INFORME INTERMEDIO DE PROYECTOS EXPLORA

Lea detenidamente las instrucciones de elaboración del informe al final de este documento.

Lea también atentamente la información solicitada en cada uno de los apartados del informe y revise la memoria técnica y el presupuesto presentados cuando hizo la solicitud de ayuda, para justificar adecuadamente todas aquellas actividades o gastos que se hayan hecho para la consecución de los objetivos que no estuvieran previstos o suficientemente detallados en la memoria y el presupuesto iniciales.

A. Datos del proyecto

A1. Datos del proyecto	
Referencia proyecto	CTQ2013-50575-EXP
Título Proyecto	SMART CHIRAL FRAMEWORKS TO CONTROL AND INHIBIT CORROSION
Investigador Principal	José Lorenzo Alonso Gómez
Entidad	Universidade de Vigo
Centro	Facultde de Químicas
Fecha de inicio	01/09/2014
Fecha final	31/08/2016
Duración	Dos años
Total concedido	84.700,00 €

A2. Descripción, en su caso, de las modificaciones producidas en el proyecto respecto a los datos que figuran en la resolución de concesión inicial (cambio de IP, de entidad, de centro, solicitud de prórrogas…)
No hay modificaciones.

B. Personal activo en el proyecto

Tiene que relacionar la situación de **todo** el personal de las entidades participantes que haya prestado servicio en el proyecto en el periodo que se justifica, o que no haya sido declarado anteriormente, y cuyos costes (dietas, desplazamientos, etc.) se imputen al mismo.

B.1. Equipo de investigación

Incluido en la solicitud original

	Nombre	NIF/NIE	Función en el proyecto	Fecha de baja	Observaciones
1	Xosé Ramón Nóvoa Rodríguez	34914531 W	Supervision of electrochemistry and corrosion studies		
2	María Magdalena Cid Fernández	35553218 W	Supervision of [14$_1$]allenophanes synthesis		

No incluido en la solicitud original

	Nombre	NIF/NIE	Función en el proyecto	Fecha	Fecha	Observaciones

				de alta	de baja	
1						
2						

B.2. Equipo de Trabajo

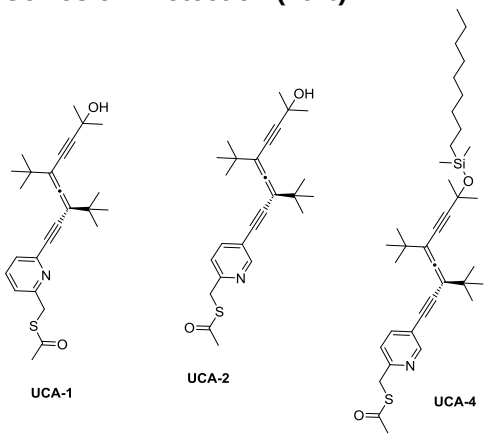
	Nombre	NIF/NIE	Función en el proyecto	Inicio	Fin	Observaciones
1	Raquel Pereira Cameselle		Supervision of chiral thioacetates synthesis for self-assemble monolayer formation and development of a synthetic orthogonal methodology to access spirocompounds	01/02/ 2015		Incorporation of a researcher with expertise in synthesis when the the PI was relocated in an independent laboratory in early 2015.
2	Ani Özçelik		Synthesis of chiral thioacetates for self-assemble monolayer formation	19/02/ 2015		Incorporation of a Master Student to undertake the synthesis of chiral thioacetates. Title of the Master thesis: Sensing with Up-standing Chiral Architectures
3	Silvia Castro Fernández		Design, synthesis and chiroptical predictions of spirobifluorenes and synthesis of [14_1]allenophanes	01/09/ 2014		PhD student Title of the PhD Thesis: From Allenes to Spiranes: a Crucial Milestone Towards Chiroptical Applications
4	Sandra Míguez Lago		Design, synthesis, chiroptical predictions and host-guest complexes of Covalent Organic Helical Cages	01/09/ 2014		PhD student Title of the PhD Thesis: Covalent Organic Helical Cages
5	Fahim Rofique		Molecular dynamics of spiro compounds	15/06/ 2015	02/07/ 2015	Visit to our group of from NYIT, New York

