



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** HORCAJADA CORTES, PATRICIA

**Referencia:** RYC-2014-15039

**Área Científica:** Química

**Correo Electrónico:** patricia.horcajada@uvsq.fr

### Título:

Bioapplications of porous materials

### Resumen de la Memoria:

With a Pharmacy BCs (2001) and a material science PhD (Nov. 2005), Patricia Horcajada possesses a highly multidisciplinary profile. Her pioneer PhD work was focused on porous materials for bone replacement and drug controlled release. She studied the bone integration on different materials, including glasses, composites, silica or zeolites, and the encapsulation and release of various drugs from these materials (anti-inflammatory, antibiotics, osteoinductor). Important capacities together with a controlled drug release, dependent on the chemical nature, pore size and structure, evidenced the potential of these materials as drug carriers.

During the Ph.D period, she performed a 3-months placement at the Institut Lavoisier (France), initiating a totally new topic dealing with the use of porous metal-organic frameworks (MOFs) as drug delivery systems. We established the proof of concept using micrometric mesoporous MOFs and the model drug ibuprofen.

She then joined the Institut Lavoisier as postdoctoral researcher and extended this concept to flexible porous MOFs, exhibiting a more controlled release of their active cargo (several weeks with zero-order kinetics). At this time, she also synthesized and fully characterized the benchmarked biocompatible mesoporous iron trimesate MIL-100.

In 2007, she gained a civil servant research position in the French Research Council (CNRS) with the aim of developing the biomedical applications of MOFs. Thereafter, she develops her expertise in bioapplications (drug delivery, imaging), which were entirely new in the group. Thereafter, her research activity is focused in three interdependent aspects: material synthesis, formulation and biomedical performances, achieving several innovative concepts. She has actively involved in the synthesis of novel biofriendly MOFs, leading to unprecedented porosities and a la carte physicochemical properties. Even more, the synthesis of therapeutically active MOFs based on bioactive cations and/or linkers as constitutive part of the framework has enabled delivering their active cargo through their progressive degradation in the biological media.

Her work on the scaling-down the MOF crystal size let to access to the nanotechnology field, obtaining small and polydispersed nanoparticles, compatible with the intravenous (iv) route, among others. Her pioneered work proved the lack of in vivo toxicity as well as the biodistribution of some iron carboxylate MOFs after the iv administration of important doses to rats. Furthermore, MOF nanoparticles were able to encapsulate exceptional loadings of diverse drugs (cosmetic, gases, drugs), including challenging antitumoral or antiretroviral molecules, and deliver them in a progressive manner, with in addition promising imaging properties.

She is currently working on the encapsulation and release of different active ingredients in biocompatible MOFs (antitumoral, antibiotics, cosmetics) for their intravenous, cutaneous, oral and pulmonary administration. In this line, she is adapting the formulation of MOFs for each route and application, paying a special attention to the biodistribution of the MOF carriers. Finally, she has recently initiated new research lines on gene therapy, bone regeneration, detoxification and vaccines.

### Resumen del Currículum Vitae:

Patricia Horcajada (36 years old) received her grade in Pharmacy from the Universidad Complutense de Madrid, Spain (1996-2001), where she also initiated her scientific career through a collaboration grant in her last BCs year and she completed her Ph.D of Pharmacy in Nov. 2005, obtaining the Premio Extraordinario. During the Ph.D period, she performed a 3-months placement at the Institut Lavoisier (France). She then joined the Institut Lavoisier, firstly as a postdoctoral researcher and later, in 2007, as civil servant researcher of the French Research Council (CNRS) with the aim of developing the biomedical applications of hybrid solids. Thereafter, she develops her expertise in bioapplications (drug delivery, imaging), which were entirely new in the group. Among her diverse scientific placements (synchrotron, U Paris 6, U PSud, U Kiel), she has recently performed a 1-year invited researcher stay (2013) in CIMUS, Santiago de Compostela (Spain).

Her unconventional and multidisciplinary scientific background (Pharmacy BCs and material science Ph.D) and her large frame of national and international collaborations in diverse fields, made possible to be involved in 24 highly multidisciplinary projects (17 National, 3 European and 4 International). In particular, she has coordinated one international and 3 international projects and she is currently coordinating 3 national projects dealing with biomedical aspects of porous hybrid solids.

With a h-index of 28, her scientific career resulted in 3 book chapters, 8 patents and 85 published or accepted publications, with more than 40 works in high impact journals (>5) and 13 articles cited more than 100 times (dec. 2014, Web of Science). These includes 1 Chem.Rev., 1 Nature Mater., 4 Angew. Chem., 2 Adv.Mater., 1 Adv. Health. Mater., 1 Chem. Sci., 1 Adv. Funct. Mater., 8 J. Am. Chem. Soc., 7 Chem. Commun., 5 Chem. Mater. and 8 J. Mater. Chem. She has received >4950 citations, with over 1000 citations per year in the last 3 years. She is the corresponding author of 26 articles (plus 2 submitted) and 3 book chapters, including 1 Chem.Rev., 1 Nature Mater., 1 Adv. Health.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

Mater., 1 Chem. Sci., 1 J. Am. Chem. Soc., 2 Chem. Commun., 1 Chem. Mater. 3 J.Mater. Chem., 1 Green Mater., 1 Nanomed., 1 Inorg. Chem., 1 Langmuir, 2 CrystEngComm.

She has participated in 56 conferences, including 31 oral presentations and 55 poster communications, in which she has contributed as invited speaker in 11 national and international conferences and as plenary lecturer in one international symposium.

She has combined research with teaching at different levels (BSc, MSc and PhD), with the supervision of students of various degrees, including 18 undergraduated, 5 BCs, 12 MSc and 16 postdocsoral researchers. As a result of her accreditation to supervise research (HDR) in 2012, she supervised 5 Ph.D students and she currently mentors 2 additional ones.

She was also awarded with the **Prime d'Excellence Scientifique** (2011-2014) and she is the secretary of the Action committee for the Mutual Assistance of the Staff of the Université de Versailles (CAESP-UVSQ).

She has also performed reviewer tasks for several journals, including Nature Comm., J. Mater Chem., JACS, Langmuir, J. Phys.Chem. A, Chem. Comm., Chem. Rev., Nanoscale, etc.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** OSUNA OLIVERAS, SILVIA

**Referencia:** RYC-2014-16846

**Área Científica:** Química

**Correo Electrónico:** silviaosu@gmail.com

### Título:

Computational investigation of carbon-based materials and enzyme catalysis

### Resumen de la Memoria:

Dr. Osuna worked on the exploration of the chemical reactivity of endohedral metallofullerenes (EMFs) during her PhD studies. At that time, computational studies investigating the reactivity of these compounds were scarce. She published the first computational paper that explored the chemical reactivity of a EMF both thermodynamically and kinetically, and of particular importance is that one of her publications corrected the erroneous assignment made experimentally on the basis of NMR analysis. These studies highlighted the importance of computations in the correct description of EMFs reactivity. In addition to that, she demonstrated the importance of including dispersion corrections for an accurate description of fullerene and related carbon materials reactivity. During her four years of postdoctoral experience (Marie Curie IOF and Juan de la Cierva fellowships), she has been working on the computational design of enzymes important for their potential applications in medicine. She computationally designed some transaminases for the manufacture of the Merck best selling drug called Sitagliptin (Januvia® for treating type-2 diabetes), new variants for the manufacture of Zocor® (Lovastatin acid is the active ingredient) and also computationally evaluated the different generated mutants created by the Codexis company. Dr. Osuna demonstrated the paramount importance of long MD simulations in the microsecond time scale for understanding the role of distant mutations on the enzyme catalytic activity. Dr. Osuna also worked on the design and computational exploration of small-molecule enzyme mimics with the final goal of designing new enzymes for the target reaction. To that aim, she was actively involved in the design of spiro-fused oligomers, called spirologozymes, which mimic the catalytic machinery of natural enzymes. The design of highly active and specific catalysts is of the utmost importance for reducing the costs associated with the synthesis of many drugs. Apart from that, she took advantage of her expertise in carbon-based materials and Molecular Dynamics simulations to work in fullerene and carbon nanotube material chemistry projects where groups from around the US were involved. Dr. Osuna also demonstrated that aromaticity plays a crucial role for the stabilization and chemical reactivity of endohedral metallofullerenes (EMF). The application of the aromaticity concept for rationalizing the preferred isomeric cage for EMF formation and for predicting the preferred additions sites for the chemical functionalization of EMF had never been performed before. She also recently started a new collaboration with the group of Dr. Y. Yamakoshi in ETH Zürich for investigating the isomerization of 1,3-dipolar EMF Prato mono- and bisadducts. During her scientific career, she has received several fellowships (FPU, Marie Curie IOF, Juan de la Cierva), and has been recently awarded a Career Integration Grant (CIG, 100000€/4 years, PI: Dr. Osuna) project for improving the computational protocol for designing new enzymes. She is the scientist in charge together with Prof. M. Swart of the I+D MINECO Project SpinEnzymeCat, whose resolution is expected for March 2015.

