



Barcelona, 3-6 de Noviembre de 2015



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(Editores)



Institut Català d'Investigació Química
Institut de Ciència de Materials de Barcelona – CSIC
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2015

Simposio de Investigadores Jóvenes (12^a. 2015. Barcelona).
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Bienvenida

El Comité Organizador da la bienvenida a todos los asistentes al XII Simposio de Investigadores Jóvenes RSEQ Sigma-Aldrich, que este año tenemos el honor de organizar en Barcelona del 3 al 6 de Noviembre.

El simposio engloba desde la investigación básica en química hasta las últimas aplicaciones, siendo una posibilidad muy enriquecedora para investigadores químicos de ambos campos. Además, en el mismo congreso se entregan los premios anuales a las mejores trayectorias (mejores C.V.s nacionales) y mejores publicaciones del 2014 en cualquier área de la Química. Este simposio cubrirá todas las ramas de la Química moderna, aunque cada vez más las distinciones se van difuminando hasta el punto que el Comité Científico ha repartido las comunicaciones en nueve áreas distintas. Las contribuciones serán distribuidas en charlas de los premiados (Sigma Aldrich y SusChem), comunicaciones *hot topic*, comunicaciones orales, comunicaciones flash (por primera vez en este simposio) y sesiones de póster. Además, el taller de empresas de este año ha querido cubrir nuevas salidas profesionales como la comunicación en revistas científicas, la divulgación en medios de comunicación y desarrollo de *software* de carácter científico.

El Comité Organizador está encantado con el número de participantes en la edición de este año y hemos intentado satisfacer toda la demanda, aún teniendo en cuenta las grandes dificultades económicas y la poca ayuda ofrecida por parte de las instituciones públicas. Asimismo, queremos destacar la alta participación de jóvenes trabajando y estudiando actualmente en el extranjero, que han querido asistir al congreso, dando una dimensión internacional a este evento nacional.

Barcelona ha sido seleccionada para acoger por primera vez una edición del simposio. Las sesiones científicas las celebraremos en la Residència d'Investigadors (con unas instalaciones immejorables) a escasos 300 m de las Ramblas de Barcelona y el Gran Teatre del Liceo. El alojamiento se realizará en tres hoteles distintos entre 5-10 minutos a pie del auditorio: el Hotel Turin, el Hotel Arc la Rambla y el Hotel Andante, todos ellos de tres estrellas y unas instalaciones fantásticas en pleno centro de Barcelona. Las comidas se realizarán en el Restaurante Cullera del Boix, a solo 300 m, y la cena de gala se celebrará en el Restaurante Brown 33, en pleno centro del Paseo de Gracia de Barcelona.

Queremos agradecer sinceramente el apoyo de todas las instituciones privadas en estos momentos de dificultad económica, por el interés mostrado en participar en la celebración del simposio y haciendo posible este evento científico.

Finalmente, damos la bienvenida a los asistentes noveles en el simposio y os recordamos que la participación y discusión es lo más importante en el avance de la ciencia. Los repetidores del simposio os pueden dar buenos consejos para que la XII edición sea un éxito. El primer consejo es que la discusión científica no se queda en la sala de actos sino que continúa durante la tarde-noche, y Barcelona os ofrecerá sin duda una excelente oportunidad para entablar colaboración para vuestro futuro. Sin más, disfrutad!

El Comité Organizador

Contacto

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Comité Científico

- **Prof. Jesús Jiménez-Barbero**

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- **Dr. Emilio J. Cocinero Pérez**

Presidente del Grupo Especializado JIQ de la RSEQ, Universidad del País Vasco (UPV/EHU).

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Institut de Ciència de Materials de Barcelona (ICMAB-CSIC).

- **Dr. Julio Lloret Fillol**

Institut Català d'Investigació Química (ICIQ).

- **Prof. Mariona Sodupe Roure**

Universitat Autònoma de Barcelona (UAB).

- **Prof. David B Amabilino**

University of Nottingham, UK.

- **Dra. Tània Gumí Caballero**

Universitat Rovira i Virgili (URV).

- **Dra. Mónica Lira Cantu**

Institut Català de Nanociència i Nanotecnologia (ICN2).

- **Dra. Mariola Tortosa Manzanares**

Universidad Autonoma de Madrid (UAM).

Comité Organizador

- **Dr. Pau Farràs Costa**
- **Dra. Arántzazu González Campo**
- **Dr. Julio Lloret Fillol**
- **Dra. Núria Aliaga Alcalde**
- **Marta Riba Moliner**
- **Cristina Oliveras González**
- **Carla Casadevall**
- **Raul Díaz Torres**
- **Wenjie Qian**
- **Arnau Call**

Patrocinadores

- Real Sociedad Española de Química (RSEQ)
- Sigma Aldrich S.A.
- Institut Català d'Investigació Química
- Institut de Ciència de Materials de Barcelona - CSIC
- Grupo Especializado de Jóvenes Investigadores Químicos de la RSEQ (JIQ)
- Fundació Banc Sabadell
- Mestrelab Research
- Bruker Corporation
- Real Sociedad Española de Química - Sección Territorial de Cataluña
- Societat Catalana de Química
- Royal Society of Chemistry, Analytical Division (RSC)



Real Sociedad Española de Química



SIGMA-ALDRICH



Institut
Català
d'Investigació
Química



INSTITUT DE CIÈNCIA DE MATERIALS DE BARCELONA

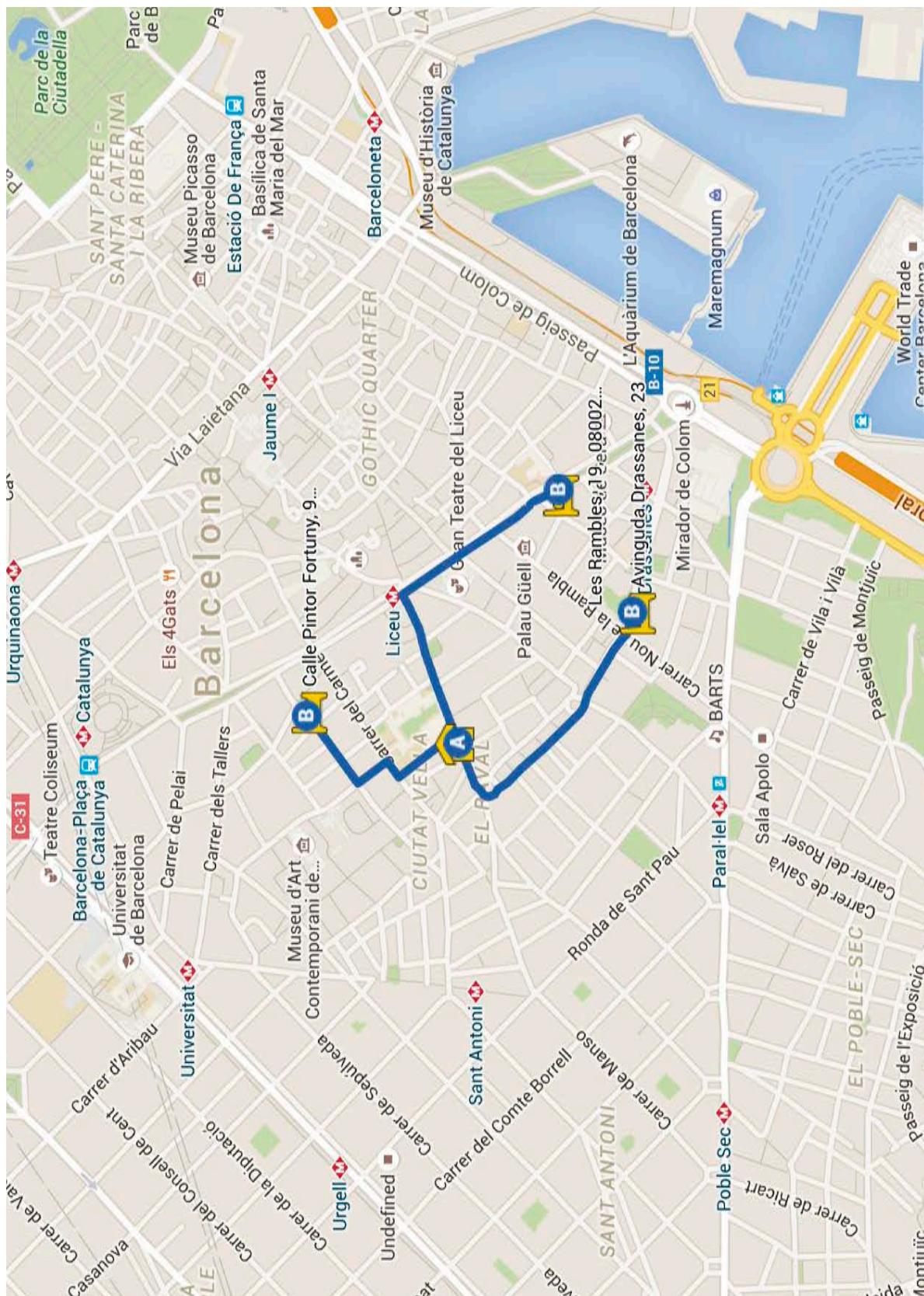


Fundació
BancSabadell



Ediciones anteriores

- **I Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
16-17 de Noviembre de 2004, Madrid
- **II Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
22-25 de Noviembre de 2005, Ciudad Real
- **III Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
16-17 de Noviembre de 2006, Tarragona
- **IV Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
20-22 de Noviembre de 2007, Burgos
- **V Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
Santiago de Compostela
- **VI Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
22-25 de Noviembre de 2009, Granada
- **VII Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
10-12 de Noviembre de 2011, Valencia
- **VIII Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
25-28 de Octubre de 2011, Torremolinos (Málaga)
- **IX Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
7-10 de Noviembre de 2012, Zaragoza
- **X Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
6-9 de Noviembre de 2013, Madrid
- **XI Simposio de Investigadores Jóvenes RSEQ - Sigma Aldrich**
4-7 de Noviembre de 2014, Bilbao