C. Progreso y resultados del proyecto

C1. Desarrollo de los objetivos planteados

Describa los objetivos y el grado de cumplimiento de los mismos (**porcentaje estimado respecto al objetivo planteado** y, en su caso, indique lo que queda por realizar en cada uno de ellos)

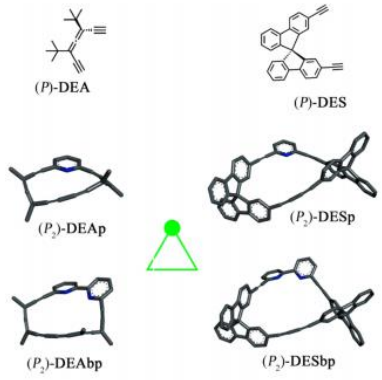
Smart Chiral Monolayers (SCMs) for Corrosion Protection (70%)

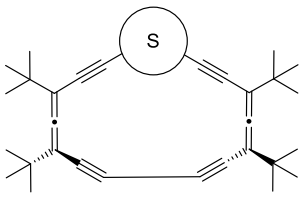


Synthesis of **S**mart **C**hiral **F**rameworks (**SCFs**) for the construction of **U**p-standing **C**hiral **A**rchitectures (**UCAs**) has been carried out. Incorporation of thioacetates directly attached to the pyridine ring will enable covalent binding to a metal substrate. On the other hand the presence of the pyridine should direct the self-assembly as well as the presence of the chiral allenes will provide strong chiroptical responses. Synthesis and enantiomeric resolution were carried out successfully for **UCA-1** and **UCA-2** where the different substitution, 2-6 and 2-5 respectively where done to study its influence on the self-assembly. Incorporation of the silane rendered **UCA-4** for both enantiomers was also carried out to study the capability of its self-assembly against corrosion.

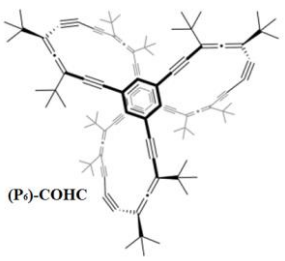
We are currently performing corrosion tests as well as deposition onto transparent electrodes in order to study the chiroptical amplification of these systems upon self-assembly and their sensitivity to detect corrosion processes.

Smart Chiral pH Sensors (SCpHSs) for Corrosion Mapping (70%)





S = pyridine **py-DEA$_2$**
S = bipyridine **bpy-DEA$_2$**



The presence of different conformations can lead to a partial cancelation of the chiroptical signal, due to the contribution of the chiral signals corresponding to each conformer. Therefore, the use of systems with narrow conformational spaces is desired in order to maximize chiroptical responses. Hence, we decided to move from previously synthetized systems bearing four chiral units to only two like **(*P*$_2$)-DEAp** and **(*P*$_2$)-DEAbp**. Our theoretical predictions suggest that these smaller macrocycles present a single conformation and strong chiroptical responses. We also theoretically predicted the reliability of spirobifluorenes (SBFs) as more stable chiral building blocks for the construction of chiroptical systems (Journal of Physical Chemistry A, 2015, 119. 1747–1753).

Synthesis of **(*P*$_2$)-DEAp** and **(*P*$_2$)-DEAbp** was performed successfully and while the first quickly photoisomerized due to the high ring straight energy, the second showed high stability and presents chiroptical sensing against pH changes (manuscript under preparation).

Another way to improve the conformational stability was performed by the synthesis of a **C**ovalent **O**rganic **H**elical **C**age (COHC) with remarkable chiroptical responses. This fascinating molecular containers undergoes host-guest complexation with ferrocenium and not with ferrocene, therefore opening the possibilities for redox chiroptical sensing that could be implemented into paints to track corrosion (Chemistry - A European Journal, 2015, 21, 18085 –18088).

Synthesis of SBF derivatives is currently under process. A Spirobifluorene Macrocycle Presenting Remarkable Chiroptical Amplification and Stability has been successfully prepared (manuscript in prepapration).

