haro. 17/01/2018.

Participation in the TV program "somos talento" (RTVE and Univesitat Autònoma de Barcelona). Gemma Fabrias. Barcelona. 17/05/2019.

20th Symposium Neurodegenerative Diseases. Fundació Marató de TV3. Digital video/dissemination. Gemma Arsequell.2018.

PARTICIPATION IN COMMITTEES AND SCIENTIFIC REPRESENTATION

Panel Member (Medical and Health Sciences). FCT projects, R. Eritja. Portugal, 2018

Member of the scientific committee of the 32nd Conference of the European Colloid and Interface Society, Ljubljana, Slovenia, Carlos Rodríguez Abreu, 2018

Senior associate editor of Journal of Surfactant and Detergents (American Oil Chemists' Society-Wiley). Carlos Rodríguez Abreu

Co-editor of the section on Emulsions and Micro-emulsions of Current Opinion in Colloid & Interface Science (Elsevier). Carlos Rodríguez Abreu

Member of the editorial board of Journal of Dispersion Science and Technology (Taylor&Francis). Carlos Rodríguez-Abreu

Member of the "Comité Español de la Detergencia, Tensioactivos y Afines (CED)", Barcelona. Jordi Esquena. from 19/07/2016

Member of International Advisory Board (IAB) of Formula Congress, and Member of Scientific Committee of Formula X Congress, . Jordi Esquena. 24-27 June, Manchester, UK.

Member of the Scientific Committee of the 8th Iberian Meeting on Colloids and Interfaces (RICI8). Jordi Esquena. 17-19 July 2019, Aveiro, Portugal.

Member of the Scientific Committee of the Okinawa Colloids Conference. Jordi Esquena. 3-8

November 2019. Naha, Japan.

Representative of "Sociedad Catalana de Química (SCQ)" in "Working Party on Formulation" from "European Association for Chemical and Molecular Sciences" (EuCheMS). Jordi Esquena. From 19/07/2016.

Member of the evaluation committees of Research projects at the "Association Nationale de la Recherche et de la Technologie", France. Jordi Esquena. From 30/04/2019

Spanish delegate at ESUO (European Synchrotron User Organization). Olga López. from 2015.

Member IFATCC (Int. Federation of Associations of Textile Chemist and Colourists) Council of delegates. M. Martí.

Member of the Comité Técnico de Normalización de AENOR: UNE/CTN40/SC 1 solideces y medida del color. M.Martí

Chair of the board of the Catalan Chemical Society and Editor of the Society's journal Revista de la Societat Catalana de Química, C. Jimeno. 2018 and 2019.

Editor of the open access journal Molecules (MDPI, Switzerland), C. Jimeno. 2019.

President of the Specialized Group in Nuclear Magnetic Resonance (GERMN) from The Spanish Royal Chemical Society (RSEQ). I. Alfonso. 2018 to present.

External evaluating member of the Nayara Braga Emidio thesis committee, University of Queensland (Australia) "Trefoil factor family: synthesis, mechanisms of action and therapeutic potential for gastrointestinal disorders". Member evaluator of projects the national plan. Juan B. Blanco.

External expert evaluator Research Foundation Flanders (FWO), Belgium. Ricardo Molina. 2016 to present.

Member of the Chemical Sciences and Technologies of the CSIC Commission. Isabel Haro. 7 June 2012 - 30 November 2018

Benefits Manager of the Chemistry Area of the CSIC Services Commission. Isabel Haro. Until 30 November 2018

Member of the IQAC-CSIC Ethics Committee. 2009 to present. Isabel Haro

Coordinator of the research group consolidated by the Generalitat de Catalunya: "Translational research group in design and synthesis for the diagnosis of rheumatic diseases" (2017SGR254). Isabel Haro.

Evaluator of the State Research Agency (formerly ANEP). 2006 to present. Isabel Haro.

Member of the magazine's Editorial Advisory Board "Current Medicinal Chemistry". 2008 to present. Isabel Haro

Appointed as evaluator of the National Agency for Quality Assessment and Accreditation of Spain (ANECA). Gemma Fabrias. 2019.