Información General del Simposio

Residència d'Investigadors del CSIC

Sala de Conferencias

Dirección: Calle Hospital 64, 08001 Barcelona

Teléfono: 93 443 27 59

Web: <http://www.residencia-investigadors.es>

Hotel Turín

Alojamiento

Dirección: Calle Pintor Fortuny 9, 08001 Barcelona

Teléfono: 93 302 48 12

Web: <http://www.hotelturin.com/>

Hotel Arc La Rambla

Alojamiento

Dirección: Les Rambles 19, 08001 Barcelona

Teléfono: 93 301 97 98

Web: <http://www.hotelarclarambla.com/>

Hotel Andante

Alojamiento

Dirección: Calle Drassanes 23-25, 08001 Barcelona

Teléfono: 93 441 25 45

Web: <http://www.andantehotel.com>

Restaurante Cullera del Boix

Comida

Dirección: Calle Hospital 3, 08001 Barcelona

Teléfono: 93 412 49 44

Restaurante Brown 33

Cena de Gala

Dirección: Passeig de Gràcia 33, 08007 Barcelona

Teléfono: 93 467 52 47

Visita guiada Ayuntamiento de Barcelona

Lugar de origen: Residència d'Investigadors del CSIC

Fecha: Martes 3 de Noviembre

Hora: 20:00

Duración de la visita: 45 minutos

Lugar de finalización: Ayuntamiento de Barcelona

	3 Martes	4 Miércoles	5 Jueves	6 Viernes
9:00		9:00 PI2: R. Martín	PI4: A.J. Martínez	
9:30		9:30 CO8: M. Ximenis	CO23: C. Romero	
9:45		9:45 CO9: D. Ventura	CO24: F. Bejarano	
10:00		10:00 CO10: A. Vellé	CO25: H. Etxabe	
10:15		10:15 CO11: G. Borrego	Sigma Aldrich	PI6: J. Lloret-Fillol
10:30		10:30 Entrega SusChem		CO39: M.A. Fuentes
10:45		10:45 Café	Café	CO40: F. Gomollón-Bel
11:00		11:00 Café (posters)	Café (posters)	JIQ
11:10		11:10 HT2: R. Recio	HT4: Y. García-Rodeja	Poster premios
11:30		11:30 CO12: M. Souto	CO26: R. Costa	HT6: T. Bello
11:45		11:45 CO13: S. Ruiz	CO27: M.E. Fernández	CO41: I. Funes
12:00	Registro	12:00 CO14: V. Rojas	CO28: D. Ferri	CO42: L. Guillade
12:15		12:15 CO15: C. Richmond	CO29: M. Frutos	CO43: A. Johnson
12:30		12:30 CO16: B. Muñoz	CO30: M. Ghirardello	CO44: V. Rubio
12:45		12:45 CO17: S. Montolio	CO31: V. Gómez	Acto Clausura
13:00		13:00 Pausa Comida	Pausa Comida	
14:15		14:15	Junta JIQ	
14:30		14:30 PI3: C. Martí-Gastaldo	PI5: R. Ponce	
15:00	Acto inauguración y entrega de premios	15:00 CO18: F. Auria	CO32: M. Navarro	PI= Ponencia Invitada
15:15		15:15 CO19: N. Bilbao	CO33: A. Mateo-Alonso	HT= Hot Topic
15:30		15:30 CO20: V. Blasco	CO34: J.I. Martínez	CO= Comunicación Oral
15:45		15:45 CO21: M.J. Cabrera	CO35: A. Martí	
16:00	PI1: M. Gulías	16:00 HT3: R. Chamorro	HT5: E.C. Gonzalo	
16:30	CO1: S. Abás	16:20 CO22: C. Casadevall	CO36: A. Irastorza	
16:45	CO2: E. Amirthalingam	16:35 Mestrelab	CO37: M.I. Gutiérrez	
17:00	CO3: F. Aparicio	16:50	CO38: C. Gozálvez	
17:15	Café	17:05 Café	Café	
17:30	RSC Talk	17:20 Workshop (Scifinder)	Divulgación	
18:25	HT1: L. Albertazzi	18:15 Flash Presentation Impares	Flash Presentation Pares	
18:45	CO4: A. Call	18:30		
19:00	CO5: A. Bauzá	18:45		
19:15	CO6: E. Cocinero	19:00 Sesión de Póster Impares	Sesión de Póster Pares	
19:30	CO7: M.P. Betoré	19:30		
20:00	Vista Guiada	21:00	CENA DE GALA	

Programa Científico y Social

Martes 3 de Noviembre

Lugar: Residència d'Investigadors del CSIC		
12:00-15:00	Registro	
Lugar: Residència d'Investigadors (Sala de Actos)		
15:00-16:00	Acto de inauguración y Entrega de los Premios RSEQ Sigma-Aldrich	
<i>Chairman: Núria Aliaga-Alcalde</i>		
16:00-16:30	PI-1	Moisés Gulías (<i>Univ. de Santiago de Compostela</i>)
		Rhodium(III)-catalyzed cycloadditions through C-H activation
16:30-16:45	CO-1	Sònia Abás (<i>Univ. de Barcelona</i>)
		A sustainable multicomponent microwave assisted reaction to prepare (2-imidazolin-4-yl)phosphonates
16:45-17:00	CO-2	Ezhil Amirthalingam (<i>Univ. de Barcelona</i>)
		Reactive oxygen species (ROS) using bi-functional microparticles for cancer theranostics
17:00-17:15	CO-3	Fátima Aparicio (<i>Université d'Angers</i>)
		Supramolecular gelation of nonlinear optically-active compounds
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
17:15-17:30	Pausa de café	
Lugar: Residència d'Investigadors (Sala de Actos)		
17:30-18:25	Careers outside the lab - a career in publishing (Rebecca Brodie)	
	<i>Chairman: Moisés Gulías</i>	
18:25-18:45	HT-1	Lorenzo Albertazzi (<i>Institut de Bioengineria de Catalunya</i>)
		Nanoscopy for nanomedicine: looking at synthetic materials one molecule at a time
18:45-19:00	CO-4	Arnau Call (<i>Institut Català d'Investigació Química</i>)
		Visible light reduction of ketones and aldehydes catalyzed by complexes based on Earth abundant elements and water as source of hydrogen atoms
19:0-19:15	CO-5	Antonio Bauzá (<i>Univ. de les Illes Balears</i>)
		Aerogen bonding interaction: a new supramolecular force?
19:15-19:30	CO-6	Emilio Cocinero (<i>Univ. del País Vasco UPV/EHU</i>)
		La espectroscopía de alta resolución en la química moderna
19:30-19:45	CO-7	Mª Pilar Betoré (<i>ISQCH - CSIC</i>)
		Activación homolítica N–H de amoníaco promovida por complejos de Iridio(I)
Lugar: Ajuntament de Barcelona		
20:00-21:00	Visita guiada al Ayuntamiento de Barcelona	

Miércoles 4 de Noviembre

Lugar: Residència d'Investigadors (Sala de Actos)		
	<i>Chairman: Carlos Martí-Gastaldo</i>	
09:00-09:30	PI-2	Rubén Martín (<i>Institut Català d'Investigació Química</i>)
	A mild Ni/Cu-catalyzed silylation via C-O cleavage	
09:30-09:45	CO-8	Marta Ximenis (<i>Univ. de les Illes Balears</i>)
	Cyclic oligosquaramide as carrier for cell internalization of alkylating agents	
09:45-10:00	CO-9	David Ventura (<i>Univ. Jaume I</i>)
	Immobilization of Ru-NHC complexes onto graphene: catalyst stabilization increases the catalytic activity	
10:00-10:15	CO-10	Alba Vellé (<i>Univ. de Zaragoza</i>)
	Dispersión de rayos X en disolución: evidencia directa de interacciones metal-metal a nivel molecular	
10:15-10:30	CO-11	Gabriel Borrego (<i>Univ. de Sevilla</i>)
	Enantioselective synthesis of β -aminophosphinic acids: biologically significant phosphorous isosters of β -amino acids	
10:30-10:45	Entrega de los Premios SusChem	
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
10:45-11:10	Pausa de café y sesión de pósteres Impares	
Lugar: Residència d'Investigadors (Sala de Actos)		
	<i>Chairman: Antonio Jesús Martínez-Martínez</i>	
11:10-11:30	HT-2	Rocío Recio (<i>Univ. de Sevilla</i>)
	Design and synthesis of new chiral SO/PO bidentate ligands in organocatalysis: enantioselective synthesis of pharmacologically significant arylamines	
11:30-11:45	CO-12	Manuel Souto (<i>ICMAB - CSIC</i>)
	Multifunctional switchable materials based on organic Donor-Acceptor systems	
11:45-12:00	CO-13	Sara Ruiz (<i>ISQCH - CSIC</i>)
	Ru-catalyzed coupling reactions for the synthesis of valuable fused heterocycles: primary amides and carboxylic acids as directing groups	
12:00-12:15	CO-14	Víctor Rojas (<i>Univ. de La Rioja</i>)
	Síntesis de nuevos glicoaminoácidos miméticos al antígeno Tn a partir de reacciones tiol-eno (TEC) o tiol-ino (TYC)	
12:15-12:30	CO-15	Craig Richmond (<i>University of Zurich</i>)
	Same catalyst, different rate law	
12:30-12:45	CO-16	Borja Muñoz-Mardones (<i>Univ. Rey Juan Carlos</i>)
	Elucidation of action mechanisms of lubricant additives	
12:45-13:00	CO-17	Silvia Montolio (<i>Univ. Jaume I</i>)
	Diseño y estudio de materiales avanzados autoorganizados basados en líquidos iónicos poliméricos	

Lugar: Restaurante Cullera del Boix		
13:00-14:30	Pausa Comida	
Lugar: Residència d'Investigadors (Sala de Actos)		
	<i>Chairman: Arántzazu González-Campo</i>	
14:30-15:00	PI-3	Carlos Martí-Gastaldo (<i>Univ. de València</i>)
	Peptide metal-organic frameworks by sidechain engineering	
15:00-15:15	CO-18	Fernando Auria (<i>Univ. de Zaragoza</i>)
	Síntesis organocatalítica de 2-oxoespiro-[indol-3,4'-(1',4'-dihidropiridinas)] quirales	
15:15-15:30	CO-19	Nerea Bilbao (<i>Univ. Autónoma de Madrid</i>)
	Tailoring 2D nanoporous networks with persistent hydrogen-bonded macrocycles	
15:30-15:45	CO-20	Víctor Blasco (<i>Univ. de València</i>)
	Design, synthesis and development of potential antimalarial drugs from thiazole derivatives	
15:45-16:00	CO-21	Mª Jesús Cabrera (<i>Univ. Autónoma de Madrid</i>)
	Aproximación a la síntesis de anguciclinonas con hidroxilos angulares mediante el uso de Oxono® como fuente de oxígeno singlete	
16:00-16:20	HT-3	Raquel Chamorro-Mendiluce (<i>Univ. Autónoma de Madrid</i>)
	Nanotubular systems self-assembled through orthogonal supramolecular interactions	
16:20-16:35	CO-22	Carla Casadevall (<i>Institut Català d'Investigació Química</i>)
	Light-driven Co-catalyzed reduction of olefins using water as a source of protons	
16:35-17:05	Chemistry software solutions - A world of possibilities outside the lab (Enrique Sánchez)	
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
17:05-17:20	Pausa de café	
Lugar: Residència d'Investigadors (Sala de Actos)		
17:20-18:15	Why SciFinder? Let's try a search! (Míriam Plana)	
	<i>Chairman: Pau Farràs</i>	
18:15-18:45	Presentaciones Flash Impares	
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
18:45-19:45	Sesión de Pósteres Impares	