The sensibility of **(*P*$_2$)-DEAbp** to track corrosion while immersed into a paint will be tested.

More information at:
http://www.smartchiralframeworks.com/research.html

C2. Actividades realizadas y resultados alcanzados	
Actividad I.a: **Design of Smart Chiral Frameworks for UCA Formation**	Miembros del equipo participantes*: J.L. Alonso-Gómez Considering our preliminary results presented in *Chem. Comm*. **2014**, *50*, 15022–15025, synthetic accessibility a systematic study of the pyridine connectivity to explore its influence in the self-assembly, structures **UCA-1** and **UCA-2** were designed, additionally in order to inhibit the corrosion, addition of a silene was proposed in **UCA-4**.
Actividad I.b: Synthesis of Smart Chiral Frameworks for UCA Formation	Miembros del equipo participantes*: A. Ozçelik and R. Pereira An appropriate rout was proposed for the synthesis of the proposed chiral framworks **UCA-1**, **UCA-2**, and **UCA-4**. Chiral resolution on HPLC using a chiral stationary phase was successful. Slow photoisomerization of **UCA-1** was observed and very slow for **UCA-2**, therefore this systems used reacted to obtain the silane **UCA-4**. The enantiomeric pairs present strong mirror image chiroptical responses.
Actividad I.c: Scanning tunneling microscopy (STM)	Miembros del equipo participantes*: F. Klappenberger (collaborator at TUM, Munich) STM studies for the preliminary results were carried out and presented in *Chem. Comm*. **2014**, *50*, 15022–15025. Based on these results it was decided to perform further STM studies on the most promising candidate after the chiroptical amplification studies on nanoparticles and metal substrates.
Actividad I.d: **Chiroptical responses of Smart Chiral Monolayers (SCMs)**	Miembros del equipo participantes*: S. Chiussi (collaborator UVigo), A. Guerrero-Martínez (collaborator UCM,Madrid), and J.L. Alonso-Gómez In order to study the chiroptical amplification of **UCA-1**, **UCA-2**, and **UCA-4**, two strategies are being performed: 1. Plasmonic nanoparticle coating with the spices bearing long alkyl chain **UCA-4** to allow colloidal behavior (preliminary tests are positive), and as a consequence to enable chiroptical responses measurement in solution (will be performed in the following weeks). 2. Formation of monolayers onto pseudo transparent substrates to enable measuring chiroptical responses via transmittance. For that, deposition of 10-30 nm thickness layer of gold onto quart plans has been performed. Currently monolayer formation of **UCA-1**, **UCA-2**, and **UCA-4** are under investigation and will be followed by chiroptical responses measurements.
Actividad I.e: Corrosion Tests of Smart Chiral Monolayers (SCMs)	Miembros del equipo participantes*: X.R. Nóvoa Currently under investigation for **UCA-4**.
Actividad II.a: Design of Allenic Macrocycles for pH Sensing (SCpHSs)	Miembros del equipo participantes*: S. Castro-Fernández and M.M. Cid Recently we showed how the conformational freedom lowers chiroptical responses intensity, *Chem. Eur.J.* **2015**, *21*,12136 –12147. That is the reason why we designed smaller macrocycles with a single conformation.
Actividad II.a: **Design of Covalent organic Helical Cages (COHCs)**	Miembros del equipo participantes*: S. Míguez-Lago and J.L. Alonso-Gómez A different way to restrict the conformational freedom, and therefore enhance the chiroptical responses is blocking the conformation by cage formation. We theoretically predicted that this COHC has a single