ORGANIZATION OF CONGRESSES

Núria Pascual; 10th EuroMabNet Meeting and 5th Antibody Validation Workshop; 27th-28th September 2018. Oxford, United Kingdom

Olga López. IX AUSE Meeting. Scientific Committee. 8th - 10th October 2019. Barcelona. 2019

M. Martí is the leader of AEQCT (Asociación Española de QUímicos y Coloristas Textiles) anual simpòsium Organization.

M. Martí is member of the Scientific Committee of 25th Int Congress of IFATCC

A.M. Manich is membre of the Scientific Committee of the International Conference on Engineering ICEUBI2019.

I. Alfonso (co-chair of the organizing committee) at the "16th Iberian Peptide Meeting / 4th ChemBio Group Meeting", Parc de Recerca Biomèdica de Barcelona-Universitat Pompeu Fabra, Barcelona, Spain, February 2018.

Amadeu Llebaria. Second International Symposium on Photopharmacology. Member of the Organizing Committee. Vic (Barcelona). November 2018

World Congress on Light and Life (17th Congress of the International Union of Photobiology and 18th Congress of the European Society for Photobiology). Member of the Organizing Committee. Amadeu Llebaria. Barcelona. August 2019.

AWARDS AND CERTIFICATIONS

R. Eritja. Honorary member Sociedad Argentina de investigación en Química Orgánica (SAIQO). 2019.

Olga López. MIT-La Caixa Seed Funds to the project "Advanced lipid nanostructures to overcome blood brain barrier" June 2018

Sara Ramos Romero. Mobility aid for doctors from the Network of Campus of International Excellence with agrifood activity of the Triptolemos Foundation. Almeria, Spain, 18th May to 10th June 2018

Wei Wen Chen. Master student. IQAC XVIII Certamen Universitario Arquímedes, Special Prize (6.000€) For the best master work in Chemistry (commemorative of the International Year of the Periodic Table). Developing a new methodology

for producing highly versatile halogenated aromatic molecules through metal-free C-H allylation. November 2019

Alexandr Shafir (IQAC) and Cuenca (IQS) as advisors. XVIII Certamen Universitario Arquímedes, Diplomas for supervising the work of Wei Wen Chen. November 2019

The Service of Dermocosmetic Assessment. Quality System of Management in accordance with the UNE-EN ISO 9001:2008 certified by AENOR with the reference ER-0430/2012. Since May 2012.

The Service of Dermocosmetic Assessment. Good Laboratory Practices (GLP) for Percutaneous Absorption Tests. First Service in the CSIC institution with this certification. From 2019

PATENT APPLICATIONS

P201830330. Dynamic combinatorial library based on pseudopeptides and its use for the detection of cysteine and other biothiols. I. Alfonso, J. Solà, M. Lafuente. Applicant: Consejo Superior de Investigaciones Científicas (CSIC). 2018.

P201830989. Gel lipídico nanoestructurado, procedimiento de preparación y uso. O. López, K. Talló, V. Moner. Applicant: Consejo Superior de Investigaciones Científicas (CSIC). 2018.

P201830343. Modelos de piel basados en membranas artificiales con lanolina. L. Coderch, V. Carrer, M. Martí, C. Alonso. Applicant: Consejo Superior de Investigaciones Científicas (CSIC). 2018.

P201830507. Multicomponent nanoparticles and use thereof. J. Blanco, N. Rubio, O. Meca, A. Cascante, L. Balcells, S. Borrós, G. Martínez. Applicant: Consejo Superior de Investigaciones Científicas (CSIC), Centro de Investigación Biomédica en Red (CIBER), Institut Químic de Sarrià (IQS), QS, Sagetis S.A. 2018.

EP19383007. Semaphorin 3a Neurodegeneration Modulators, Compositions and uses thereof. Á. Messeguer, I. Alfonso, M. Corredor, J. Bujons, A. moure, Y. Pérez, A. Solomon. Applicant: Consejo Superior de Investigaciones Científicas (CSIC), Tel-Aviv University (TAU). 2019.