Jueves 5 de Noviembre

Lugar: Residència d'Investigadors (Sala de Actos)		
	<i>Chairman: Emilio Cocinero</i>	
09:00-09:30	PI-4	Antonio Jesús Martínez-Martínez (<i>University of Strathclyde</i>)
	Functionalisation of aromatic compounds: switching the regioselectivity away from <i>ortho</i>	
09:30-09:45	CO-23	Carlos Romero-Nieto (<i>University of Heidelberg</i>)
	Paving the way to novel phosphorus-based architectures: a non-catalyzed protocol to access six-membered heterocycles	
09:45-10:00	CO-24	Francesc Bejarano (<i>ICMAB - CSIC</i>)
	In solution and on surface studies of novel polychlorotriphenylmethyl (PTM) radicals for molecular electronics applications	
10:00-10:15	CO-25	Haizea Echave (<i>Univ. del País Vasco UPV/EHU</i>)
	Stereoselective direct aldol reaction of α -keto amides catalyzed by ureidopeptide-based brønsted bases	
10:15-10:45	Novel Materials of Today for Applications of Tomorrow – Adelina Braun	
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
10:45-11:10	Pausa de café y sesión de pósteres Pares	
Lugar: Residència d'Investigadors (Sala de Actos)		
	<i>Chairman: Rocio Ponce</i>	
11:10-11:30	HT-4	Yago García-Rodeja (<i>Univ. Complutense de Madrid</i>)
	Diels-Alder reactivity and selectivity at the interior of the polycyclic aromatic hydrocarbons: a computational study	
11:30-11:45	CO-26	Rubén D. Costa (<i>Friedrich-Alexander-Universität Erlangen-Nürnberg</i>)
	Hybrid organic-inorganic materials for integrated optoelectronic devices	
11:45-12:00	CO-27	Mª Eloisa Fernández (<i>Univ. de Granada</i>)
	Síntesis, caracterización estructural y magnética de un compuesto tetranuclear Zn_2Dy_2 con propiedades de molécula imán	
12:00-12:15	CO-28	Daniel Ferri (<i>Univ. de València</i>)
	Mesoporous systems capped with an azoaniline derivative for transport and controlled delivery applications	
12:15-12:30	CO-29	María Frutos (<i>IQOG - CSIC</i>)
	Ruthenium(II) 1,2,3-triazolylidene carbenes: synthesis, structure and catalytic activity	
12:30-12:45	CO-30	Mattia Ghirardello (<i>ISQCH - CSIC</i>)
	Towards new glycosyltransferase ligands	
12:45-13:00	CO-31	Mª Victoria Gómez (<i>Univ. de Castilla-La Mancha</i>)
	Broad band microcoils for inline/insitureaction monitoring	
Lugar: Restaurante Cullera del Boix		
13:00-14:30	Pausa Comida	

Lugar: Residència d'Investigadors (Sala de Actos)		
	<i>Chairman: David González-Rodriguez</i>	
14:30-15:00	PI-5	Rocío Ponce (Univ. de Málaga)
Semiconductores para electrónica y fotónica orgánica		
15:00-15:15	CO-32	Miquel Navarro (Universität Bern)
	Bodipy functionalised mesoionic NHC complexes: synthesis & fluorescence modulation	
15:15-15:30	CO-33	Aurelio Mateo-Alonso (Polymat)
	Distorted molecular and low-dimensional materials	
15:30-15:45	CO-34	Jose Ignacio Martínez (University of Nottingham)
	Chain walking of allylrhodium species towards esters during rhodium-catalyzed nucleophilic allylations of imines	
15:45-16:00	CO-35	Almudena Martí (Univ. de València)
	Selective recognition and sensing of succinate vs. other aliphatic dicarboxylates	
16:00-16:20	HT-5	Elena Cándida Gonzalo (CIC Energigune)
	Electrochemical characterization and in situ synchrotron study of P2- and O3- $\text{Na}_{2/3}\text{Fe}_{2/3}\text{Mn}_{1/3}\text{O}_2$ as cathode material for Na ion batteries.	
16:20-16:35	CO-36	Aitziber Irastorza (Univ. del País Vasco UPV/EHU)
	Palladium-catalyzed $\text{C}(\text{sp}^2)\text{-H}$ acetoxylation directed by 1,2,3-triazoles	
16:35-16:50	CO-37	Mª Isabel Gutiérrez-Jiménez (Univ. de La Rioja)
	Synthesis of S-glycodipeptides through sulfa-michael addition and lactone aminolysis sequence	
16:50-17:05	CO-38	Cristian Gozávez (Polymat)
	Polymolecular assemblies for electronic applications	
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
17:05-17:20	Pausa de café	
Lugar: Residència d'Investigadors (Sala de Actos)		
17:20-18:15	La Divulgación Científica	
	<i>Chairman: Arántzazu González-Campo</i>	
18:15-18:45	Presentaciones Flash Pares	
Lugar: Residència d'Investigadors (Sala de Exposiciones)		
18:45-19:45	Sesión de Pósteres Pares	
Lugar: Restaurante Brown 33		
21:00-00:00	Cena de gala	

Viernes 6 de Noviembre

Lugar: Residència d'Investigadors (Sala de Actos)		
		<i>Chairman: Pau Farràs</i>
10:00-10:30	PI-6	Julio Lloret-Fillol (<i>Institut Català d'Investigació Química</i>)
	Well defined iron water oxidation and light-driven cobalt reduction catalysts	
10:30-10:45	CO-39	M. Ángeles Fuentes (<i>University of Strathclyde</i>)
	C-H bond functionalization of phenyl-substituted benzotriazole using trans-metal trapping chemistry	
10:45-11:00	CO-40	Fernando Gomollón-Bel (<i>ISQCH - CSIC</i>)
	Obtención de nuevos inhibidores enzimáticos para transglicosilasas de <i>Aspergillus fumigatus</i> mediante click chemistry	
11:00-11:15	Charla JIQ	
11:15-11:30	Entrega de premios a los mejores póster	
	<i>Chairman: Julio Lloret-Fillol</i>	
11:30-11:50	HT-6	Tamara Bello (<i>Univ. del País Vasco UPV/EHU</i>)
	Enantiopure tetrasubstituted pyrrolidines as scaffolds for novel and potent proteasome inhibitors	
11:50-12:05	CO-41	Ignacio Funes-Ardoiz (<i>Institut Català d'Investigació Química</i>)
	A mechanistic approach to the overpotential control in Cu-based water oxidation catalysis	
12:05-12:20	CO-42	Lucía Guillade (<i>Univ. de Vigo</i>)
	Approaches to the synthesis of tripartin	
12:20-12:35	CO-43	Alice Johnson (<i>ISQCH - CSIC</i>)
	Luminescent NHC gold complexes from propargyl functionalised imidazolium salts	
12:35-12:50	CO-44	Víctor Rubio-Giménez (<i>Univ. de València</i>)
	Charge transport in metal-organic framework ultrathin film	
12:50-13:00	Acto de Clausura	

Programa de Pósteres

Sesión de Pósteres Impares (Sala de Exposiciones, miércoles 4 de Noviembre)

Sesión de Pósteres Pares (Sala de Exposiciones, jueves 5 de Noviembre)

Póster con Presentación Flash

FP01 - Juan V. Alegre-Requena (ISQCH – CSIC)

One-pot synthesis of unsymmetrical squaramides and their application in organocatalytic henry reactions

FP02 - Cintia Anton-Torrecillas (Univ. De Alicante)

Syntheses and Cytotoxicity of (R)- and (S)- 7-Methoxycryptopleurine

FP03 - Celeste Are (Univ. de Barcelona)

Enantioselective synthetic approach to the marine alkaloids of the madangamine group

FP04 - Miguel Espinosa (Univ. de València)

E,Z-stereodivergent synthesis of N-tosyl α,β-dehydroamino esters via a Mukaiyama-Michael addition

FP05 - Alberto Macario (Univ. de Valladolid)

The structure of o-anisic acid by microwave spectroscopy

FP06 - Julia Guillemé (Univ. Autónoma de Madrid)

Polar Self-assembled Subphthalocyanine Columnar Stacks

FP07 - Vanessa Herrero García (Univ. de Zaragoza)

Nanopartículas de óxido de hierro funcionalizadas con ácidos nucleicos y péptidonucleicos para la liberación controlada mediante hipertermia

FP08 - Elena López-Mayo (Univ. de Granada)

Textile-metal-organic framework composites for Personal Protection

FP09 - Priscila López Rojas (Univ. de La Laguna)

Síntesis y estudios in silico de derivados 1,2,3-triazolil naftoquinónicos y cumarínicos con potencial actividad antimalárica

FP10 - Elena Contreras (Univ. de La Rioja)

Modulación de propiedades antibióticas por luz

FP11 - Alberto Martínez-Cuezva (Univ. de Múrcia)

Molecular switches based on interlocked di(acylamino)pyridines

FP12 - María José Mayoral (Univ. Autónoma de Madrid)

Dual mode self-assembly of discotic cone-shaped molecules

FP13 - Alexandre Pinto (*Univ. de Barcelona*)

Enantioselective total synthesis of (-)-lepadin A-C and (+)-lepadin D

FP14 - Mª de Gracia Retamosa (*Univ. del País Vasco UPV/EHU*)

New organocatalytic properties of densely substituted 4-nitropyrrolidines

FP15 - Sheila Ruiz-Botella (*Univ. Jaume I*)

Unveiling the Importance of π -Stacking in Borrowing-Hydrogen Processes Catalysed by Iridium Complexes with Pyrene Tags

FP16 - Montse Vallejo-López (*Univ. del País Vasco UPV/EHU*)

How pyridine interacts with freons: π or σ intermolecular bonds?

Pósteres

PO1 - María Albert Soriano (*Univ. de Alicante*)

1,3-bis(carboximetil)imidazol como ligando en estructuras metal-orgánicas con actividad catalítica

PO2 - Melanie Aliaga Lavrijzen (*ISQCH - CSIC*)

Síntesis de catalizadores de oro(I) y su estudio en reacciones multi-componente

PO3 - Estefanía Almenar Sánchez (*Univ. de València*)

Fluorescence sensing of diacetonediperoxide (DADP)

PO5 - Susan Azpeitia Coscarón (*Univ. del País Vasco UPV/EHU*)

Silyl-thioether multidentate ligands: synthesis of Rh(III) complexes via Rh(I)/Rh(III) mixed valence and cyclooctenyl intermediates

PO6 - Eider Badiola Aramendi (*Univ. del País Vasco UPV/EHU*)

Enantioselective direct Michael addition of cyanoacetates to α' -oxy enones

PO7 - Julio Bastos Arrieta (*Univ. Politècnica de Catalunya*)

Modificación personalizada de superficies reactivas con nanopartículas funcionales: presente y futuro

PO8 - Francisco Berga Montaner (*Univ. de les Illes Balears*)

Nuevos métodos colorimétricos para la detección de fitato: características y aplicabilidad de sistemas metal-indicador para la determinación de fitato urinario

PO9 - Francisco Berga Montaner (*Univ. de les Illes Balears*)

Uso del fitato solo o en combinación con vitámeros B6 para la prevención de la formación de productos de glicación avanzada

PO11 - Francisco Jesús Carmona (*Univ. de Granada*)

Control del tamaño y la morfología de las partículas de MOFs. Influencia en la incorporación de metalofármacos

PO12 - Javier Castells Gil (*Univ. de València*)

Chemical coating of metal-organic frameworks for enhanced water stability

PO13 - María Catalá Reig (*Univ. Jaume I*)