### Resumen del Currículum Vitae:

Dr. Silvia Osuna (b. 1983, Castelló d'Empúries) is currently a Juan de la Cierva postdoctoral researcher at the Institute of Computational Chemistry and Catalysis (IQCC) at the University of Girona. Dr. Osuna obtained her PhD with academic honours in 2010 at the University of Girona (Spain) under the supervision of Prof. Miquel Solà and Prof. Marcel Swart. She received the PhD thesis award (Premio Extraordinario) for the best thesis defended in 2010 at the Chemistry department of the University of Girona. Upon graduation, she then moved to the University of California, Los Angeles (UCLA, USA) for a two-year postdoctoral position with the Marie Curie International Outgoing Fellowship (IOF) at the group of Prof. K. N. Houk. In October 2012, she moved to IQCC for her third year of the IOF fellowship and was awarded the highly competitive Juan de la Cierva postdoctoral position. During these four postdoctoral years, she has been working on the computational design of enzymes important for their potential applications in medicine, and has also worked on the computational exploration of fullerene and carbon nanotubes reactivity in collaboration with many groups located in the EU and US. During her scientific career, she has received several fellowships, and has been recently awarded a Career Integration Grant (CIG) project for improving the computational protocol for designing new enzymes. She has participated in 8 research projects, has been invited to give several seminars, has participated in more than 50 conferences, in 2 of which as an invited speaker, has been Chairman at one of the sessions, and has co-organized two conferences (satellite meeting ICQC 2012, and Girona Seminar 2014). She is now co-organizing the upcoming Girona Seminar 2016, as well as the meeting of the Xarxa de Química Teòrica i computacional (XRQTC) to be held in Girona next June 2015. She has been Guest Editor for the special Hot-Topic issue Nanoreactors and Molecular Prisons published at Curr. Org. Chem. in September 2013 and has been invited to review more than 20 papers. She has also been selected as a member of the evaluation committee of several master, undergraduate and PhD theses. She is starting to create her own research group at the IQCC, composed of two PhD students and one undergraduate student. This new research line started by Dr. Osuna gives a new perspective to the host IQCC group. In fact, the computational design of enzymes is a cutting-edge approach included in very few European group research interests. Her scientific production includes 2 book chapters, and 43 publications (+2 submitted) in international peer-reviewed journals (among them, one Nature



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

**AYUDAS RAMÓN Y CAJAL  
CONVOCATORIA 2014**

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

Chem. Biol., one Nature Commun.; one Angew. Chem. Int. ed., one ACS Nano, eight J. Am. Chem. Soc. and eleven Chem. Eur. J.). Her publications accumulate 595 citations (Scopus, 19 January 2015), providing an H index of 15. Dr. Osuna has also participated in many activities to disseminate science to the popular public, and has published three dissemination papers in the journals: LifeSciencesLab, Anales de Química, and Investigación y Ciencia.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** SANCHEZ COSTA, JOSE  
**Referencia:** RYC-2014-16866  
**Área Científica:** Química  
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### Título:

Development of new advanced materials for technological applications

### Resumen de la Memoria:

The research undertaken throughout my research career has been centred on the areas of Coordination Chemistry, Inorganic Chemistry and Material Science. Within these disciplines, the main objective underpinning my research work is the development of new advanced materials whose electronic, optical and magnetic properties can be fine-tuned at the molecular and nanometric scale, and the study of their properties, as this allows modulating and obtaining the required performances for their ultimate technological application in the fields of energy storage, catalysis, memory devices or sensing materials.

During my PhD in condensed matter Physical-Chemistry from the University of Bordeaux (France) and later throughout three European post-doctorates in the University of Mainz (Germany), University of Leiden (The Netherlands) and University of Barcelona (Spain), I became an expert in the design, synthesis and characterization at the molecular level (bulk and crystalline studies) of novel functional materials. I focused mainly in the development of new Spin-Crossover (SCO) bi-stable complexes, which present exceptional properties for being used as memory devices and sensors. In addition, I worked in other areas in organic, inorganic and material science such as Metal Organic Frameworks, homo- and heterogeneous catalysis, supramolecular assemblies, etc.

A major accomplishment of my career was the introduction and coordination of the research carried out in the functional switchable materials research area within the Inorganic Chemistry Department of the University of Barcelona. Initially in the group of Pr. J. Ribas Gispert as Juan de la Cierva fellow and later as a founder member of the Magnetism and Functional Molecules Group together with Dr. Guillem Aromí, I was responsible for starting up new research lines. Using the knowledge I previously acquired, I autonomously initiated an ambitious research area aiming at engineering new molecular materials to achieve i) novel multifunctional SCO compounds and ii) high nuclearity cluster materials.

The technological application of these materials requires their surface deposition and nanopatterning. With this purpose, in 2012 I was awarded with the highly competitive and prestigious IEF Senior Marie Curie European research grant, and I am currently directing as Principal Investigator an initiative at the Laboratoire de Chimie de la Coordination (LCC-CNRS) in Toulouse (France). As a result, my research work is currently shifting towards mastering nano-structuration processes and other innovative nano-chemistry methods, key for the development of functional hybrid materials controlling their growth at the nanometric scale and so their physicochemical properties. I am also specialising in cutting-edge characterization techniques specific for nanosystems and in techniques aiming at integrating the obtained nanomaterials into functional nano-devices.

In such a way, the knowledge I acquired in coordination chemistry and material science in previous research is being extended to the highly promising Nanotechnology area.

### Resumen del Currículum Vitae:

The most significant contributions I attained throughout my career can be summarized as follows:

**Publications** ♦ I published 57 CSI articles in high quality international journals receiving more than 1200 citations and an h-index of 20. I am corresponding author of 8 publications and signed 11 as first author. I regularly collaborate as referee with several high quality journals of Elsevier (Inorganic Chimica Acta and Polyhedron) and of the Royal Chemical Society (Dalton Trans., ChemEngComm, Chem.Comm.), International congresses and invited lectures ♦ The results I obtained during my scientific career have also had great diffusion in international congresses. I attended 24 international congresses, presenting 10 oral and 14 poster communications and imparted 10 seminars in international institutions. I was also part of the organizing committee of the MOLMAT 2012 international conference.

**Participation in National and International projects** ♦ I participated in a total of 15 projects (2 International, 5 European, 7 national and 1 regional projects). In addition, more than a dozen of the proposals I wrote directed to the crystallographic study the SCO phenomena were awarded with placements to perform measurements in the ALS Synchrotron of the University of California Berkeley.

**Funding as Principal Investigator** ♦ I acquired an extensive expertise in managing projects at national and international level, which allowed me to develop leading, management, administration and coordination competences and the ability to identify research funding opportunities and writing project proposals to carry out my own research initiatives. These have been crucial to develop my research career, to start up new research lines and to establish my consolidated independent position. From the previous list, I was the Principal Investigator in the 2 International projects, in 2 of European projects and in 3 of the National projects.

**Awards** ♦ Apart from the highly competitive and prestigious IEF Senior Marie Curie European grant and the ♦Juan de la Cierva♦ distinctions, I was also awarded by the Royal Society of Chemistry, by the AGAUR and the ALS from the University of California Berkeley,



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

amongst others.

Student supervision and training ♦ Throughout my career I developed great experience managing and mentoring people. To date, I co-supervised 4 PhD students and a MSc student and directed 3 additional MSc and 9 undergraduate students.

Teaching ♦ I imparted several seminars in the Master Courses Program at the Leiden Institute of Chemistry and a total of 445 lecture practical teaching hours at the Inorganic Chemistry department of the University of Barcelona. In 2009 I obtained the Lecturer professor and Assistant professor official credentials from the Regional and National Agencies for the Education Quality (AQU and ANECA respectively).

Collaborations ♦ Throughout numerous and fruitful transnational experiences, I built-up an excellent multidisciplinary network of international collaborations involving more than 40 renowned scientists.