	conformation and remarkable chiroptical responses.
Actividad II.a: **Design of Macrocycles: Opening access to new chiral macrocycles: from allenes to spiranes**	Miembros del equipo participantes*: S. Castro-Fernandez and J.L. Alonso-Gómez Allenes are valuable for the construction of systems with remarkable chiroptical responses, but they present stability limitations when conjugated with electron rich groups or under ring strength energy. Therefore we performed a theoretical study to proof that systems bearing sipiranic chiral elements are good competitors, *J. Phys. Chem*. *A* **2015**, *119*, 1747−1753.
Actividad II.b: Synthesis of Allenic Macrocycles for pH Sensing (SCpHSs)	Miembros del equipo participantes*: S. Castro-Fernandez These new macrocycles with single conformation present higher *g*-factor that the larger systems, *manuscript under preparation*.
Actividad II.b: Synthesis of Covalent organic Helical Cages (COHCs)	Miembros del equipo participantes*: S. Míguez-Lago Synthesis of both enantiomers of a COHC and complexation studies with ferrocenium, *Chem. Eur.J.* **2015**, *21*,18085 –18088.
Actividad II.b: Synthesis of Spiranic Macrocycles: Opening access to new chiral macrocycles: from allenes to spiranes	Miembros del equipo participantes*: S. Castro-Fernandez, R. Jang (collaborator, CSU, China), H. Xu (collaborator, CSU, China) Synthesis of a macrocycle bearing chiral spiranes confirmed the strong chiroptical responses theoretically predicted by us, *manuscript under preparation*.
Actividad II.b: Orthogonal Synthesis of Spirobifluorenes (SBFs)	Miembros del equipo participantes*: R. Pereira Synthesis of diethynylspiranes (DESs) was less efficient than expected, in order to improve accessibility to larger amounts and access to more complex structures, development of orthogonal synthesis of spirobifluorenes is under progress.
Actividad II.c: pH Chiroptical Sensing of Allenic Macrocycles	Miembros del equipo participantes*: S. Castro-Fernández and M.M. Cid Reversible chiroptical responses of macrocycle **bipy-DEA$_2$** were observed by changing the pH.
Actividad II.c: **Redox Chiroptical Sensing of Covalent Organic Helical Cages (COHCs)**	Miembros del equipo participantes*: S. Míguez-Lago and J.L. Alonso-Gómez Coupling of redox processes and complexation abilities of COHCs are now under investigation and could serve are corrosion reporters.
Actividad II.d: Corrosion Tests of Thin Films Incorporating Chiral Frameworks	Miembros del equipo participantes*: X.R. Nóvoa Pending

C3. Problemas y cambios en el plan de trabajo

Describa las dificultades y/o problemas que hayan podido surgir durante el desarrollo del proyecto, Indique cualquier cambio que se haya producido respecto a los objetivos o el plan de trabajo inicialmente planteados, así como las soluciones propuestas para resolverlos.

- The low stability of small allenophane **py-DEA$_2$** due to the ring strain energy can be undertaken by substituting the allenic chiral building block as proposed in the initial project. Another way can be to restrict to a single conformation an allenic macrocycle by the formation of a covalent organic helical cage (COHC). Therefore, we have designed, synthetized and tested this COHCs for complexing organometallic sandwich compounds that can undergo redox processes, therefore opening the gate for redox-chiroptical sensing that could report corrosion processes.
- Synthesis of diethynylspiranes (DESs) was less efficient than expected, to overcome this limitation, development of a methodology to access orthogonal spirobifluorenes is under process.
- In order to facilitate the study of chiroptical amplification of self-assemble chiral frameworks, deposition onto Plasmonic nanoparticles is being performed to study them in solution. On the other hand to facilitate the study of self-assemble monolayers by transmittance, the construction of pseudo transparent metallic substrates is under progress.

C4. Colaboraciones con otros grupos de investigación directamente relacionadas con el proyecto

Relacione las colaboraciones con otros grupos de investigación y el valor añadido para el proyecto. Describa, si procede, el acceso a equipamientos o infraestructuras de otros grupos o instituciones.

- **S. Chiussi** (http://newmaterials.uvigo.es/) from the Applied Physics of the Universidade de Vigo to build transparent substrates for monolayer formation and chiroptical responses analysis.
- **A. Guerrero-Martínez** (http://pendientedemigracion.ucm.es/info/quisupra/index.html)from the Physical Chemistry Department of the Universidad Complutense de Madrid to perform chiroptical frameworks deposition onto plasmonic nanoparticles in order to enable the study of their chiroptical amplification in solution.