Fluor-containing pseudopeptidic tripodal small cages

PO14 - Sara Cembellín Santos (*Univ. Complutense de Madrid*)

Síntesis de heterociclos a través de reacciones de ciclación de [3]-cumulenoles

PO15 - Andrés José Chueca López (*ISQCH - CSIC*)

Light emission from ionic NHC-cycloplatinated compounds

PO16 - Sandra Codony Gisbert (*Univ. de Barcelona*)

Synthesis of novel anilines with anti-influenza activity

PO17 - Paula Cruz Franch (*Univ. Rey Juan Carlos*)

Diseño de nuevos materiales mesoporosos de titanio y su aplicación en procesos de polimerización por apertura de anillo de ε-caprolactona

PO18 - Ismael Francisco Díaz Ortega (*Univ. de Granada*)

Síntesis y caracterización estructural de nuevas moléculas imán basadas en compuestos de coordinación de iones lantánidos

PO19 - Luis Escobar González (*Institut Català d'Investigació Química*)

Synthesis and binding studies of super aryl-extended calix[4]pyrroles

PO20 - Cintia Ezquerro Parmo (*Univ. de La Rioja*)

Materiales híbridos titania/organometálico mesoporosos fotoactivos bajo luz visible

PO21 - Javier Fernández Ariza (*Univ. Autónoma de Madrid*)

Phthalocyanine-ferrocene hybrids as components of donor-acceptor ensembles

PO22 – Belén Fernández (*Univ. de Granada*)

Highly active anti-diabetic metal-organic framework

PO23 - Raluca Maria Fratila (*Univ. de Zaragoza*)

Bioorthogonal “click” functionalization of magnetic nanoparticles

PO24 – Isaac Giménez Sonsona (*Univ. de Zaragoza*)

Activación de organocatalizadores urea por ácidos de Brønsted externos y su empleo en la reacción de Friedel-Crafts

PO25 - Antonio Gimeno Prat (*Univ. de Zaragoza*)

Síntesis y reactividad de benzamiduro complejos de Pt(II)

PO26 - Beatriz Gómez Nieto (*Univ. Autónoma de Madrid*)

Direct determination of minor and major elements in biological micro-samples using solid sampling high-resolution continuum source graphite furnace atomic absorption spectrometry

PO27 - Asier Gómez San Juan (IQM - CSIC)

Potent and selective inhibitors of re-emerging Chikungunya virus replication

PO28 - David González Rodríguez (Univ. Autónoma de Madrid)

Polar self-assembled molecular materials

PO29 - María José González Soria (Univ. de Alicante)

Synthetic and mechanistic studies on the solvent-dependent copper-catalyzed formation of indolizines and chalcones

PO30 - Lingaraju Gorla (Univ. Jaume I)

New pseudopeptidic ligands: synthesis and metal recognition behavior

PO31 - Santiago Guisán-Ceinos (Univ. Autónoma de Madrid)

Síntesis y propiedades fotocrómicas de (S_{Fc}, S_S)-*p*-sulfinil ferrocenil azobencenos enantiopuros

PO32 - María Susana Gutiérrez (Univ. de les Illes Balears)

Study of substitution flexible ligands on iron oxide nanoparticles by microwave assisted synthesis

PO33 - María Antonia Herrero (Univ. de Castilla-La Mancha)

Chemical modulation of the CNHs and its applications

PO35 - Mario Hoyos Núñez (ICTP - CSIC)

Modificación de fibras de sepiolita para la preparación de materiales híbridos basados en polifluoreno

PO36 - Anabel Izaga Sebastián (ISQCH - CSIC)

Activación pionera tioureas quirales con complejos de Au

PO37 - Verónica Juste Navarro (ISQCH - CSIC)

Síntesis de *N*-óxidos de 4,5-dihidrooxazoles mediante reacciones de iluros de nitrona y aldehídos

PO38 - Rebeca Lara Garnica (Univ. de La Rioja)

Compuestos luminiscentes ciclometalados de Pt(II) y Pt(IV) basados en la unidad 2-fenilbenzotiazol

PO39 - Eduardo López González (Univ. de Valladolid)

Study of the cell structure of LDPE foams irradiated at different doses

PO40 – Carlos López Roig (Univ. de les Illes Balears)

Functionalization of aluminium oxy-hydroxide with long-chain amidosquaric acids

PO41 - Raúl Losantos Cabello (*Univ. de La Rioja*)

Síntesis de compuestos fotoprotectores

PO42 - María Maciá Delgado (*Univ. Jaume I*)

Nuevos organocatalizadores para la reducción enantioselectiva de iminas empleando Cl₃SiH como reductor

PO43 - Mateo Martín Salgado (*Univ. de Salamanca*)

Síntesis asimétrica de APN's basada en una reacción dominó

PO44 – Carlos Martínez Aquino (*Univ. de València*)

Dosimeter for detection of formaldehyde and future perspectives

PO45 - Carmen Mejuto Nieblas (*Univ. Jaume I*)

First homoleptic MIC and heteroleptic NHC–MIC coordination cages from 1,3,5-triphenylbenzenebridged tris-MIC and tris-NHC ligands

PO46 - José Manuel Méndez Arriaga (*Univ. de Granada*)

Síntesis y caracterización de nuevos complejos metálicos de derivados triazolopirimidínicos con potencial actividad leishmanicida

PO47 - Andrea Mirats Arce (*Univ. Autònoma de Barcelona*)

H₂O₂ formation induced by Cu²⁺-Aβ(1-16) complexes.

PO48 - Zaira Monasterio Peiteado (*Univ. del País Vasco UPV/EHU*)

Novel cationic alkynes as scaffolds for thermal and Cu(I) catalyzed azide-alkyne cycloaddition reactions

PO49 - Natalia Muñoz Padial (*Univ. de Granada*)

Isoreticular series of zirconium metal-organic framework. Catalytic applications

PO50 – Javier Navarro Ruiz (*Univ. Autònoma de Barcelona*)

Relevance of silicate surface morphology in interstellar H₂ formation

PO51 - Daniel Nuevo Vialás (*Univ. Jaume I*)

Modulación funcional de membranas monolíticas tubulares y aplicación en procesos de separación

PO52 - Francisca Orvay Pintos (*Univ. de les Illes Balears*)

Interacciones ADN-oligoescuaramidas cíclicas

PO53 - Alberto Pérez Bitrián (*ISQCH - CSIC*)

Pt(III) vs. Pt(IV) en la oxidación de complejos de Pt(II)

PO54 - Maria Del Mar Pérez Ferrer (*Univ. de les Illes Balears*)

SNF472 inhibe la calcificación cardiovascular en ratas inducida por vitamina D

PO55 - Jorge Pérez Miqueo (*Univ. del País Vasco UPV/EHU*)

Catalizadores fotomodulables de iridio(III) para la reacción de hidrosililación de iminas

PO56 - Edgar Peris Salom (*Univ. Jaume I*)

Task specific Supported Ionic Liquid-Like Phases (SILLPs) for Strecker reactions under continuous flow conditions

PO57 - David Roca López (*Univ. de Zaragoza*)

Estudio mecanístico de cicloadiciones catalizadas por un organocatalizador bifuncional derivado de pirrolidina y escuaramida

PO58 - Adrián Rodríguez Rodríguez (*Univ. de les Illes Balears*)

Simple HPLC determination of urinary theobromine: Cocoa products consumption and urinary theobromine levels in healthy children

PO59 - Sara Rojas Macías (*Univ. de Granada*)

Zn-NanoMOFs: estudio de su estabilidad coloidal y aplicación como sistemas de transporte/liberación de fármacos

PO60 - Andrea Ruiz-Olalla Fernández (*Univ. del País Vasco UPV/EHU*)

Synthesis of 1-benzyl-1,2,3,4-tetrahydroisoquinoline alkaloids via organocatalyzed Pictet-Spengler reaction

PO61 - Mercedes Santiago Calvo (*Univ. de Valladolid*)

FTIR studies to characterize the kinetics of nanocomposite polyurethane foams

PO62 - Andreea L. Turcu (*Univ. de Barcelona*)

Direct reductive alkylation of amine hydrochlorides with aldehyde bisulfite adducts

PO63 - Victoria Valdivia Giménez (*Univ. de Sevilla*)

“Sulfolefinas”: Ligandos sulfinamido-olefinas para adiciones conjugadas enantioselectivas catalizadas por rodio

PO64 - Adriana Valls Ten (*Univ. Jaume I*)

Síntesis de nuevos compuestos tripodales pseudopeptídicos como receptores de cloruros

PO65 - Álvaro Vega Vega (*Univ. de Valladolid*)

BO radical-metal interaction: computational study of structure and bonding

PO66 - Álvaro Vega Vega (*Univ. de Valladolid*)

Theoretical study of tetratomic {C,H,N,Zn} compounds: molecular structure and bond characteristics

PO67 - Carlos Vila Descals (*Univ. de València*)

N-Alkylation of benzoxazinone and quinoxalinone derivatives with organozinc reagents via *umpolung*

Premios RSEQ Sigma-Aldrich

Dr. Moisés Gulías Costa



Moisés Gulías estudió en la Universidad of Santiago de Compostela donde obtuvo su título de Doctor en el año 2006 bajo la supervisión del Prof. José L. Mascareñas. Durante sus estudios de doctorado llevó a cabo una estancia en la Universidad de Stanford (2004) con el Prof. Barry M. Trost.

Entre 2007 and 2009 fue becario postdoctoral Marie-Curie postdoctoral en el grupo de Matthew J. Gaunt (Universidad de Cambridge).

En 2010 volvió a la Universidad de Santiago de Compostela como investigador Parga-Pondal. Sus intereses científicos incluyen el descubrimiento de nuevas metodologías para activación de enlaces no reactivos que faciliten la síntesis de moléculas complejas y el desarrollo de nuevos métodos de catálisis enantioselectiva. En el 2015 Moisés Gulías ha recibido el premio Thieme Chemistry Journal Award.

Publicaciones recientes:

- 1) "Rhodium-Catalyzed (5+1) Annulations Between 2-Alkenylphenols and Allenes: A Practical Entry to 2,2-Disubstituted 2H-Chromenes", N. Casanova, A. Seoane, J. L. Mascareñas, M. Gulías* Angew. Chem. Int. Ed., 2015, 54, 2374-2377.
- 2) "Rhodium (III)-catalyzed dearomatizing (3+2) annulation of 2-alkenylphenols and alkynes", Seoane, A.; Quinones, Noelia; Casanova, N.; Mascareñas, Jose L.; Gulias, M.* J. Am. Chem. Soc., 2014, 136, 7607-7610.
- 3) "Straightforward Assembly of benzoxepines by Means of a Rhodium (III)-Catalyzed C-H Functionalization of o-Vinylphenols", Seoane, A.; Quinones, Noelia; Casanova, N.; Mascareñas, Jose L.; Gulias, M.* J. Am. Chem. Soc. 2014, 136, 834-837.
- 4) "Rhodium(III)-catalyzed intramolecular annulations involving amide-directed C-H activations: synthetic scope and mechanistic studies", Quinones, Noelia; Seoane, A.; Mascareñas, Jose L.; Gulias, M.* Chem. Sci. 2013, 4, 2874-2879.