Multidisciplinaryity ♦ Having worked in various European and International centres of excellence with teams from different areas of research in different countries, has given me the opportunity to get to know many research environments, participate and lead a wide range of scientific projects and work closely with highly relevant and specialized researchers.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** PRIMO ARNAU, ANA  
**Referencia:** RYC-2014-16209  
**Área Científica:** Química  
**Correo Electrónico:** aprimoar@itq.upv.es

### Título:

Preparación y aplicación de grafenos y nuevos materiales a partir de biomasa

### Resumen de la Memoria:

I did my PhD at the Institute of Chemical Technology (ITQ, UPV-CSIC) under the supervision of Prof. Corma (FPU scholarship, overall degree mark 2.5/4). My research field was heterogeneous catalysis developing solid catalysts containing Pd to promote C-C bond forming reactions. The quality of my PhD can be quantitatively assessed by the high number of citations (289) received by the 7 articles of this period.

After my PhD, I moved in 2007 (24 months) to the Institute Charles Gerhardt at Montpellier (CNRS-ENSCM) to join the group of Profs. Brunel and Quignard. I worked on natural biopolymers as scaffolds for metal nanoparticles and Cu complexes. I also applied these biomass wastes to metal oxides preparation. There, I supervised an Erasmus student (Matz Liebel). The number of publications of this period was 4. My role on these publications can be deduced considering that my supervisors had not worked before on Pd or Au catalysis for C-C bond formation and also because in one of the publications I was corresponding author.

After my postdoctoral stage I rejoined the ITQ, now in Prof. Hermenegildo García group. An evidence of my present role and my growing responsibility and independence is that this group never worked on biopolymers before I joined the team, but after my incorporation they use them. The increasing responsibility in research design, experimental work planning and article writing can be demonstrated by the fact that since 2013 I have been corresponding author of 5 publications (Chem. Eur. J., 2015, 21, 324, Angew. Chem., 2014, 53, 12581, ChemSocRev, 2014, 43, 7548, Angew. Chem., 2013, 52, 11813 and ChemCatChem, 2013, 5, 1020). Training 4 young researchers (Benjamin Soreé, Eric Aguado, Josep Martinez and Juan Carlos Ruiz) and Master project supervision (Esther Dominguez) and 3 PhD students (Marcos Latorre, Sana Frindy and Ivan Esteve) is steadily gaining importance in my career as a sign of gradual increase in maturity and independence.

Also, in the last three years I have been participating in 2 R&D projects for Abengoa Solar aimed at solar fuel production and novel graphene synthesis. My role in this research can be demonstrated by the use of biopolymers as platforms for material production based on the knowledge that I gained at Montpellier and also because I am co-inventor of the PCT and Spanish patents applied by Abengoa for these processes. I am also involved with INALCO in the preparation of organic-inorganic composites. Natural biopolymers are also employed by Meristem and Industrias Morera for nutrient delivery in agriculture.

After joining Prof. García group in 2009 I have been participating in the SUDOE project Train2 aimed at collaboration and exchange between groups from transpyrenees regions. I was partner responsible and as consequence of this activity I have delivered the course **◆Nanodevice fabrication and applications◆** at the University of Zaragoza. I am also participating in **3** European projects (Figaro, Being Energy and Novacam) and in an international exchange collaboration funded by CSIC (i-link, with KAU at Saudi Arabia) and I have been recently awarded with my first research project as principal investigator by the UPV.

Moreover, I have started collaborations with groups of the Universities of Strassbourg (Prof. Keller), Salerno (Prof. Vittoria), Fez (Prof. el Kadib) and Bucharest (Prof. Parvulescu)

### Resumen del Currículum Vitae:

- ◆Chemistry degree, University of Valencia, 2001
- ◆PhD in chemistry, Technical University of Valencia, 2006
- ◆H index: 15
- ◆Number of citations: 937
- ◆Average citation per article: 26.03

#### SCIENTIFIC PUBLICATIONS

- ◆Number of publications: 35 (+ 5 book chapters)

Journal Name	Quotes
ChemSocRev (2014)	1
Angew.Chem. (2014)	-
Angew.Chem. (2013)	18
Angew.Chem. (2009)	73
Nature Commun. (2014)	-
JACS (2011)	104



## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

### Turno de acceso general

Small (2014)	-
ChemSusChem (2012)	10
Chem. Commun. (2012)	15
Chem. Commun. (2011)	35
Chem. Commun. (2010)	36
J. Mater. Chem.(2012)	19
Adv. Synth. Catal. (2012)	20
Adv. Synth. Catal. (2011)	23
Carbon (2015)	-
Carbon (2014)	2
Chem. A Eur. J. (2014)	-
Chem. A Eur. J. (2014)	2
Chem. A Eur. J. (2013)	9
Chem. A Eur. J. (2011)	10
Chem. A Eur. J. (2007)	40
Chem. Mater. (2009)	41
ACS catal.(2014)	3
ChemCatChem (2015)	-
ChemCatChem (2013)	6
ChemCatChem (2013)	3
ChemCatChem (2012)	4
J. Catal.(2007)	66
J. Catal.(2006)	31
Langmuir (2013)	2
PhysChemChemPhys(2011)	190
App. Catal. A Gen (2004)	71
App. Catal. A Gen (2003)	65
New. J. Chem. (2004)	6
Inorg. Chim. Acta (2003)	7

◆Hot paper: It should be commented that one of the papers (JACS (2011)) is a hot paper according to the ISI database. A hot paper is defined as an article less than 2 years old that has a number of citations among 0.1/100 of the most cited papers in the research field.

◆Research front: One of my articles (PhysChemChemPhys (2011)) appears as a core paper (by ISI database) in a research front focused on visible light photocatalysis.

◆Highlighted papers: 2 of my recent papers have been selected by ◆Chemistry Views◆ of Wiley (Chem. Eur. J. (2014)) and ◆Advanced Engineering News◆ (Chem. Eur. J. (2013)) as the most interesting papers for highlighting to the corresponding audience.

◆Corresponding author: In 6 of my publications, I am corresponding author, including 1 Chem. Eur. J. (2015), 1 Angew. Chem. (2014), 1 ChemSocRev (2014), 1 Angew. Chem. (2013), 1 ChemCatChem (2013) and 1 Chem. Commun. (2010)

◆First author: I am first author in 12 of my research articles.

◆Exponential growth of annual citations: In the last 5 years the number of citations has increased from 38 (2009), 52 (2010), 88 (2011), 148 (2012), 194 (2013) to 289 (2014). This exponential growth shows the increasing impact of my research.

#### SUPERVISION OF PhD, FINAL PROJECTS AND MASTERS

◆PhD: I am co-supervisor of 3 PhDs, Marcos Latorre, Sana Frindy and Ivan Esteve.

◆Erasmus Mundi (EMAG): I am co-supervising 1 Erasmus Mundi (EMAG) together with the ◆Cadi Ayyad University◆ at Marrakech (Morocco) cosupervised with Prof. Lahcini.

◆Master degree : I have co-supervised 1 Master degree (Esther Domínguez)

◆Degree projects: I have co-supervised 4 degree projects (Benjamin Soree, Eric Aguado, Josep Martinez and Juan Carlos Ruiz).

#### R&D PROJECTS:

◆Participation in R&D projects as principal researcher: 1 (◆Primeros proyectos de investigación◆ de la Universidad Politécnica de Valencia)

◆Participation in R&D projects as researcher: 7

◆Participation in R&D project as scientific coordinator: 1 (European project, Training 2 Sudoe in Nanomaterials and International Erasmus mundi program)

#### CONGRESS:

◆Oral Presentations: 2 (RSEQ and UBIOCHEM IV)

◆Total congress participations: 7

PROJECTS WITH COMPANIES: 4 (Abengoa, Meristem, A. Alcorense, I. Morera)





MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** MARTINEZ LILLO, FRANCISCO JOSE

**Referencia:** RYC-2014-16431

**Área Científica:** Química

**Correo Electrónico:** lillo@uv.es

### Título:

DEVELOPMENT OF NEW COMPOUNDS BASED ON HIGHLY ANISOTROPIC METAL IONS AND EXPERIMENTAL RESEARCH ON THEIR MAGNETIC PROPERTIES