More information at :

http://www.smartchiralframeworks.com/collaborations.html

C5. Colaboraciones con empresas o sectores socioeconómicos directamente relacionados con el proyecto

Relacione las colaboraciones con empresas o sectores socioeconómicos y el valor añadido que aporta al proyecto.

We are currently on search for companies that may be interested in our results.

C6. Actividades de internacionalización y otras colaboraciones relacionadas con el proyecto
Indique si ha colaborado con otros grupos o si ha concurrido, y con qué resultado, a alguna de las convocatorias de ayudas (proyectos, formación, infraestructuras, otros) de programas europeos y/o a otros programas internacionales, en temáticas relacionadas con la de este proyecto. Indique el programa, socios, países y temática y, en su caso, financiación recibida.

- Network Chiroptics (http://www.chiroptics.net/)

CTQ2015-71924-REDT, Redes de Excelencia, CHIROPTICal systemS, MINECO, 1/12/2015 – 30/11/2017, 25.000 €

The CHIROPTIC S network combines complementary expertise to achieve the goal of tailoring and characterizing chiroptical systems. The understanding of chiroptical properties and synthesis of powerful chiroptical molecules by the Chiral Frameworks team combined with the expertise of the Scanning Tunneling Microscopy team recently enabled the construction of Up-standing Chiral Architectures with tremendous potential for sensing applications. The Photochemical Switches team joins the network with the aim of providing more functionality to these chiroptical systems; the Nuclear Magnetic Resonance and Chiroptical Simulations teams will explore molecular recognition to improve the design and characterization capabilities; the Plasmonic Nanoparticles team, also current collaborator, will expand the applicability of chiroptical systems to nanoparticles; and, finally, the Surface and Gas Spectroscopies, Atomistic Structural Determination, Electrochemistry, and Surface Processing and characterization teams will be integrated into the network to move towards the constructions of simple sensing devices up to LabOnChips through chiral amplification. CHIROPTIC S aims at establishing the proof-of-principle for chiroptical sensing, in order to open up the opportunity of exploiting the unique sensing applications of chiroptical systems.

The main expected impacts of this project will be establishing the basis for the use of CHIROPTICal systemS for Sensing. Geometrically Linear, Tweezer-like, and Switch-like molecules will be Designed and Synthesized to undergo Molecular Recognition into Host–Guest complexes and stable self-assemblies onto Surfaces and Nanoparticles. Chiral Amplification of these LabOnChip compatible systems will be used for Sensing by chiroptical Spectroscopies.
While this project is based on previously demonstrated principles, their combination is unexplored. Significant research and development at both fundamental scientific and technological levels will be required to build the scientific and technological capacity in this area to the appropriate level for transferring to industry. Therefore, technological development will be complemented by producing new fundamental knowledge and rational design principles in chirality, surface preparation, and sensing devices. The development of new sensing devices in solution and on surfaces would improve the diagnostic abilities of crucial ailments within the challenge of Horizon 2020 “Health, demographic change and wellbeing”.

Partners

R. Novoa, UVigo, Spain, **Electrochemistry**.
S. Chiussi, UVigo, Spain, **Surface Processing and Characterization**.
A. Guerrero, UCM, Spain, **Plasmonic Nanoparticles**.
J. L. Alonso-Gómez, UVigo, Spain, **Chiral Frameworks**.
A. Navarro, UFPE, Basil, **Nuclear Magnetic Resonance**.
A. Kartouzian, TUM, Germany, **Surface and Gas Spectroscopies**.
F. Klappenberger, TUM, Germany, **Scanning Tunneling Microscopy**.
D. Duncan, Diamont, UK, **Atomistic Structural Determination**.
A. G. Petrovic, NYIT, New York, **Chiroptical Simulations**.
H. Dube, LMU, Germany, **Photochemical Switches**.