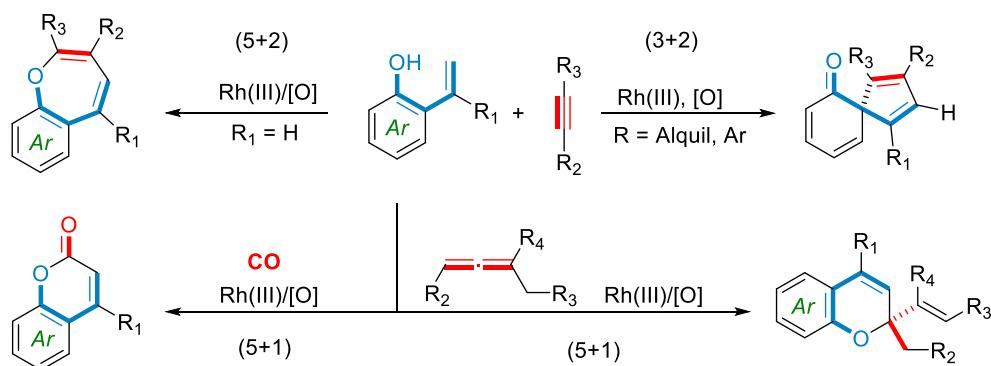
Rhodium(III)-catalyzed cycloadditions through C-H activation

Moisés Gulías

Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS) and Departamento de Química Orgánica. 15782, Universidade de Santiago de Compostela
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The discovery of methods that allow assembling relatively complex organic products from simple and non-expensive precursors constitutes a major goal in synthetic chemistry. In this context, cycloaddition reactions are very appealing, allowing a rapid increase on molecular complexity while matching the requirements of atom economy, selectivity and minimizing the chemical waste.

Recently we started a new line of research which aims to develop new types of cycloadditions through the metal-catalyzed activation of relatively inert C-H bonds.^{1,2} Thus, we have demonstrated that readily available 2-alkenyl phenols can be transformed in different types of hetero- and carbocycles through annulations with alkynes,³ allenes⁴ or carbon monoxide^{3a} using a rhodium(III) complex as catalyst.



- For reviews on C-H activation: For selected reviews on C-H activation: (a) C. S. Yeung, V. M. Dong, *Chem. Rev.* **2011**, 111, 1215. (b) G. Song, F. Wang, X. Li, *Chem. Soc. Rev.*, **2012**, 41, 3651. (c) J. Wencel-Delord, F. Glorius, *Nat. Chem.* **2013**, 5, 369. (d) K. M. Engle, T.-S Mei, M. Wasa, J.-Q. Yu, *Acc. Chem. Res.* **2012**, 45, 788.
- N. Quiñones, A. Seoane, R. García-Fandiño, J. L. Mascareñas, M. Gulías *Chem. Sci.* **2013**, 4, 2874.
- (a) A. Seoane, N. Casanova, N. Quiñones, J. L. Mascareñas, M. Gulías *J. Am. Chem. Soc.* **2014**, 136, 834. (b) A. Seoane, N. Casanova, N. Quiñones, J. L. Mascareñas, M. Gulías *J. Am. Chem. Soc.* **2014**, 136, 7607.
- N. Casanova, A. Seoane, J. L. Mascareñas, M. Gulías *Angew. Chem. Int. Ed.* **2015**, 54, 2374.

Dr. Carlos Martí-Gastaldo



Carlos Martí-Gastaldo se licenció en Químicas en la Universidad de Valencia, recibiendo el premio extraordinario de licenciatura.

Completó su tesis doctoral en el Instituto de Ciencia Molecular (ICMol) bajo la dirección de los Prof. Eugenio Coronado y J. R. Galán Mascarós en 2009, recibiendo el premio extraordinario de doctorado.

En 2010 obtuvo una Marie Curie y se trasladó a la Universidad de Liverpool (Reino Unido) para trabajar en el grupo del profesor Matthew J. Rosseinsky. Durante este periodo trabajó en el desarrollo de MOFs biomiméticos basados en péptidos.

En 2013 inició su carrera científica independiente tras recibir una URF Fellow de la Royal Society of Chemistry. En 2014 se incorporó al ICMol como investigador Ramón y Cajal para desarrollar MOFs estables para su aplicación en fotocatálisis, transporte iónico y aplicaciones optoelectrónicas.

Carlos es co-autor de más de 50 trabajos publicados en revistas de alto impacto con más de 1750 citas y ha sido reconocido con premios, como el “Young Researcher Olivier Kahn Recognition Award” (2009), el “NanoMatMol” (2010), el “Suschem Postdoc” (2011) o el “Premio Científico-Técnico Ciudad de Algemesí” (2015).

Publicaciones recientes:

- 1) “Chemical and Structural Stability of Zirconium-based Metal-Organic Frameworks with Large Three-Dimensional Pores by Linker Engineering” S. Kalidindi, S. Nayak, M.E. Briggs, S. Jansat, A. Katsoulidis, G.J. Miller, J.E. Warren, D. Antypov, M. Prestley, C. Martí-Gastaldo, M.J. Rosseinsky Angew. Chem. Int. Ed. (2015), 127, 223-228.
- 2) “Sidechain control of porosity closure in single and multiple peptide-based porous materials by cooperative folding” C. Martí-Gastaldo, D. Antypov, J. E. Warren, M. E. Briggs, P. A. Chater, P. V. Wiper, G. J. Miller, Y. Z. Khimyak, G. R. Darling, N. G. Berry, M. J. Rosseinsky Nature Chem. (2014), 6, 343-351.
- 3) “Enhanced stability in rigid peptide-based porous materials” C. Martí-Gastaldo, J. E. Warren, K. S. Stylianou, N. O. Flack, M. J. Rosseinsky Angew. Chem. Int. Ed. (2012), 51, 11044-11048.
- 4) “Coexistence of Superconductivity and Magnetism by chemical design” E. Coronado, C. Martí-Gastaldo, E. Navarro-Moratalla, A. Ribera, S. J. Blundell, P. Baker Nature Chemistry (2010), 12, 1031-1036.

Peptide Metal-Organic Frameworks by sidechain engineering

Carlos Martí-Gastaldo

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Peptides have recently emerged as naturally occurring linkers for the design of metal organic frameworks (MOFs) provided their multiple coordination modes, torsional adaptability and chirality. The use of peptide struts provides unprecedented guest adaptability, modulation of the framework's flexibility and control over its chemical and mechanical stabilities triggered by suitable choice of the amino acids in the peptidic sequence. In this talk we will review recent advances in the design of peptide-based porous materials with key focus on how chemical engineering of the peptide sidechain renders control over their structural flexibility, stability, chemical function and accessible porosity.

[1] Rabone, Y. F. Yue, S. Chong, K. Stylianou, J. Bacsa, D. Bradshaw, G. Darling, N. Berry, Y. Khimyak, A. Ganin, P. Wiper, J. B. Claridge, M. J. Rosseinsky, *Science* **2010**, 329, 1053.

[2] C. Martí-Gastaldo, J. E. Warren, K. S. Stylianou, N. O. Flack, M. J. Rosseinsky *Angew. Chem. Int. Ed.* **2012**, 51, 11044.

[3] A. P. Katsoulidis, K. Park, D. Antypov, C. Martí-Gastaldo, G. J. Miller, J. E. Warren, C. M. Robertson, F. Blanc, G. R. Darling, N. G. Berry, J. A. Purton, D. J. Adams, M. J. Rosseinsky *Angew. Chem. Int. Ed.* **2014**, 53, 193.

[4] C. Martí-Gastaldo , D. Antypov, J. E. Warren, M. E. Briggs, P. A. Chater, P. V. Wiper, G. J. Miller, Y. Z. Khimyak, G. R. Darling, N. G. Berry, M. J. Rosseinsky *Nature Chem.* **2014**, 6, 343.

[5] C. Martí-Gastaldo , J. E. Warren, M. E. Briggs, J. A. Armstrong, K. M. Thomas, M. J. Rosseinsky *Chem. Eur. J.* **2015** (accepted).

Dra. Rocío Ponce Ortiz



Licenciada en Ingeniería Química por la Facultad de Ciencias de la Universidad de Málaga en 2003. A continuación, se integró con una beca FPDel (Junta de Andalucía) en el grupo de investigación del Prof. Juan Teodomiro López Navarrete, defendiendo la Tesis Doctoral en Febrero de 2008. Desde Octubre de 2008 hasta Octubre de 2011, realizó una estancia postdoctoral en el grupo de investigación del Prof. Tobin J. Marks en Northwestern University (Illinois, USA), gracias a la concesión de una beca postdoctoral del MICINN y una beca europea Marie Curie IOF (International Outgoing Fellowship). Fruto de esta etapa postdoctoral destaca la publicación de 23 artículos de investigación original en revistas de alto prestigio, 3 artículos de revisión y un capítulo de libro. En Octubre de 2011 se reincorporó a la Universidad de Málaga, consiguiendo un contrato Ramón y Cajal en Noviembre de 2013.

Actualmente es autora de 57 artículos de investigación, con un índice de citación (h) de 26. Cabe destacar la reciente concesión de una Bolsa de Investigación L’Oreal-UNESCO “For Women in Science”.

Publicaciones recientes:

1. “On the Biradicaloid Nature of Long Quinoidal Oligothiophenes: Experimental Evidence Guided by Theoretical Studies” R. Ponce Ortiz, J. Casado, V. Hernández, J. T. López Navarrete, P. M. Viruela, E. Ortí, K. Takimiya, T. Otsubo. *Angew. Chem. Int. Ed.* 2007, 46, 9057.
2. “Organic n-Channel Field-Effect Transistors Based on Arylenediimide-Thiophene Derivatives” R. Ponce Ortiz, H. Herrera, R. Blanco, H. Huang, A. Facchetti, T. J. Marks, Y. Zheng, J. L Segura. *J. Am. Chem. Soc.* 2010, 132, 8440.
3. “Rational Design of Ambipolar Organic Semiconductors: Is Core Planarity Central to Ambipolarity in Thiophene-Naphthalene Semiconductors? R. Ponce Ortiz*, H. Herrera, C. Seoane, J. L. Segura, A. Facchetti, T. J. Marks. *Chem. Eur. J.* 2012, 18, 532-543.
4. “Polymer Solar Cells with Enhanced Fill Factors” X. Guo, N. Zhou, S. J. Lou, J. Smith, D. B. Tice, J. W. Hennek, R. Ponce Ortiz, J. T. López Navarrete, S. Li, J. Strzalka, L. X. Chen, R. P. Chang, A. Facchetti, T. J. Marks, *Nature Photonics* 2013, 7, 825.
5. “The unusual electronic structure of ambipolar dicyanovinyl-substituted diketopyrrolopyrrole derivatives” A. Riaño, P. Mayorga Burrezo, M. J. Mancheño, A. Timalsina, J. Smith, A. Facchetti, T. J. Marks, J. T. López Navarrete, J. L. Segura, J. Casado, R. Ponce Ortiz*. *J. Mater. Chem. C* 2014, 2, 6376.