### Resumen de la Memoria:

After receiving his degree in Chemistry (2000) at the University of Valencia (Spain), Francisco José Martínez Lillo spent 11 months in the Institute of Ceramic Technology (ALICER-ITC) in Castellón (Spain) to carry out pilot projects and developments which were addressed to industrial production processes. In 2002, he returned to the University of Valencia to get his PhD (with Quality Award) under supervision of Prof. Juan Faus (Prof. Miguel Julve group). The PhD thesis was focused on the study of the magnetic properties of Re(IV) compounds. During this period, he obtained the first oxalate-based Single-Molecule Magnet (SMM), the first hexachlororhenate(IV) salt which exhibits ferromagnetic behaviour, and the first reported examples of polymorphs and supramolecular isomers in the Re(IV) coordination chemistry. In 2007, he got his first post-doctoral position at the Excellence Centre CEMIF.CAL (Italy) within the research group of Prof. Giovanni De Munno, where he was trained in X-ray diffraction techniques and, at the same time, also worked on projects dealing with the coordination chemistry of some biomolecules, such as vitamins and nucleosides. In addition, he developed biological investigations focused on metal-based anti-tumor drugs. In 2008, thanks to the funding from the European Network of Excellence MAGMANET, he performed a short post-doctoral stay in the group of Prof. Dante Gatteschi at the University of Florence (Italy), with direct supervision given by Prof. Roberta Sessoli. In this pioneering group in the Molecular Magnetism field, he was mainly trained in the use of SQUID magnetometry and EPR techniques. Between 2008 and 2010, he was hired at the Université Pierre et Marie Curie of Paris (France) where, under the supervision of the Emeritus Profs. Michel Verdaguer and Pierre Gouzerh, he performed magneto-structural studies on hexanuclear salicylamidoxime-based Mn(III) nanomagnets, which revealed new and important insights in this type of systems. He proposed a structural classification of these hexanuclear Mn(III) complexes in four classes depending on the coordination of the axial carboxylate and demonstrated the structural flexibility of such systems, their sensitivity to solvent effects and their ability to achieve high energy barrier values by simple desolvation. In 2011, he received a Marie-Curie Fellowship funded under the European Commission's Seventh Framework Programme, the hosting institution being the University of Edinburgh (UK). The research project was developed within the group of Prof. E. K. Brechin. The over-arching aim of the research program was the introduction of the highly anisotropic Re(IV) metal ion into hexanuclear Mn(III) cages in order to enhance the energy barrier of such systems. Moreover, a series of major accomplishments has also shown the scientific success of this project, as the first cationic compounds based on phenolic oximes. This being a step towards making more advanced materials, since this allows to tune the solubility, reactivity, purification, stability and substrate specificity of such systems. The first salt ever reported in which both cation and anion are nanomagnets, and the first complexes based on the highly anisotropic Re(IV) and Mn(III) metal ions exhibiting SMM behaviour. Here, he has recently opened new research lines based on High Pressure techniques.

### Resumen del Currículum Vitae:

Francisco José Martínez Lillo received his degree in Chemistry (2000) at the University of Valencia (Spain). Then, thanks to a grant from IMPIVA, he spent eleven months in the Institute of Ceramic Technology (ALICER-ITC) in Castellón (Spain) where, in collaboration with other institutes of technology and national ceramic companies, he carried out several pilot projects and developments which were later successfully introduced into industrial production processes. In 2002, he returned to the University of Valencia in order to get his PhD under supervision of Prof. Juan Faus, within the research group of Prof. Miguel Julve. The PhD thesis was focused on the study of the magnetic properties of polynuclear compounds based on Re(IV). In 2007, he carried out his first post-doctoral appointment hosted by the research group of Prof. Giovanni De Munno in the Excellence Centre CEMIF.CAL (Italy), and where two previous pre-doctoral stages (in 2005 and 2006) were also performed, to carry out X-ray diffraction studies as well as develop biological investigations with metal-based anti-tumor drugs. In 2008, he performed a six month post-doctoral stay in the group of Prof. Dante Gatteschi at the University of Florence (Italy), with direct supervision given by Prof. Roberta Sessoli. In this pioneering group in the Molecular Magnetism field, he was mainly trained in the use of SQUID magnetometry and EPR techniques. Between 2008 and 2010, he was hired at the Université Pierre et Marie Curie of Paris (France) under the supervision of the Emeritus Profs. Michel Verdaguer and Pierre Gouzerh, where he performed magneto-structural studies on salicylamidoxime-based Mn(III) nanomagnets, which revealed new and important insights in this type of systems. In 2011 he was awarded a Marie-Curie Fellowship, funded under the European Commission's Seventh Framework Programme, and the hosting institution being the University of Edinburgh (UK). The research project was focused on the development of new nanomagnets based on the highly anisotropic Mn(III) and Re(IV) metal ions, within the research group of Prof. E. K. Brechin. Here, he has recently opened new research lines focused on combined studies of High Pressure Crystallography and High Pressure Magnetochemistry. During his post-doctoral period, he has mentored several undergraduate and Erasmus students from different European countries, he was in charge of designing and supervising their research projects. In June 2014, he has started the co-direction of a Thesis work at the University of



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

**AYUDAS RAMÓN Y CAJAL  
CONVOCATORIA 2014**

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

Edinburgh. He is an active Referee in ACS, Wiley and Elsevier journals. In a high number of his publications (more than 35 publications in high-impact scientific journals) he is the first author (85 percent of the papers) or corresponding author (50 percent of the papers), some of them have been highlighted as 'Hot Article' and also as Front Cover. Moreover, he has co-authored two book chapters. He is/has been member of the Associazione Italiana di Cristalografia (AIC), Real Sociedad Española de Química (RSEQ) and also of the European Network of Excellence: Molecular Approach to Nanomagnets and Multifunctional Materials (MAGMANet).



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** FERNANDEZ GARCIA, BEATRIZ  
**Referencia:** RYC-2014-14985  
**Área Científica:** Química  
**Correo Electrónico:** fernandezbeatriz@uniovi.es

### Título:

New Analytical Strategies For Quantitative and Spatially Resolved Analysis Using Solid-State Mass Spectrometry Techniques

### Resumen de la Memoria:

The main research line during my career has been the development of quantitative methodologies for the direct analysis of materials using solid state spectrometry techniques as well as instrumental developments in this research field. Particularly, I am a recognized worldwide researcher in complementary analytical techniques such as glow discharge sources coupled to either optical emission (GD-OES) or mass spectrometry (GD-MS), and laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS). GD sources and LA-ICP-MS are an advantageous tandem for the characterization of practically any type of solid sample, offering to different research fields powerful analytical tools to assist the synthesis procedures and also for quality control purposes. Although qualitative analysis can be carried out on a routine basis, quantification still remains as an important challenge for many kind of samples; it is in this particular field where my research line has been mainly devoted.

Concerning glow discharge sources, I have been involved in the development of new methodologies for the quantitative and depth profiling analysis of solids by GD-OES and GD-MS since the beginning of my research career. The broad experience acquired during these 14 years on GD plasmas has allowed to me to get a leadership position worldwide. The research carried out with GD sources has been tackled through different aspects, including basic studies, instrumental developments and applications to the analysis of samples of high technological interest. I have studied the effect of light elements on GD plasmas and developed appropriate corrections for quantitative analyses. Also, I have carried out instrumental developments in the frame of a European Project to develop a GD-ToFMS prototype (successfully commercialized nowadays). Among the different high technological materials successfully investigated by pulsed GDs it should be included ultra-low energy implants, nanostructured materials, photovoltaic devices and polymer-based coatings.

Regarding laser ablation analyses, the combination of laser ablation and ICP-MS represents one of the most powerful techniques for the direct determination of elemental composition and isotope ratios in solid samples. Today's success of LA-ICP-MS is partially related to the technological progress in lasers and ICP-MS instrumentation and no generally applicable protocols can be suggested for the wide variety of samples that are currently investigated by means of LA-ICP-MS. So far, several calibration strategies have been developed, but in all of them we can find several specific limitations and, thus, new methodologies must be still developed to find universal calibration methods. Since my postdoctoral Stage at CNRS, the research carried out with LA-ICP-MS has tackled through different aspects such as basic studies, instrumental developments and, particularly, development of accurate and precise calibration methods for the analysis of samples of Geological, Biological and Biomedical interest. Also, I would like to stress that thanks to the experience and knowledge acquired during my Postdoc using LA-ICP-MS, I have started a new research line in the Analytical Spectrometry Research Group of the University of Oviedo focused to new analytical strategies for quantitative and spatially resolved analysis by LA-ICP-MS.

### Resumen del Currículum Vitae:

I completed my PhD at the Dept. of Physical and Analytical Chemistry of the University of Oviedo (2002-2006). The European PhD was awarded with the Extraordinary Doctorate Prize of the University of Oviedo and with the San Alberto Magno Doctoral Thesis Award of the Official College of Chemists from Asturias and León. During my PhD I published 9 articles in International peer-reviewed journals and I spent 3 months at the Swiss Federal Laboratories for Materials Testing & Research (Thun, Switzerland) and 2 months at the Dept. of Chemistry of Clemson University in USA.