- *Research Project* **Molecular and Supramolecular Systems for Chiroptical Sensing (MolSupraSens)**

CTQ2014-58629-R, Retos de Investigación 2015 – 2017, **100.430 €**

The aim of this project is to build molecular and supramolecular Smart Chiral Frameworks (SCF) with strong chiroptical responses, sensitive to interactions with biomarkers, to explore their use for the construction of sensors (Figure 1). Appropriate combination of funtionalized spacers and chiral axes, allows the design and synthesis of Open, Cyclic, and Cage-shaped frameworks (Figure 2). Molecular Recognition of these systems along with their strong chiroptical responses will enable their use in biosensing. Host–Guest inclusion complexes of cycles and cages with will allow their use as biosensors in solution. Self-assembly of open SCFs can be used for the construction of Up-standing Chiral Architectures (UCAs) that for the moment have low stability. This project aims at improving the stability of these UCAs to funtionalized surfaces for their use as transductors. Furthermore, Host–Guest inclusion complexes of helical cages will be tailored for their further self-assembly directed by the invited guests in order to generate regular chiral networks, we call them Netanes. This very ambitious goal would open the use of SCFs in optoelectronics. Finally, it is expected that the self-assembly of open SCFs into chiral gles will induce significant chiroptical amplification, thus permitting the use of these chiral systems as transducers. Overall, this project aims to obtain Smart Chiral Frameworks and provide the necessary methodology for implementating them in Biosensing.

More information at:
http://www.smartchiralframeworks.com/funding.html

D. Difusión de los resultados del proyecto

D1. Publicaciones científico-técnicas (con peer-review) derivadas del proyecto y, en su caso, patentes

Autores, título, referencia de la publicación*…

Scientific articles

Morpholgical Self-assembly of Enantionpure Allenes for Upstanding Chiral Architectures at Interfaces
Y-Q. Zhang, M. A. Öner, I. R. Lahoz, B. Cirera, C-A. Palma, S. Castro-Fernández, S. Míguez-Lago, M. M. Cid, J. V. Barth, J. L. Alonso-Gómez, F. Klappenberger
Chemical Communications, **2014**, *50*, 15022–15025.

A Combined Experimental-Computational Investigation to Uncover the Puzzling (Chiro-optical Response of Pyridocyclophanes: One- and Two-Photon Spectra
D. Padula, I. R. Lahoz, C. Díaz, F. E. Hernández, L. Di Bari, A. Rizzo, F. Santoro, M. M. Cid
Chemistry - A European Journal, **2015**, *21*, 12136–12147.

Opening access to new chiral macrocycles: from allenes to spiranes
S. Castro-Fernández, M. M. Cid, C. S. López, J. L. Alonso-Gómez
Journal of Physical Chemistry A, **2015**, *119*. 1747–1753.

A Covalent Organic Helical Cage with Remarkable Chiroptical Amplification
S. Míguez-Lago, A. L. Llamas-Saiz, M. M. Cid, J. L. Alonso-Gómez
Chemistry - A European Journal, **2015**, *21*, 18085 –18088.

Chiroptical Amplification through Conformational Confinement: the Narrow Borderline between Ring Strain and Stability of Allenophanes
in preparation

A Spirobifluorene Macrocycle Presenting Remarkable Chiroptical Amplification and Stability
in preparation
More information at:
http://www.smartchiralframeworks.com/journal-articles.html

Patents

We contacted PONS (https://www.ponspatentesymarcas.es/) to study the possibility of protecting with a patent the main results of this project.

*Resalte en negrita las realizadas por el IP

D2. Asistencia a congresos, conferencias o workshops relacionados con el proyecto
Nombre del congreso, tipo de comunicación (invitada, oral, póster), autores

Chiroptical Amplification through Conformational Confinement and Self-Assembly
October, 13th **2015** Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
Invited talk, J.L. Alonso-Gómez

Chirality Transfer from Single Molecules to Surface-Confined Nanostructures
July, 20th **2015** XXXV Congreso Bienal de la Real Sociedad Española de Química, A Coruña, Spain
Oral presentation, José Lorenzo Alonso-Gómez, Yi-Qi Zhang, Murat Anil Öner, Inmaculada R. Lahoz, Borja Cirera, Carlos-Andres Palma, Silvia Castro-Fernández, Sandra Míguez-Lago,a M. Magdalena Cid, Johannes V. Barth and Florian Klappenberger