Semiconductores para electrónica y fotónica orgánica

R. Ponce Ortiz

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La búsqueda de nuevas tecnologías capaces de reemplazar a la tecnología actual basada en silicio representa uno de los campos de investigación científica más dinámico en la actualidad.¹ La electrónica y fotónica orgánica aparecen como alternativas viables, usando materiales orgánicos como componentes activos de los dispositivos. Estos materiales presentan propiedades deseables tales como bajo coste, excelente procesabilidad y compatibilidad con sustratos plásticos, lo que permite la fabricación de circuitos y células solares mecánicamente flexibles mediante el uso de técnicas económicas como la impresión.²

Para avanzar de forma eficiente en este campo de investigación mediante el diseño racional de nuevos semiconductores orgánicos es necesario establecer relaciones claras estructura molecular/estructura del estado sólido/propiedad de los materiales estudiados. En esta comunicación, mostraré ejemplos de mi investigación reciente en donde se analiza el comportamiento de semiconductores orgánicos para electrónica y fotónica mediante técnicas espectroscópicas, cálculos químico-cuánticos y análisis de las propiedades electrónicas.³

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Dr. Julio Lloret Fillol



Dr. Julio Lloret Fillol nació en Carcaixent (Valencia) en 1977. Se licencio en la Universidad de Valencia y obtuvo el grado de doctor en 2006 en la misma Universidad bajo la supervisión del Prof. Pascual Lahuerta y la Prof. Julia Perez-Prieto, trabajando en la síntesis de compuestos quirales organometálicos de dinucleares rodio (II), sus aplicaciones catalíticas y estudios teóricos. En Diciembre de 2006 se trasladó al grupo del Prof. Lutz H. Gade en la Universidad de Heidelberg (Alemania) como becario postdoctoral del Ministerio de educación y ciencia (2006-2008) y con una Marie Curie IEF (2008-2010). Su trabajo se centró principalmente en catálisis enantiselectiva y en el estudio de los mecanismos de reacción con complejos organometálicos de titanio, zirconio y hafnio. En Abril del 2010, se unió a la Universidad de Girona como Ramón y Cajal y allInstitut de Química Computacional i Catàlisi donde empezó su carrera científica independiente gracias al programa Marie Curie Reintegration Grant para desarrollar “modular ligands for water splitting”.

En Noviembre de 2014 se incorporó al Instituto Catalán de Investigación Química (ICIQ) como líder de grupo de investigación bajo el programa CELLEX. Recientemente se le ha concedido un proyecto “Consolidator Grant” del “European Research Council” (Co-ERC) para desarrollar nuevas transformaciones reductivas utilizando luz y agua. Actualmente, sus líneas de investigación se focalizan en el desarrollo de la catálisis sostenible y la activación de pequeñas moléculas. Julio Lloret es co-autor de más de 55 publicaciones en revistas de alto impacto y ha sido reconocido con el premio GEQO 2014 a Jóvenes Investigadores.

Publicaciones recientes:

- 1) “Evidence for an Oxygen Evolving Fe–O–Ce Intermediate in Iron-Catalysed Water Oxidation” Zoel Codolà, Laura Gómez, Scott T. Kleespies, Lawrence Que, Jr.,* Miquel Costas* and Julio Lloret-Fillol* Nature Communications 01/2015, 6:5865
- 2) 2.- “Triggering the generation of an iron(IV)-oxo compound and its reactivity towards sulfides by Ru^{II} photocatalysis” Anna Company,* María González-Béjar, Gerard Sabeña, Laura Gómez, Miquel Costas,* Julia Pérez-Prieto* Julio Lloret-Fillol* J. Am. Chem. Soc. 2014, 4624-4533
- 3) “Photoinduced catalytic water reduction to hydrogen by new cobalt complexes based on pentadentate nitrogenate ligands” Arnau Call, Zoel Codolà, F. Acuña-Pares Julio Lloret-Fillol* Chem. Eur. J.. 2014, 20, 6171
- 4) “Highly Effective Water Oxidation Catalysis with Iridium Complexes through the use of NaO4” Zoel Codolà; João M. S. Cardoso; Beatriz Royo; Miquel Costas; Julio Lloret-Fillol* Chem. Eur. J. 2013, 19, 7203-7213
- 5) “Efficient Water Oxidation Catalysts Based on Readily Available Iron Coordination Complexes” Julio Lloret Fillol,* Zoel Codolà, Isaac Garcia-Bosch, Laura Gómez, Juan José Pla, Miquel Costas,* Nat. Chem. 2011, 807-813

Well-Defined Iron Water Oxidation and Light-Driven Cobalt Reduction Catalysts

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One of the most appealing research areas is the mechanism understanding of multi-electron multi-proton processes, being central in the activation of small molecules such as the water oxidation to O₂ (WO) or reduction to H₂ (WR) processes.[1] In this line, we have discovered that readily available iron coordination complexes based on aminopyridine ligands are highly efficient homogeneous WO but also WR catalysts.[2-5] We present here one of the few examples of homogeneous and well-defined WO catalysts based on 1st row transition metals, which allows for a mechanistic studies. To gain insight into the mechanism of the Fe-catalyzed WO catalysis, we carried out a detailed study through kinetics, spectroscopic monitoring of intermediates, isotopic effects, isotopic labeling, electronic effects and DFT calculations.[3-5] The roles of the high oxidation state oxo-iron (IV) and (V) and new Fe-O-Ce species in the O-O forming event as well as possible intermediates in the oxidation of organic substrates[5] will be discussed.

Likewise, cobalt complexes based on aminopyridine ligands form robust homogeneous catalytic systems for light-driven reductions, in which their electronic and structural properties can be easily tuned.[6] By a combination of experimental and computational studies we have obtained key information about intermediate species and the mechanism for the photochemical reduction of water to H₂ but also ketones, aldehydes and olefins. The mechanism aspects will be discussed on this basis.

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Premios SusChem-JIQ

Cayetana Zárate Sáez
PREDOC-MESTRELAB



Cayetana Zárate se graduó con Premio Extraordinario de Fin de Carrera en la Universidad de Valladolid en 2012. Durante sus dos últimos años de licenciatura trabajó en catálisis de oro en el grupo del Profesor Pablo Espinet gracias a la concesión de dos becas de colaboración. En Octubre de 2012 se trasladó a Tarragona para trabajar en el grupo de Rubén Martín y en Julio de 2013 recibió el título de Master in Synthesis and Catalysis por la Universidad Rovira i Virgili.

En Julio de 2015 comenzó una estancia predoctoral en la Universidad de Princeton, en el grupo del Profesor Paul J. Chirik. Sus estudios de doctorado en el grupo de Rubén Martín se centran en el área de la activación catalítica de enlaces C-O.

Publicaciones recientes:

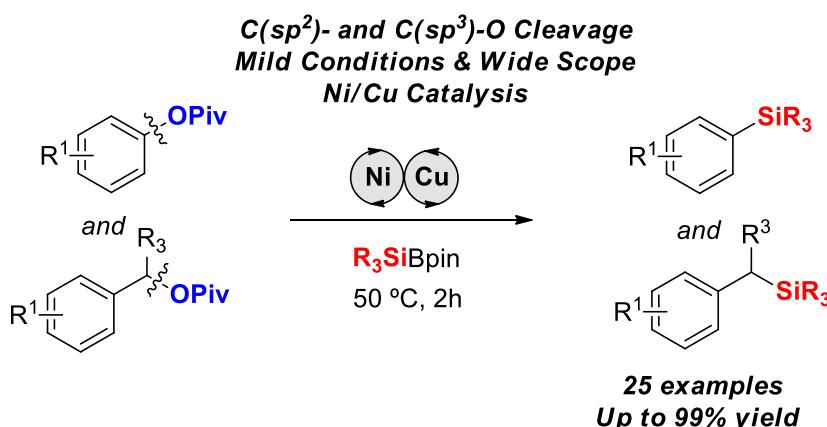
- 1) Ipsi-Borylation of Aryl Ethers via Ni-Catalyzed C-OMe Cleavage. Zarate, C.; Manzano, R.; Martin, R. J. Am. Chem. Soc. 2015, 137, 6754–6757
*Entre las publicaciones más leídas en Mayo de 2015
- 2) A Mild Ni/Cu-Catalyzed Silylation via C–O Cleavage. Zarate, C.; Martin, R. J. Am. Chem. Soc. 2014, 136, 2236–2239
*Uno de los 10 artículos más leídos en Febrero de 2014
- 3) Metal-catalyzed activation of ethers via C–O bond cleavage: a new strategy for molecular diversity. Zarate, C.; Cornella, J.; Martin, R. Chem. Soc. Rev. 2014, 43, 8081–8097
*Artículo más leído en Agosto de 2014.

A Mild Ni/Cu-Catalyzed Silylation via C-O Cleavage

C. Zarate,¹ R. Martin^{1,2*}

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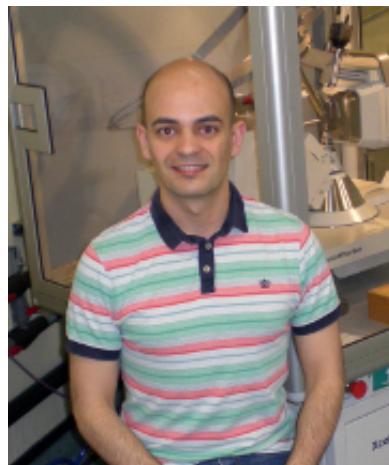
In recent years, the utilization of C-O electrophiles as coupling partners has received a great deal of attention due to their lack of toxicity and the readily availability of phenol as compared to commonly employed aryl halides as counterparts.¹ While formidable advances have been realized in this area of expertise, to the best of our knowledge, the development of a catalytic C-Si bond forming event using simple and traditionally considered inert C-O electrophiles has no precedents in the literature. This is surprising regarding the considerable value of aryl silanes in medicinal and material science.² Herein, we report a Ni/Cu-catalyzed silylation of unactivated aryl esters via C(sp²)- and C(sp³)-O bond cleavage.^{3,4}



Our catalytic synergistic Ni/Cu-catalyzed silylation of C(sp²)- and C(sp³)-O is characterized by its mild reaction conditions, robustness and wide substrate scope, including challenging substrate combinations.

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- ⁽³⁾ C. Zarate, R. Martin, *J. Am. Chem. Soc.*, **2014**, *136*, 2236.
- (4) Reaction conditions: aryl and benzyl pivalate (1.0 equiv.), Et₃SiBpin (1.2 equiv.), Ni(COD)₂ (10 mol %), PCy₃ (20 mol %), CuF₂ (30 mol %), CsF (1.0 equiv.) in toluene (0.25 M), 50 °C, 2 h.

Dr. Antonio Jesús Martínez Martínez
POSTDOC-MESTRELAB.



Antonio J. Martínez-Martínez, licenciado en Química por la Universidad de Murcia en 2005, se doctoró en dicha Universidad en 2012 con la máxima calificación de Sobresaliente 'Cum Laude' y Premio Extraordinario de Doctorado.