In 2006 I moved to the IPREM (Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux) at CNRS in Pau (France) working as a Postdoctoral researcher on the direct characterization of solid materials. During this period, I was awarded with a 2 years Postdoctoral Fellowship from the Spanish Government (MEC/Fulbright). Afterwards, I extended my stage by signing a Research Contract with the CNRS leading to a total Postdoctoral Stage of 29 months. During my postdoc I acquired leadership skills and team work abilities with the supervision of 2 students, I actively participated in 2 research projects (R&D, including Technology Transfer) and I published 8 articles in International peer-reviewed journals.

In September 2008 I moved to the University of Oviedo where I am working in the Analytical Spectrometry Research Group. I was awarded



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

with a Juan de la Cierva Contract from the Spanish Government and I have initiated 2 new research lines in the Group: the characterization of solar cells using GD sources and the development of accurate quantification methods for LA-ICP-MS analysis. I am currently the corresponding author of the published articles, co-director of 4 Doctoral Thesis (two of them already defended in 2012 and 2014) and director of 9 Master Thesis Projects. I have published 49 articles in International peer-reviewed journals (including 4 Anal. Chem., 1 Progress in Photovoltaics and 2 TrAC reviews with 169 citations), 2 book chapters and I am the first author of a Spanish Patent with Previous Examination (currently in negotiations for its fabrication and commercialization). I am either the first or the second author in 37 publications and the corresponding author in 20. My research has been presented in 80 National and International conferences including 7 invited lectures.

I have established multidisciplinary National and International collaborations such as those with the German National Metrology Institute (PTB, Berlin), the Center for Materials & Microsystems of Trento (Italy) and the National Institute of Standards and Technology (NIST, USA). I have secured funding as a Principal Investigator in 7 R&D&I Projects (1 funded in competitive tenders by public bodies and 6 contracts with Companies and Technological Centers). I have actively participated in 2 European projects (Marie Curie Research Training Network & Specific Targeted Research Project). I received invitations to contribute to JAAS & ABC Special Issues devoted to young outstanding scientists in Analytical Chemistry. I am reviewer of 10 International journals and I was Guest Editor of an ABC special issue. I have co-chaired 1 International and 1 National Conference and I have been member of the Scientific Committee in a National Conference.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** ARDA FREIRE, ANA  
**Referencia:** RYC-2014-15969  
**Área Científica:** Química  
**Correo Electrónico:** aarda@cicbiogune.es

### Título:

Structural studies of molecular recognition processes by NMR and modeling

### Resumen de la Memoria:

My research career started during my PhD in the field of Natural Products Chemistry. In particular, in the structural elucidation of the configuration of chiral centers. Specifically, I was involved in the extension of the J-based analysis, which had been applied to chiral centers containing alkyl and hydroxyl groups, to nitrogen containing moieties. After chemical synthesis of different structural models (known configuration), we demonstrated the applicability of the method to nitrogen containing fragments. This allowed us to successfully apply the methodology to a newly discovered Marine Natural Product. The proposed configuration was later confirmed by total synthesis by us. Through a short stay (3 months) at the University of Salerno in Italy, I learned to acquire and interpret specific NMR experiments for extracting NMR coupling constants. This work was published in different peer reviewed journals.

After that period I decided to direct my research toward a biological applicable Chemistry. I thus moved to a reference group in the field of Carbohydrate Chemistry, at Utrecht University in The Netherlands. In particular I was involved in the NMR study of complex glycan structures for the generation a Carbohydrate Database, one of the urgent demands within the glycan community. With the state-of-the-art in NMR instrumentation, analysis and assignment software, I was able to fully characterize (NMR) biologically relevant glycan structures, as well as protein-glycan complexes.

In the year 2008 I moved to a worldwide reference group in the study of biomolecular interactions by NMR: the group of Prof. Jesús Jiménez-Barbero at Centro de Investigaciones Biológicas (CSIC) in Madrid. There, I have been involved in a variety of different projects, with the common aim of unravelling the structural features that steer molecular recognition processes as well as molecular and supramolecular organizations, by pushing the possibilities of NMR spectroscopy, and with the assistance of molecular modelling. Through different international collaborations I have studied for instance, the specificity, in terms of epitope, of the recognition of HNK1 related carbohydrates by antibodies. I have explored the selective recognition of mannosides by synthetic receptors. I have demonstrated the conformational switch of a molecular machine upon pH change, and elucidated the folding of chiral metalloptides.

More recently, I have focused on the recognition processes that rule the so-called 'sugar code'. The recognition of glycans by specific receptors (lectins and antibodies) relies on the presence of specific epitopes. We have recently demonstrated that other important issues such as ligand presentation or receptors oligomeric state might change assumed selectivities and specificities. It is thus important to assess which are the roles of these and other structural elements (conformational entropy, multivalency presentation) in order to understand the 'sugar code'. In parallel, the detailed study of the interatomic interactions that take place in these recognition processes are also object of interest in my research, such as CH- $\pi$  interactions or the potential hydrophobic effect caused by sugar polyfluorination.

In November 2014 I moved to CICbioGUNE, a young Institution with an enthusiastic thrilling scientific atmosphere, where I pretend to carry on my research.

### Resumen del Currículum Vitae:

#### Education:

March 2006. PhD (cum laude) in Chemistry from the University of La Coruña.

#### Research experience:

11/2014- current. CICbioGUNE, Bilbao. Postdoctoral research associate.

10/2008 - 11/2014. Centro de Investigaciones Biológicas (CIB-CSIC), Madrid. Postdoctoral research associate. Research advisor: Jesús Jiménez-Barbero. From December 2009 - November 2012 as Juan de la Cierva fellow.

11/2006 - 10/2008. Bijvoet Centre for Biomolecular Research, Utrecht (NL). Postdoctoral position. Research advisor: Johnannis P. Kamerling.

09 - 12/2003. Università degli Studi di Salerno (IT). Short term research scholar at Facoltà di Farmacia. Supervisor: Dr. Luigi Gomez-Paloma.

10/2000 - 03/2006. University of A Coruña, La Coruña (ES). PhD fellow. PhD supervisors: Dr. Carlos Jimenez and Dr. Jaime Rodríguez.

#### Scientific publications:

- PLOS ONE. Accepted.

- Glycobiology. Accepted.

- FEBS J. 2014 Accepted.

- Chem. Eur. J. 2014, 20 (46), 15208-15.

- Chem. Eur. J. 2014, 20 (20), 60811-91

- Chem. Eur. J. 2014, 20 (24), 7363-72.

- Chembiochem. 2014, 15, 250-8.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

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  - Chem. Eur. J. 2011 17 (17), 4821-9.
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  - Eur. J. Org. Chem. 2010, 64-71.
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  - Eur. J. Org. Chem. 2006, 3645-51.
  - Tetrahedron 2005, 61, 10093-8.
  - J. Nat. Prod. 2004, 45, 1190-2.
  - Tetrahedron Lett. 2004, 45, 3241-3.
- BOOK chapters in New Applications of NMR in Drug Discovery and Development, 2013, 7-42, Print ISBN: 978-1-84973-444-8.
- BOOK chapter in SPR - Carbohydrate Chemistry 2012, 38, 192-214. Book series from the Royal Society of Chemistry. Print ISBN: 978-1-84973-439-4.
- BOOK chapter in SPR - Carbohydrate Chemistry 2009, 35, 334-356. Book series from the Royal Society of Chemistry. Print ISBN: 978-1-84755-880-0.
- Participation to conferences:
- Invited speaker:
- Glycopharm Workshop, Siena, Italy, January 2014.
  - Carbohydrate Research New Investigator Symposium, Bangalore, India, January 2014.
  - 9th Spanish-Italian Symposium on Organic Chemistry (SISOC 9), Tenerife, Spain, February 2012.
  - European Young Investigator Workshop, Lyon, France April 2011.
  - Reunión Bienal del GERMN-II Reunión Ibérica de RMN, Bilbao, Spain, September 2010.
- Oral communications: 6 in International meetings.
- Poster communications: 18 in international and national meetings.
- Participation in I+D Projects: 4 european projects, 5 national projects, and 2 projects with companies.
- Teaching: Workshop:
- Receptor-ligand interactions by NMR. GERMN NMR meeting. Alacá de Henares 2014.
  - Master Universitario en Química Orgánica Experimental e Industrial. Resonancia Magnética Nuclear. Valencia 2012.
  - Curso de actualización: Structure of carbohydrate molecules. NMR and recognition. Lisboa 2011.
  - Master Química Médica Universidad San Pablo-CEU. Reconoc



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** ROCA MOLINER, MARIA TERESA

**Referencia:** RYC-2014-16592

**Área Científica:** Química

**Correo Electrónico:** m.teresa.roca@uv.es

### Título:

On the role of protein dynamics in enzyme catalysis: towards rational design of new drugs

### Resumen de la Memoria:

The main research line of Maria Teresa Roca Moliner during her career is to provide a deeper comprehension of the remarkable catalytic power of enzymes. Enzymes catalyze biochemical reactions and play a major role in performing and controlling most biological processes. Thus, it is important to understand the action of enzymes on a detailed molecular level by the fact that many diseases can be controlled by developing drugs that block the action of enzymes in crucial biological pathways of the bacteria or viruses that cause these diseases. So if we can learn enough about enzyme mechanisms, we may someday learn to manipulate them and treat any kind of disease.