KNOWLEDGE TRANSFER

Promotion and management of the relationships between IQAC researchers and companies and research organizations is carried out by Dr. Isabel Masip, Knowledge Transfer Manager of the CSIC Deputy Vice-Presidency of Knowledge Transfer in our Institutional Delegation in Catalonia.

Different collaborative approaches are offered by IQAC:

- Technical and scientific consultancy taking advantage of IQAC researchers' expertise.
- Research and technological support contracts to solve technological needs and industrial challenges.
- Licensing of technologies protected by patents or by other intellectual property protection modes.

Our currently patented technologies and materials available to be transferred to companies through licensing agreements include:

LIFE SCIENCES

Medical diagnosis

- IQAC_061. Dynamic system for rapid cystinuria diagnosis
- IQAC_047. Immunoassay for rapid diagnosis of infectious diseases caused by *Pseudomonas aeruginosa*.
- IQAC_053. Immunoassay for detection of infections caused by *Staphylococcus aureus*.
- IQAC_059. Immunoassay for detection of lipoprotein (a) to determine cardiovascular risk

Immunology

- IQAC_060. Non-glycosidic analogues of α -GalCer as NKT cell activators.

Metabolic Diseases

- IQAC_052. Treatment of non-alcoholic fatty liver disease.

CHEMICAL TECHNOLOGY

Cosmetics

- IQAC_063. Synthetic Human Skin model based on an artificial membrane containing lanoline
- IQAC_065. High diluted nanostructured lipid hydrogels with no gelling agents.

Biosensors

- IQAC_058. Multiplexing liquid system in biosensor microchambers.

Biocatalysis

- IQAC_056. Enzymatic process to obtain L-Homoserine and other functionalized molecules. Licensed
- IQAC_057. Industrial (poly)hydroxylate compounds by enzymatic catalysis. Licensed

Genetic tools

- IQAC_064. Multicomponent particles for genetic modification of eukaryotic cells and selection of modified cells

SPIN-OFF ACTIVITIES

bicosome®



Bicosome S.L. is a spin-off company founded in 2012 by scientists of the Biophysics of Lipids and Interfaces group from the Institute of Advanced Chemistry of Catalonia (IQAC). The objective was to create a company that could transform the knowledge of the research group into dermatological and cosmetic products that improve people's quality of life.

Our company develops and commercializes advanced skincare ingredients based on a patented platform, under license of the CSIC. The Bicosome technology is based on skin delivery systems inspired on the skin's own biological transporters, the epidermal lamellar bodies. These systems are formed by discoidal structures enclosed into lipid vesicles forming a double encapsulation structure able to stabilize, transport and deliver active molecules into target skin layers, potentiating their efficacy. In addition, the structure and composition of the Bicosomes per se reinforces the skin structure, contributing to the overall improvement of the skin condition.

Interaction mechanism of Bicosome systems with the skin:

Bicosome systems interact with the skin through a mechanism that uses and imitates the skin's biological processes. When Bicosomes are applied on the skin, its outer vesicle fuses on the skin surface and the small discoidal structures penetrate selectively through the inter-corneocytes spaces reaching target skin layers.

Once inside the skin, the disks respond to internal physiological stimulus and release the active molecules, whereas their own lipid structure is slowly integrated into the skin lipid matrix, reinforcing its architecture.

Bicosomes represent a combination of scientific knowledge, tangible efficacy and ecological consciousness resulted from a deep understanding and respect for skin biology.

Business model

Bicosome business model is based on generating resources basically in two ways.
Commercialization of our own line of ingredients

Development and commercialization of a proprietary line of active ingredients based on the patented Technology.

Partnering

The company also partners for the development of exclusive products commercialized through license agreements.

Proprietary products

Each Bicosome product has a specific target in the skin. This allows for the active ingredient to work in the right layer of the skin, achieving its best performance. Recently, Bicosome technology has been redesigned to adhere to hair fibres and promote the penetration of active ingredients into the hair, giving rise to our Bicohair line of products.

Bicosome currently has 8 ingredients marketed in 20 countries through 14 distributors.





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