Realizó su tesis doctoral en el Grupo de Química Organometálica bajo la supervisión de los Profs. José Vicente y María Teresa Chicote trabajando en la síntesis y aplicaciones de complejos de organopaladio en síntesis orgánica. Durante esta etapa realizó dos estancias en la Universidad de Glasgow (UK) en el grupo de Química Computacional del Prof. John McGrady (actualmente en la Universidad de Oxford, UK).

En 2012 se incorporó como 'EPSRC Postdoctoral Research Assitant' en el Grupo del Dr. Charles O'Hara de la Universidad de Strathclyde (Glasgow, UK), donde actualmente continúa trabajando.

Sus líneas de investigación se enfocan en el diseño racional de compuestos bimetálicos que incorporan metales con distintas polaridades y el estudio de sus aplicaciones en síntesis orgánica, especialmente en la activación de enlaces C-H. Entre otras, actualmente desarrolla colaboraciones con los grupos del Prof. Robert Mulvey (de la misma Universidad) y del Prof. Holger Braunschweig de la Universidad Julius-Maximilians de Würzburg (Germany).

Publicaciones recientes:

- 1) A. J. Martínez-Martínez, A. R. Kennedy, R. E. Mulvey, C. T. O'Hara. "Directed ortho-meta'-and meta-meta'-dimetalations: A template base approach to deprotonation", *Science* 2014, 346, 834-837. Recientemente destacado en *Nature Chem.* 2015, 7, 8; y en *Chemical & Engineering News* 2014, 92, 35.
- 2) A. J. Martínez-Martínez, D. R. Armstrong, B. Conway, B. J. Fleming, J. Klett, A. R. Kennedy, R. E. Mulvey, S. D. Robertson, C. T. O'Hara. "Pre-inverse-crowns: synthetic, structural and reactivity studies of alkali metal magnesiates primed for inverse crown formation", *Chem. Sci.* 2014, 5, 771-781.
- 3) A. R. Kennedy, S. M. Leenhouts, J. J. Liggat, A. J. Martínez-Martínez, K. Miller, R. E. Mulvey, C. T. O'Hara, P. O'Keefe, A. Steven. "Dehydromethylation of alkali metal salts of the utility amide 2,2,6,6-tetramethylpiperidide (TMP)", *Chem. Commun.* 2014, 50, 10588-10591.

Functionalisation of aromatic compounds: switching the Regioselectivity away from *ortho*

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Directed *ortho*-Metallation (DoM) represents the leading method for functionalising aromatic compounds. In this reaction a basic organometallic compound is used to deprotonate the position adjacent to a functional group residing on an aryl ring (transforming inert C---H bonds to reactive and useful C---metal ones).¹ The addition of electrophiles allows the simple preparation of valuable organic synthons (*e.g.* in the pharmaceutical industry). However, on the downside, this strictly *ortho*-limitation prevents functionalisation at remote C---H positions. Selective C---H bond metallation at hitherto inaccessible positions (*i.e.* *meta*) of aromatic systems is currently one of the hottest topics in organometallic chemistry;² however, these transformations are still of limited wide applicability and often require laborious preparations of specific groups which are able to *meta*-direct C---H bond transformations.

In this work, the intrinsic *ortho*-selectivity typically displayed by single---metal reagents in functionalised aromatics is overcome by using a novel template metallation approach. This methodology is based on the pre---organized structure of mixed alkali metal magnesium reagents.³ It exhibits remarkable direct *ortho,meta'* or *meta,meta'*---C---H bond dimetallation, both feats are unachievable by any known methodology, and the latter completely overrides the normal *ortho*-preference. Additionally, the reactions proceed with broad functional group tolerance under mild reaction conditions. Finally, the metallation of several different polyaryl hydrocarbon systems, which are generally unreactive towards conventional metallation chemistry, will be discussed.⁴

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 3. a) A. J. Martínez---Martínez, D. R. Armstrong, B. Conway, B. J. Fleming, J. Klett, A. R. Kennedy, R. E. Mulvey, S. D. Robertson, C. T. O'Hara, *Chem. Sci.* **2014**, *5*, 771; b) A. J. Martínez---Martínez, A. R. Kennedy, R. E. Mulvey, C. T. O'Hara, *Science* **2014**, *346*, 834.
 4. A. J. Martínez---Martínez, B. J. Fleming, S. Justice, A. R. Kennedy, I. D. H. Oswald, C. T. O'Hara, *2015, unpublished results.*

Comunicaciones Hot Topic

Nanoscopy for Nanomedicine: looking at synthetic materials one molecule at a time

L. Albertazzi

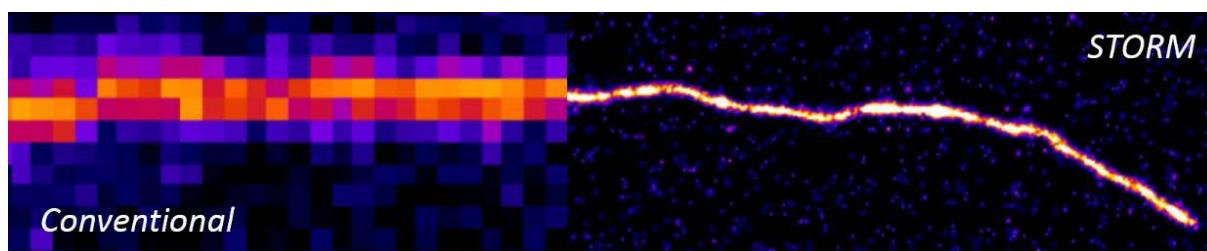
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The use of nanocarriers for intracellular delivery of therapeutic moieties is a great challenge for synthetic chemistry and nanotechnology. Supramolecular materials such as micelles, liposomes self-assembled nanoparticles and nanofibers play a pivotal role in this framework. A crucial factor limiting the design of effective materials is the lack of understanding about material-cell interactions that hampers the rational design of nanosized carriers. This is particularly relevant for supramolecular materials as their complex structure pose several unanswered questions.

Here we discuss the use of super resolution microscopy to image materials in vitro and in mammalian cells. This novel technique, allowing to obtain a resolution down to 20nm, had a dramatic impact in the field of cell biology, however its use in the field of chemistry is poorly explored. Super resolution microscopy offers nanometric resolution and multicolor ability. Therefore it is an ideal tool to study nano-sized supramolecular assemblies of multiple components in vitro and in cells, unveiling materials behavior that was impossible to study before due to lack of suitable techniques.

We employed Stochastic Optical Reconstruction Microscopy (STORM) to image biomaterials, with special emphasis on supramolecular polymers, in vitro unveiling novel information on materials structure and dynamics, a key issue of supramolecular materials (1)

Moreover we propose a methodology to image nano-sized materials in cells, tracking them during their membrane targeting, cell uptake and intracellular targeting. We show how 2-color STORM can be used to perform nanometric-accurate colocalization unveiling at the molecular level materials-cell interactions. The use of the information obtained thanks to these novel microscopy methodologies for the “STORM-guided” design of novel biomaterials will be discussed.



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Design and synthesis of new chiral SO/PO bidentate ligands in organocatalysis: enantioselective synthesis of pharmacologically significant arylamines.

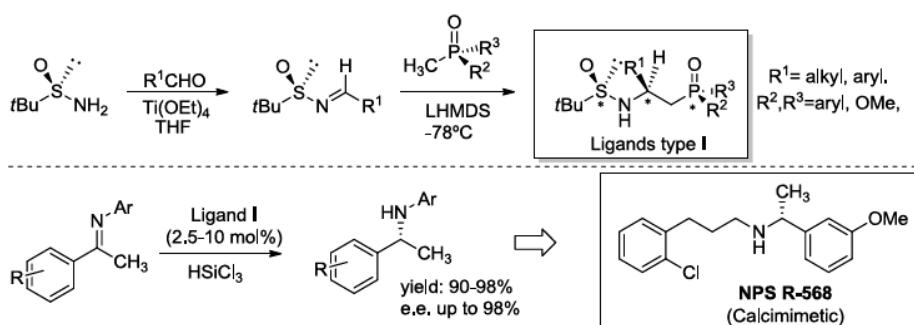
R. Recio,¹ A. Chelouan,¹ G. Borrego,¹ N. Khiar,² I. Fernández¹

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Despite the historical need for and continued interest in chiral imines, their enantioselective synthesis remains a challenging task even today. In this sense, the development of new metal-free, readily available chiral catalytic systems for the enantioselective reduction of keto-imines has become an important goal in the field of asymmetric catalysis.¹ One of the organocatalytic approaches to carry out enantioselective C=N reductions involves the use of trichlorosilane in the presence of chiral Lewis bases. On these bases, we have synthesized a new family of chiral sulfinamide-phosphinate type I derivatives as chiral PO/SO bidentated organocatalyzers, in two simple steps, from the readily available enantiopure N-tert- butylsulfamide. These ligands present four diverse diversity points: the configurations at sulfur and at phosphorus, the nature of the substituent at the chiral carbon of the linker and the nature of the phosphinyl group. These ligands have been applied to the asymmetric hydrosilylation of differently substituted imines, with good to high enantioselectivities. The methodology has been successfully extended to the stereoselective synthesis of (R)-NPS R568, a new type of calcium receptor agonist.²



Acknowledgment: Acknowledgements: Financial supports from the "Ministerio de Ciencia e Innovación" (grant No. CTQ2013-49066-C2-1/2-R and "Junta de Andalucía" (grant No.P11-FQM-8046)

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Nanotubular systems self-assembled through orthogonal Supramolecular interactions

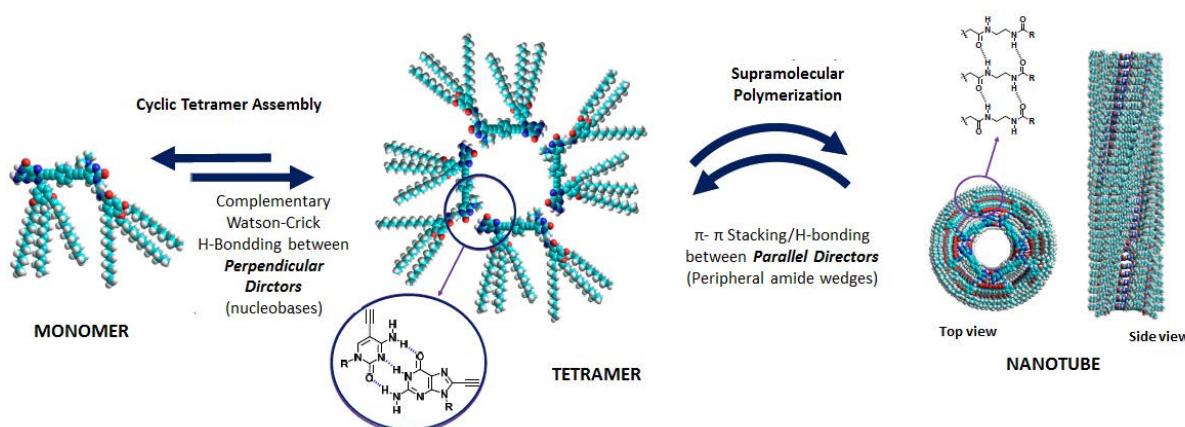
R. Chamorro-Mendiluce,¹ V. Vázquez-González, M.J. Mayoral,¹ M. T. Aranda,¹ N. Bilbao,¹ C. Montoro-García,¹ J. Camacho-García,¹ A. López-Pérez¹ and D. González-Rodríguez*¹

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Our project aims at the preparation of macrocyclic self-assembled systems with a fine control on their size, shape and chemical functionality, which will constitute the section of self-assembled nanotubes.¹⁻⁴ To this purpose we have designed two different linear and planar molecules bearing hydrogen-bonding moieties (**perpendicular directors**) and peripheral amide wedges (**parallel directors**). These monomers are expected to self-assemble into nanotubes through p-p interactions and hydrogen bonding of the amide groups.