The potential of this important field can be explored and clarified in an efficient way by computational approaches that actually consider the activation barriers of the reactions that are being catalyzed and other effects that contribute to the catalytic process.

First of all, we study the catalytic processes by obtaining the activation free energy barriers using the hybrid Quantum Mechanics/Molecular Mechanics Molecular Dynamics methods. In this step, we rationalize the catalytic power of enzymes in terms of interactions that stabilize the transition state in order to find the key factors to the catalysis. Comparing the charge distributions and the interactions with the environment of the transition structures obtained with the known inhibitors we can predict or design new efficient inhibitors.

It is well-known that proteins sample numerous conformational states and vibrational coupling between the protein and the substrate could exist. Recent isotopic substitution studies have been proposed to affect catalysis by changing ultrafast vibrations that couple to the reaction coordinate. Thus, we explore the protein motions that could be coupled with the catalytic reaction (dynamical effects).

In conclusion, detailed analysis of transition state structures and a better understanding of enzyme action allow us to perform a rational approach to the computational design of novel and potent drugs. The results will be shared with experimental groups in order to validate them in vitro and in vivo and in the future will yield new medicines to treat diseases such as Parkinson, Alzheimer, Cancer.

### Resumen del Currículum Vitae:

María Teresa Roca Moliner was graduated in Chemistry in June 2000 at the Universitat Jaume I. She obtained a predoctoral fellowship by Ministerio de Educación y Ciencia and carried out her European PhD degree in Chemistry at the Universitat Jaume I. The Thesis was defended in 2005 and she obtained the maximum grade **sobresaliente Cum Laude por unanimidad** (premio extraordinario de doctorado). Her work was an excellent application of statistical QM/MM methods to investigate fundamental hypothesis regarding enzyme catalysis.

In 2006 she obtained a postdoctoral fellowship of excellence by Generalitat Valenciana and started her postdoctoral research under the supervision of the Nobel Laureate in Chemistry 2013, Prof. Arieh Warshel at University of Southern California, Los Angeles (USA). Her work was focused on the study of the thermal stability in enzymes and it was resolved the origin of the relationship of the thermal stability and the catalytic power of enzymes for the first time. She was awarded by **The 2008 Arthur Adamson Postdoctoral Recognition Award** for the scholarly excellence and innovative postdoctoral research.

In 2009 she obtained a Juan de la Cierva contract under the supervision of Prof. Iñaki Tuñón at Universitat de Valencia. In July 2012 she got a postdoctoral researcher contract at Universitat Jaume I under the supervision of Juan Andres Bort and in September 2013 she obtained a contract as Assistant Professor at Universitat de Valencia. Nowadays, her research is mainly focused on the role that dynamics effects play enzyme catalysis for the rational design of effective inhibitors.

She has supervised the Master Thesis of two predoctoral students and she continues supervising their PhDs. She has participated in 16 research projects which financial entities were Universitat Jaume I - Fundació Bancaixa, Generalitat Valenciana, British Royal Society, Ministerio de Educación y Ciencia, Ministerio de Ciencia e Innovación, National Institutes of Health of USA and CNRS Funding (France). And she has been the main researcher of two projects which financial entities are Universitat de Valencia and Generalitat Valenciana.

She is currently author of 31 publications in international journals with high impact factor and two in preparation. Most highlights include: 1 Chem. Soc. Rev. (selected as hot paper in Chemical Science), 2 PNAS, 9 JACS (one selected as hot paper in Reports Ltd Faculty of 1000, one highlighted in Nature Chemistry and one and another one selected as cover picture), 1 Curr. Opin. Chem. Biol., 1 Chem. A Eur. J.,



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

with 548 citations (h-index 15) (Web of Science). She has acted as referee several times for the American Chemical Society, Royal Society of Chemistry and Elsevier.

Furthermore, the candidate has presented her results in 24 prestigious international conferences as an oral communication or a poster, among which it is worth highlighting WATOC, ESPA, Isotopes, Biophysical Society Meeting, Gordon Conference and 237th ACS National Meeting. It is worth pointing out that the candidate has taught different subjects of Physical Chemistry at Chemistry degree, Pharmacy Degree and Electronic Engineering degree, in an interuniversity Master of Biomedical Engineering and in an interuniversity European Master of Theoretical and Computational Chemistry, a total of 840 hours. She is qualified as Profesor Titular de Universidad by ANECA.





MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** GINER CASARES, JUAN JOSE

**Referencia:** RYC-2014-14956

**Área Científica:** Química

**Correo Electrónico:** jjginer@cicbiomagune.es

### Título:

Plasmonic substrates for biomedicine

### Resumen de la Memoria:

Dr. Giner-Casares achieved the basis of his research knowledge on physical chemistry of Langmuir monolayers studied by a combination of experimental and computational techniques. During a postdoc in the Max Planck Institute for Colloids and Interfaces, the applicant extended the Langmuir technique to novel inorganic/organic polyoxometalate surfactants and acquired intensive knowledge on synchrotron radiation based techniques. Currently, Dr. Giner-Casares is working at CIC biomaGUNE focusing on the interfacial self-assembly of plasmonic nanoparticles aimed at functional materials for biomedicine.

Dr. Giner-Casares obtained his Ph. D. in the Department of Physical Chemistry at the University of Córdoba (Spain) in 2009 under the supervision of Prof. Dr. Luis Camacho. Two main topics were studied: experimental studies using interfacial spectroscopy and microscopy techniques on photoactive Langmuir monolayers, and computational studies using molecular dynamics on lipid bilayers and monolayers. Additionally, he performed research on organic electronics. During the Ph. D. Period, the applicant realized two research stays in international labs in UK and USA, as well as two research stays in collaboration with Prof. Dr. Javier López-Cascales (Polytechnic Univ. Cartagena). Dr. Giner-Casares employed a large array of experimental and computational techniques focused on understanding structure at the nanoscale, receiving the doctorate extraordinary award.

In August 2009, Dr. Giner-Casares joined the Max Planck Institute of Colloids and Interfaces (Potsdam, Germany) as a postdoctoral researcher under the guidance of Prof. Dr. Helmuth Möhwald and firstly working in Langmuir monolayers as biophysical models. In 2010 the applicant was awarded an Alexander von Humboldt fellowship, extending his research to novel polyoxometalate surfactants and working intensively on synchrotron based radiation techniques. He performed research on the crystallographic structure of mixed Langmuir monolayers containing organic dyes by synchrotron X-ray scattering, additionally leading a coordinated project Germany-Spain at DESY synchrotron (Hamburg, Germany). During 4 months at 2011 and 2012 each, Dr. Giner-Casares served as temporary **Profesor Sustituto Interino** at the Department of Physical Chemistry, University of Córdoba. Besides teaching, the applicant cosupervised a Ph. D. Thesis on Langmuir monolayers containing organic dyes. Additionally, he supervised three research stays of Ph. D. Students from the group of Prof. Dr. Salette Reis (University of Porto, Portugal) on biophysical studies.

In March 2013, he joined the BioNanoPlasmonics Lab led by Prof. Dr. Luis Liz-Marzán at CIC biomaGUNE (Donostia-San Sebastián, Spain). From March 2014 he is working as a Juan de la Cierva fellow. Dr. Giner-Casares is seeking to apply the acquired knowledge on physical chemistry of interfaces to design plasmonic functional materials for biomedicine, therefore further enhancing his capabilities for performing independent research and promoting his leadership.