Chiroptics through Chiral Axes
June, 5th **2015** InTechSE, Vigo, Spain
Invited talk, J.L. Alonso-Gómez

Chiral Amplification in Molecular and Supramolecular Frameworks
October, 3rd **2014** Columbia University, New York, USA
Invited talk, J.L. Alonso-Gómez

Smart Chiral Frameworks From individual to collective chirality
July, 15th **2014** CIQUS, Santiago de Compostela, Spain
Invited talk, J.L. Alonso-Gómez

Up-standing Chiral Architectures through Topological Self-Assembly of Enantiopure Allenes
February, 12–14th **2014**, NanoPT, Porto, Portugal
Oral presentation, José Lorenzo Alonso-Gómez, Yi-Qi Zhang, Murat Anil Öner, Inmaculada R. Lahoz, Borja Cirera, Carlos-Andres Palma, Silvia Castro-Fernández, Sandra Míguez-Lago,a M. Magdalena Cid, Johannes V. Barth and Florian Klappenberger

More information at:
http://www.smartchiralframeworks.com/oral-presentations.html

D3. Otras publicaciones derivadas de colaboraciones mantenidas durante la ejecución del proyecto y que pudieran ser relevantes para el mismo, así como artículos de divulgación libros y conferencias
Autores, título, referencia de la publicación…

Scientific articles

Conformational stable alleno-acetylenic cyclophanes bearing chiral axes
I. R. Lahoz, S. Castro-Fernández, A. Navarro-Vázquez, J. L. Alonso-Gómez, M. M. Cid
Chirality, **2014**, *26*, 563–573

Preparation and characterization of a halogen-bonded shape-persistent chiral alleno-acetylenic inclusion complex
S. Castro-Fernandez,´ I. R. Lahoz, A. L. Llamas-Saiz, J. L. Alonso-Gómez, M. M. Cid, A. Navarro-

Vazquez
Organic Letters **2014**, *16*, 1136–1139.

Acetylenic homocoupling methodology towards the synthesis of 1,3-butadiynyl macrocycles: [14_2]-Alleno-acetylenic cyclophanes
I. R. Lahoz, A. Navarro-Vázquez, J. L. Alonso-Gómez, M. M. Cid
European Journal of Organic Chemistry **2014**, *9*, 1915–1924.

Divulgation articles

Transferencia de quiralidad desde moléculas discretas a nano-estructuras confinadas en superficies
J. L. Alonso-Gómez
Interempresas **2016**, *in press.*

Books and book chapters

Structure Elucidation in Organic Chemistry: The Search for the Right Tools
Editors: M.M. Cid and J. Bravo
ISBN: 978-3-527-33336-3, **2015**,Wiley-VCH.

Absolute Configuration and Conformational Analysis of Chiral Compounds via Experimental and Theoretical Prediction of Chiroptical Properties: ORD, ECD, and VCD
A. G. Petrovic, N. Berova, J. L. Alonso-Gómez,
in *Struct. Elucidation Org. Chem. Search Right Tools*, **2015**, pp. 65–104.

On the Search for the Appropriate Techniques for Structural Elucidation of Small Molecules
M.M. Cid, J. Bravo
in *Struct. Elucidation Org. Chem. Search Right Tools*, **2015**, pp. 493–520.

More information at:
http://www.smartchiralframeworks.com/journal-articles.html

Conferences

Chiroptical Systems on the Road to Sensing
December, 7–10th **2015** IC3TC, Lisbon, Portugal
Invited talk, J.L. Alonso-Gómez

De Eixos Quirais a Sensores Quirópticos
September, 8th **2015** Charlas Informativas de Propuestas de Trabajos Finde Grado, Vigo, Spain
Oral presentation, J.L. Alonso-Gómez

[14_2] Alenofanos Quirales: Síntesis, Propiedades Quirópticas y Aplicaciones
December, 11th **2014** Jornadas de Seguimiento MINECO, Madrid, Spain
Invited talk, J.L. Alonso-Gómez