### Resumen del Currículum Vitae:

Dr. Giner-Casares could secure his own salary at CIC biomaGUNE with a Juan de la Cierva fellowship starting in March 2013 (JCI-2012-12517). The applicant was ranked #1 in the **Basic Sciences** category of applicants, with a score of 100/100. The candidate is seeking to apply the acquired knowledge on physical chemistry of interfaces to design plasmonic functional materials for biomedicine. Additionally, Dr. Giner-Casares applied simultaneously for a Marie Curie Career Integration Grant in the 2013 call (FP7-PEOPLE-2013-CIG), with a three years proposal. The proposal was scored 88.40/100, being ranked in category B: Proposal on the reserve list, unfortunately not being awarded eventually.

Dr. Giner-Casares was selected as a temporary part-time lecturer **Profesor Sustituto Interino** in the Department of Physical Chemistry of the University of Córdoba during two semesters, in 2011 and 2012 each. Dr. Giner-Casares took advantage of this position to promote his research within the university environment, simultaneously with the research work at the Max Planck Institute of Colloids and Interfaces (Potsdam, Germany). Therefore, the candidate cosupervised a Ph. D. Thesis on Langmuir monolayers. Additionally, he supervised three research stays of Ph. D. Students from the group of Prof. Dr. Salette Reis (University of Porto, Portugal) on biophysical studies.

Dr. Giner-Casares was awarded an Alexander von Humboldt postdoctoral fellowship with duration of 24 months, starting in May 2010, to



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

work under the guidance of Prof. Dr. Helmuth Möhwald at the MPI of Colloids and Interfaces (Potsdam, Germany). The proposal for this fellowship was mainly related to biophysical studies. This was the first topic for motivating synchrotron-based studies at the air/water interface of the applicant in this postdoc period. Sixteen papers were published by the candidate within different topics, based on the experimental work of the candidate at the Max Planck Institute as well as on different collaborations.

Dr. Giner-Casares intensively used synchrotron radiation for characterizing widely different Langmuir monolayers, mainly by Grazing Incidence X-ray Diffraction (GIXD) and X-ray reflectivity. Dr. Giner-Casares was awarded for a coordinated European project in DESY entitled **Two dimensional supramolecular assemblies of organic dyes at the air/water interface** (I-20110062 EC). Dr. Giner-Casares was the PI of this project, being positively ranked by the selection committee because of the relevance of the proposed research, allocating 30 synchrotron shifts during 2011 and 2012. The coordination of this international project demonstrates the independence and leadership capabilities of the candidate.

Dr. Giner-Casares has experimentally realized for the first time Langmuir monolayers of novel inorganic/organic surfactants where the chains merely serve anchoring at the air/water interface and the organization is dictated by the hydrophilic head group. The publication **Polyoxometalate Surfactants as Unique Molecules for Interfacial Self-Assembly** was published in 2012 in The Journal of Physical Chemistry Letters (pag. 322-326). The candidate is the first and corresponding author, being the only responsible for designing and performing the experiments.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** OÑA BURGOS, PASCUAL

**Referencia:** RYC-2014-16620

**Área Científica:** Química

**Correo Electrónico:** pob081@ual.es

### Título:

A New Approach to Small Molecule Activation Based on Multi-nucleating Catalysts

### Resumen de la Memoria:

I studied Chemistry at the University of Almeria (UAL) (Andalucía, Spain), where I earned my PhD in December 2008, receiving the best qualification Sobresaliente cum laude, under the supervision of Prof. Fernando López-Ortiz and Prof. Ignacio Fernández. The thesis was focused in organic synthesis of phosphorous-based compounds as metallation directing groups, and mechanistic studies through extensive use of multinuclear NMR and X-ray diffraction methods.

After my PhD, I expanded my horizons through three consecutive postdoctoral research opportunities:

1) I spent 7 months in the industry working at Deretil's R&D department. My most important contribution was the optimization and development of a new and low-cost process for the synthesis of Ferroactive® (<http://deretilagrnutritional.com/productos/ferroactiv/>). As a matter of fact, the company sells this fertilizer the amount of 21 million of euros per year, representing one of its most important products. During this period I also initiated some collaborations in the academia such as the group of Ignacio Rodríguez working in titanium-mediated catalytic processes.

2) Right after my step in the industry, I worked for 2 years and 7 months in the research group of Prof. Frank Breher at the Karlsruhe Institute of Technology (KIT), where I was supported by an Alexander von Humboldt Foundation fellowship. My research was focused on: i) Synthesis of new ambidentate-based heterobimetallic complexes and their full characterization with special emphasis on their electrochemical properties and catalytic activity; ii) Rare Earth complexes with applications in luminescent materials and sulphur dioxide (SO<sub>2</sub>) fixation; iii) Main group chemistry; iv) Application of frustrated Lewis pairs (FLPs) to hydrogenation processes; and v) Synthesis of metallic clusters and wires.

3) Several days after finishing my von Humboldt period in Germany, I enjoyed an International Outgoing Fellowship (IOF) under the 7th FP People Marie Curie Actions. I joined an extraordinary 1 year in Prof. D. Tilley's research group at UC Berkeley. This prestigious fellowship included an extra year of returning phase which I enjoyed at the UAL in the Prof. Fernández's group. My research in this 1+1 year program established the synthesis of dinuclear homobimetallic complexes that could potentially reduce carbon dioxide into useful chemicals. In fact, during this period of time I could develop the first tetranuclear well-defined copper catalyst able of fixing CO<sub>2</sub> and reducing it into formate (a Nature Chem. paper is currently under submission).

Nowadays, I am back at the University of Almería leading together with Prof. Fernández the research group Advanced NMR Methods and Metal-based catalysts ([www2.ual.es/NMRMBC](http://www2.ual.es/NMRMBC)), which was created in 2013 and we are both building the bases of the group and establishing a body of research knowledge that is allowing me to supervise PhD thesis and developing my own lines of research.

I have authored 30 publications and 1 international patent. I have recently submitted 2 more papers, and 5 additional papers are in preparation. In overall, I have published 11 papers during my PhD period, and 19 during my postdoctoral stages. So far in my career, I have given 7 oral communications and 5 invited lectures. My overall H-index is 11 with a total of citations of 343.

### Resumen del Currículum Vitae:

07/2003 Undergraduate studies in Chemistry, University of Almería, Spain.

10/2006 M. Sc. in chemistry, University of Almería, Spain.

Sobresaliente (best mark possible).

Prof. Fernando López Ortiz.

12/2008 PhD. in Chemistry, University of Almería.

◆ Cum laude por unanimidad ◆ (best mark possible).

Prof. Fernando López Ortiz and Prof. Ignacio Fernández.

06/2009-12/2009 Post doctoral research at Deretil. S.A. R&D Institute.

Mr. Manuel Santiandreu (Head of R&D Institute in Deretil.SA).

01/2010-08/2010 Post doctoral research hired by the Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany.

Prof. Frank Breher.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

09/2010-08/2012 Postdoctoral Fellowship Alexander von Humboldt at KIT.  
Prof. Frank Breher.

09/2012-09/2014 International Outgoing Fellowship (IOF) of the 7th FP People Marie Curie Actions at University of California, Berkeley, United State outgoing phase and University of Almería, Almería, Spain returning phase.  
Prof. Don Tilley and Prof. Ignacio Fernández.

Spanish: mother language; English: fluently spoken and written; German: good spoken and written.

So far in my career, I have participated in 9 research projects. It is worth mentioning that I have enjoyed grants from the Spanish Ministry of Science, from the Alexander von Humboldt Foundation and from the 7th FP People Marie Curie Actions.

### Laboratory skills

I have acquired a broad experience in schlenk lines, dry-box techniques and SPS solvents. I have vast experience in multinuclear double and triple magnetic resonance techniques, acquisition and analysis of 1D and 2D NMR spectra, editing sequences and designing experiments. I have also acquired experience in the acquisition and interpretation of EPR, CV, FT-IR, Raman spectroscopies and X-ray crystallography for structural elucidation, LC (UPLC and HPLC) with chiral and non-chiral stationary phases as well as semi-preparative HPLC, GC-MS and ESI-MS spectroscopy for organometallics complexes characterization.

After my postdoctoral stage at KIT I have initiated fruitful collaborations with several internationally-recognized research groups, notably those directed by Prof. Breher, Prof. Roesky, Prof. Paradies and Prof. Bräse (KIT). During my time at University of California, Berkeley, I started collaborations with Prof. Tilley and Prof. Toste.