May We Use Chiral Structures for Sensing?
October, 2nd **2014** New York Institute of Technology, New York, USA
Invited talk, J.L. Alonso-Gómez

Materiais Chirais Intelixentes ¿Poderían detectar biomarcadores do cancro?
May, 8th **2014** CHUS, Santiago de Compostela, Spain
Invited talk, J.L. Alonso-Gómez

More information at:
http://www.smartchiralframeworks.com/oral-presentations.html

E. Gastos realizados hasta la mitad del periodo de ejecución del proyecto

E1. Gastos de personal (indique número de personas, situación laboral y función desempeñada)					**Previsto en la sol. original (S/N)**
	Nombre	**Situación laboral**	**Función desempeñada**	**Importe**	
1	CASTRO FERNANDEZ SILVIA	Contratada a tiempo completo	Design, synthesis and chiroptical predictions of spirobifluorenes and synthesis of [14$_1$]allenophanes	24.021,11	S
2	ANI OZÇELIK	Contratada a tiempo completo	Synthesis of chiral thioacetates for self-assemble monolayer formation	22.512,74	S
Total gastos de personal:				**46.533,85**	

E2. Material inventariable (describa el material adquirido)				
	Equipo	**Descripción del equipo**	**Importe**	**Previsto en la sol. original (S/N)**
1	Agitador Magnético	Agitador con calefacción para la agitación y calentamiento de las reacciones	358,79	N
2	Armario	Armario frigorífico para conservar productos	562,00	N
3	Armario	Armario con ventilación para guardar reactivos	821,10	N
Total gastos material inventariable			**1.741,89**	

E3. Material fungible (describa el tipo de material por concepto o partida, p. ej., reactivos, material de laboratorio, consumibles informáticos, etc.)			
	Concepto	**Importe**	**Previsto en la sol. original (S/N)**
1	Reactivos y disolventes	8.820,54	S
2	Material vidrio, jeringas, lámpara UV, otro material fungible	8.320,92	S
3	Gases inertes, bala y mantenimiento	395,07	S
Total gastos material fungible		**17.536,53**	

E4. Viajes y dietas (describa la actividad del gasto realizado y **las personas que han realizado la actividad)**. Debe incluir aquí los gastos derivados de la asistencia a congresos, conferencias, colaboraciones, reuniones de preparación de propuestas relacionados con este proyecto, etc.)

	Concepto	**Relación con el proyecto**	**Importe**	**Nombre del participante**	**Previsto en sol. original (S/N)**
1	Asistencia bienal	Búsqueda de colaboraciones en el congreso y dar a conocer los resultados	795,95	Jose Lorenzo Alonso Gómez	S
2	Viaje a Munich	Realización de medidas y reunión para consecución de objactivos	771	Jose Lorenzo Alonso Gómez	S
3	Inscripción congreso IC3TC 2015	Búsqueda de colaboraciones en el congreso y dar a conocer los resultados	300	Jose Lorenzo Alonso Gómez	S
	Stay at UVigo	Estudio de sistemas espiránicos con dinámica molecular	362,85	Fahim Rofique	S
Total viajes y dietas			**2.229,8**		

E5. Otros gastos (describa la actividad del gasto por concepto, y si procede, las personas que han realizado la actividad)

	Concepto	Relación con el proyecto	Importe	Nombre del participante	Previsto en la sol. original (S/N)
1	CACTI	Uso servisios centrales de la Universidad (NMR, MS)	117,4		N
2					
Total otros gastos			**117,4**		

E6. Descripción de gastos no contemplados en la solicitud original (si ha realizado algún gasto no contemplado en la solicitud original, se **debe** justificar la necesidad de su adquisición en este apartado)

Gasto	Justificación
Gastos CACTI	Realización de medidas indispensables para el desarrollo de la síntesis y caracterización de los compuestos: RMN, MS.
Agitador magnético y armarios de reactivos	El traslado a un laboratorio independiente ha requerido de la adquisición de nuevo inventariable

E7. Total ejecutado (costes directos únicamente)

Importe total concedido (Gstos Directos)	**70.000,00**
Importe total ejecutado durante el periodo	**68.159,47**