During these three periods, I have authored 30 publications: 2 Angew. Chem. Int. Ed.; 3 J. Am. Chem. Soc.; 2 Chem. Sci.; 3 Chem. Commun.; 4 Org. Lett.; 6 Chem. Eur. J.; 4 Organometallics; 4 Dalton Trans; 1 Synlett; and 1 J. P. P.; 2 paper has been submitted and 5 additional papers are in preparation. I am authored of 3 front covers in Chem. Eur. J. and 1 more in Dalton Trans. During 2014 already in the Fernández group I have authored my first international patent focused on NMR topics, and another one is in progress. I have given 7 oral presentations (the last one in the ACS meeting in San Francisco) and 5 invited lectures and three more are already programmed in 2015. In terms of leadership skills, I have helped to train and mentor during my career several PhD students and master students at both KIT and Berkeley, and currently in Almería I am co-advising two graduate students. I dedicated 504 hours to teaching undergraduates at KIT (English as the vehicle language). I have also taught 1st year undergraduate students of Chemistry and Environmental at UAL with an overall dedication of 2 ECTS credits in 2014.



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

Turno de acceso general

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

**Nombre:** CONCELLON FERNANDEZ, MARIA DEL CARMEN  
**Referencia:** RYC-2014-16021  
**Área Científica:** Química  
**Correo Electrónico:** carmen.concellon@gmail.com

### Título:

Organocatálisis asimétrica asistida por interacciones no covalentes

### Resumen de la Memoria:

En 2002 la Dra. Concellón comienza su Tesis Doctoral bajo la supervisión del Prof. J. M. Concellón estudiando las aplicaciones y usos de reactivos metálicos de bajo estado de oxidación en síntesis orgánica. Resultado de esta investigación son 12 publicaciones. Cabe destacar 3 (J. Org. Chem, 2006, 71, 7919; Org. Lett. 2006, 8, 5979; J. Org. Chem. 2007, 72, 5421), relacionadas con la catálisis orgánica. En 2007 la Dra. Concellón comienza su etapa postdoctoral en el grupo del Prof. A. D. Smith en el campo de la organocatálisis asimétrica. Estos estudios dieron lugar a 8 publicaciones entre las que cabe destacar: Angew. Chem. Int. Ed. 2009, 48, 8914. En 2009, la Dra. Concellón se traslada a la U. de Oviedo donde continua desarrollando métodos catalíticos basados en reactivos metálicos (Synlett 2011, 262-264; Tetrahedron 2012, 68, 1736). En 2010 la candidata comienza una línea de investigación independiente, llevando a cabo el diseño, la síntesis y la evaluación de nuevos aditivos que mejoran el comportamiento de la prolina en procesos catalizados por la misma, y que evitan grandes esfuerzos en la preparación de sofisticados organocatalizadores "de novo". Así, la Dra. Concellón ha presentado el uso de sales de guanidinio derivadas del TBD (una guanidina bicíclica aquiral) como aditivos en reacciones catalizadas por prolina. En disolventes no polares, los grupos N-H de esta sal de guanidinio, que se encuentran preorganizados, ofrecen un gran potencial para formar enlaces de hidrógeno dobles con la función carboxilato de la prolina, así como con compuestos carbonílicos como cetonas o aldehídos, modificando su inherente reactividad. La naturaleza de los aniones de las sales de TBD es totalmente decisiva. Más de 20 sales han sido preparadas y estudiadas en la reacción aldólica catalizada por prolina, exhibiendo todas ellas diferentes cualidades y efectos. La sal tetrafluoroborato de guanidinio es privilegiada, mejorando en gran medida la diastereo y enantioselectividad de la reacción aldólica catalizada por prolina (Org. Lett. 2011, 13, 3032). Esta sal, además, permite llevar a cabo por vez primera la reacción aldólica entre cloroacetona y aldehídos aromáticos empleando prolina como organocatalizador (Chem. Eur. J. 2012, 18, 5188). Así mismo, la candidata, ha descrito cómo el empleo de diferentes sales de guanidinio, en conjunción con prolina, permiten preparar independientemente aldeos tanto de configuración relativa sin- como anti-, en todos los casos con ee muy elevados (J. Org. Chem. 2010, 77, 10375). Siguiendo esta línea, la candidata describe la síntesis de  $\alpha$ -azido- $\beta$ -hidroximetilcetonas con total regio, y alta diastereo y enantioselectividad, utilizando prolina y la sal tetrafenil borato de guanidinio (Chem. Commun. 2014, 50, 2598-2600). Además, la Dra. Concellón ha publicado 2 trabajos donde el TBD, y no sus sales, es utilizado como catalizador: Org. Biomol. Chem. 2012, 10, 1976; y Tetrahedron 2012, 68, 6438. Finalmente, de forma colateral, la candidata ha publicado el uso de Oxone para transformar cetonas  $\alpha,\beta$ -insaturadas en los correspondientes acetatos vinílicos en un novedoso proceso tipo Baeyer-Villiger donde se describe por primera vez la migración de un grupo vinilo en esta reacción (Org. Lett. 2013, 15, 2810).

### Resumen del Currículum Vitae:

La candidata, Dra. Concellón, se licenció en Química en el año 2001 en la Universidad de Oviedo. A continuación se trasladó a la Universidad de Bristol (UK), donde trabajó en el grupo del Prof. T. Gallagher durante 10 meses bajo la financiación de una beca Erasmus de postgrado. Finalizado este periodo, la candidata comenzó, en 2002, su Tesis Doctoral en la Universidad de Oviedo bajo la supervisión del Catedrático José M. Concellón y con la financiación correspondiente a una beca FPI. Durante los siguientes 4 años la candidata desarrolla 2 estancias cortas, una de ellas en la Universidad de Bristol (grupo del Prof. T. Gallagher), en 2003, y la otra en la Universidad de Oxford (grupo del Prof. S.G. Davies), en 2004. En 2006, la Dra. Concellón defiende su Tesis Doctoral y a continuación se traslada a la Universidad de St Andrews (UK), donde durante 2 años y 6 meses (contrato de un año y beca postdoctoral MEC/Fullbright) llevará a cabo su investigación post-doctoral en el grupo del Prof. A.D. Smith. En 2009, la candidata se incorpora a la Universidad de Oviedo con un contrato de 3 meses para trabajar en el grupo del Catedrático José M. Concellón. En 2010, la Dra. Concellón toma posesión de un contrato Juan de la Cierva. Desde entonces y hasta la actualidad, la candidata no sólo ha trabajado en las líneas de investigación propias del grupo receptor, sino que ha comenzado una nueva línea de investigación totalmente independiente. En términos de docencia la Dra. Concellón se inicia en la misma durante su periodo post-doctoral impartiendo clases de problemas y prácticas de laboratorio. Continúa con su labor docente una vez reincorporada en la Universidad de Oviedo, impartiendo clases de problemas, tutorías grupales y prácticas de laboratorio siendo incorporada al plan docente del Dpto. de Química Orgánica e Inorgánica. Ha dirigido 3 Tesis Doctorales, una Tesina y un Trabajo Fin de Máster.

En resumen, el trabajo de la candidata ha dado lugar a una patente y 40 artículos científicos, todos ellos publicados en revistas de carácter internacional. Así mismo, cabe decir, que la candidata ha presentado su trabajo en congresos, nacionales e internacionales. Cabe enfatizar el éxito de la candidata en su actual periodo de investigación ya que, a pesar de los grandes cambios estructurales sufridos en el grupo de investigación del que forma parte la Dra. Concellón, ha desarrollado una nueva línea de investigación independiente, sin relación con la química tradicional del grupo. Este trabajo ha dado lugar a 7 artículos científicos en revistas internacionales en los que la candidata es



MINISTERIO  
DE ECONOMÍA  
Y COMPETITIVIDAD

## AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2014

**Turno de acceso general**

SECRETARÍA DE ESTADO  
DE INVESTIGACIÓN  
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL  
DE CIENCIA, TECNOLOGÍA  
E INNOVACIÓN

DIRECCIÓN GENERAL  
DE INVESTIGACIÓN  
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL  
DE RECURSOS HUMANOS  
PARA LA INVESTIGACIÓN

◆corresponding author◆. Fruto de toda su labor, la candidata posee un índice h de 16, ha sido habilitada por la ANECA como Profesor Contratado Doctor, Profesor Ayudante Doctor y Profesor de Universidad Privada y es censor habitual de Tetrahedron Letters y Green Chemistry. Esto prueba la habilidad de la Dra. Concellón para desarrollar su actividad investigadora de forma exitosa en todos los grupos de investigación de los que ha formado parte, independientemente de la gran diversidad de campos de investigación en los que se han encuadrado sus proyectos. Cada periodo de investigación, incluyendo las estancias cortas en el extranjero, han dado lugar a una publicación científica como mínimo.