The role of perpendicular and parallel directors to generate self-assembled nanotubes will be studied in detail in the global process. The former provide a highly stable p-conjugated macrocyclic trough hydrogen bonding between complementary nucleobases, while the parallel directors induce the supramolecular polymerization process of the macrocyclic self-assembled system.

The supramolecular equilibrium has been studied by UV-Vis Spectroscopy, Fluorescence Spectroscopy, Circular Dichroism and Nuclear Magnetic Resonance in solution, as well as visualized by imaging techniques (Transmission Electron Spectroscopy, Scanning Electron Spectroscopy and Atomic Force Microscopy).



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Diels-Alder Reactivity and Selectivity at the interior of the Polycyclic Aromatic Hydrocarbons: A computational study

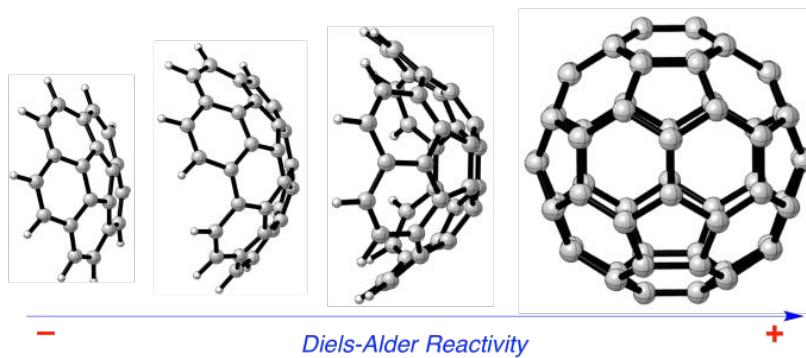
Yago García-Rodeja and Israel Fernández *

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A computational study (at the DFT level) using the so-called Activation Strain Analysis (ASA) [1] and the Energy Decomposition Analysis (EDA) [2] methods was carried out to understand the physical factors controlling the Diels-Alder reactivity and selectivity between different polycyclic aromatic hydrocarbons (PAHs) [3] and cyclopentadiene and their relationship to C₆₀.

It was found that: **(i)** the [6,6]-pathway is both kinetically and thermodynamically favored (with the exception of corannulene) over the [5,6]-pathway. **(ii)** There is a convergence to the C₆₀ energy barrier for the [6,6] attack when the size of the buckybowl is increased. **(iii)** Both the decrease of the strain energy and the increased of the interaction energy between the deformed reactants are responsible for the observed trend of [4+2]-reactivity. **(iv)** The complete regioselectivity of the process can be ascribed to the higher interaction between the deformed reactants as a result of higher orbital and electrostatic interactions along the entire [6,6]-pathway as compared to the corresponding [5,6]-path. **(v)** the more stabilizing orbital interactions for the [6,6]-pathway can be attributed to the better HOMO-LUMO overlap along the entire reaction coordinate.

In summary, it can be concluded that whereas the [6,6]-regioselectivity is controlled by the interaction energy between the deformed reactants along the reaction coordinate, the reactivity of the buckybowls depends on the interplay between the activation strain energy and the transition state interaction.



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Electrochemical characterization and In situ Synchrotron study of P2- and O3- $\text{Na}_{2/3}\text{Fe}_{2/3}\text{Mn}_{1/3}\text{O}_2$ as cathode material for Na ion batteries.

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Lithium-ion batteries (LIBs) continue to attract world-wide attention not only because of their proven application in portable electronic devices (cell phones, laptops...) but also because of their promising application for transportation (electric vehicle).[1]

Na-ion based cathode materials are getting more interest recently ever since they were firstly investigated in 1980's.[2,3] Some reasons for this raising interest are its natural abundance, geographical distribution, low cost and similar electrochemical behaviour to lithium. Layered oxides, NaMO_2 (M = Cr, Mn, Fe, Co, Ni, and mixture of 2-3 transition metal) are playing an important role because of their high capacity and structural simplicity. All layered oxides can be classified by oxygen layer stacking and surrounding environment for sodium.[4]

We have focused our research on Na-Mn-Fe-O system and studied the stability of the P2- and O3- $\text{Na}_{2/3}\text{Fe}_{2/3}\text{Mn}_{1/3}\text{O}_2$ phases. They have been synthesized as pure phases and structural and physicochemical characterizations have been performed by our group. [5] Their electrochemical performances have been analyzed and the energy densities are 386.05 mW h g⁻¹ and 423.878 mW h g⁻¹ for P2- and O3- phase.

In situ synchrotron X-ray diffraction method has been used to study the structural evolution of both phases during cycling under relatively high current rates.[6,7]

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Enantiopure Tetrasubstituted Pyrrolidines as Scaffolds for Novel and Potent Proteasome Inhibitors

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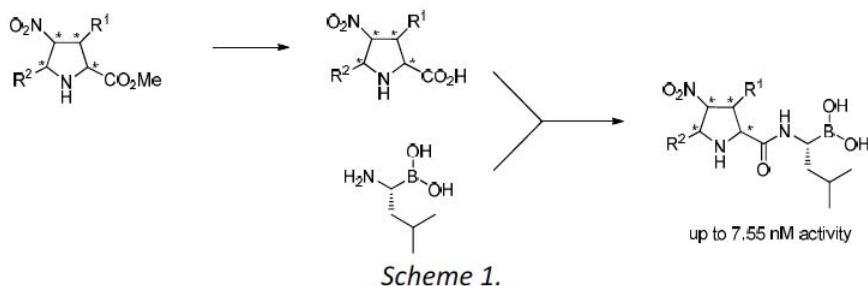
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The ubiquitin proteasome system (UPS) is a highly conserved intracellular pathway responsible for the degradation of unneeded and damaged proteins. It plays a pivotal role in fundamental pathways such as cell cycle regulation, DNA repair, apoptosis and different types of malignancies. Therefore, the development of proteasome inhibitors has emerged as a very active field in medicinal chemistry, pharmacology and oncology.

Several proteasome inhibitors have been described in the literature being Bortezomib the first one approved by the US Food and Drug Administration (FDA) for the treatment of multiple myeloma and mantle cell lymphoma.

On the other hand, the synthesis of hybrid ferrocene-pyrrolidine ligands via 1,3-dipolar cycloadditions has been described by our group,¹ as well as its use in (3+2) cycloaddition reactions between stabilized azomethine ylides and different π -deficient dipolarophiles. This reaction allows the preparation of an offspring of unnatural *endo*- and *exo*-D and L- densely substituted and functionalized by proline derivatives with excellent enantiomeric excesses.

Within this context, the aim of this work has been to combine both ideas synthesizing novel proteasome inhibitors possessing both boronic acid and enantiopure pyrrolidinic moieties. (Scheme 1).²



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² Patent. Enantiopure Tetrasubstituted Pyrrolidines as Scaffolds for Proteasome Inhibitors and Medicinal Applications Thereof. (2014) EP14382058-WO 2015/124663

Comunicaciones Orales

A sustainable multicomponent microwave assisted reaction to prepare (2-imidazolin-4-yl)phosphonates

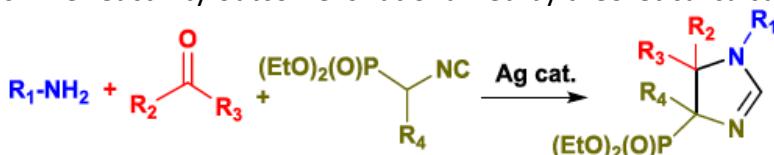
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2-Imidazoline-containing compounds constitute a valuable class of agents that modulate the α_2 -adrenergic receptors, and often show a high affinity for imidazoline binding sites (IBS). The biological profile of these IBSs has been examined due to their involvement in the control of blood pressure, depression, insulin secretion, neurodegenerative disorders, and tolerance and dependence on opioids. Moreover, 2-imidazolines are an important class of heterocyclic scaffolds. Inspired by a previous study by Orru [1] and seeking new applications of isocyano derivatives, we envisaged the possibility of performing a MCR between diethyl isocyanomethylphosphonate (PhosMic) or α -substituted PhosMic derivatives, ketones and amines (Scheme 1). Notably, although isocyano derivatives can be found extensively in the literature as reactants in multicomponent reactions, the use of PhosMic in IMCRs has received less attention. The proposed reaction would give direct access to (2-imidazolin-4-yl)phosphonate compounds. The potential biological interest of these new azaheterocyclic phosphonates is mostly associated with the tetrahedral structure of the phosphoryl group, which may act as a “transition state analogue” in enzymatic peptide hydrolysis. This work addresses the synthesis of 2-(imidazolin-4-yl)phosphonates through an environmentally friendly multicomponent heterocyclic reaction following green chemistry considerations. We envisioned the use of microwave irradiation, which is an outstanding tool for sustainable organic chemistry, maximizing synthetic efficiency, diversity and complexity. We disclose a general microwave protocol for a silver-catalysed three-component reaction towards the synthesis of (2-imidazolin-4-yl)phosphonates. The reactivity outcome is rationalized by theoretical calculations.



Scheme 1

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Reactive oxygen species (ros) using bi-functional microparticles For cancer theranostics

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The aim of this work is to develop a novel microtool for producing and sensing Reactive Oxygen Species (ROS) potentially useful in cancer treatment. For this study, we will be using two species acting as a photosensitizer: either Cytochrome C, an apoptotic agent containing heme group, or zinc porphyrin derivatives.¹ Both the species are known to have peroxidase activity and, upon light excitation, therefore they would release ROS necessary for initiating apoptosis leading to cell death. On the other hand, in order to sense ROS production, BODIPY 581/591 will be used: this fluorescent dye shows a shift in the fluorescence emission peak upon oxidation, allowing the detection and quantification of singlet oxygen species.²

Our approach is to prepare and optimize a protocol for functionalizing bi-functional microparticles (build up of gold and polysilicon) with both BODIPY 581/591 and one selected photosensitizer. Finally, the photochemical behaviour of the bi-functionalized microparticles will be studied in an *in vitro* experiment, in order to test their capability and efficiency in sensing ROS in living cells.

Acknowledgement:

Financial support from the Ministerio de Ciencia e Innovación (MICINN) (project TEC2011-29140-C03-02, TEC2014-51940-C2-2-R, TEC2011-29140-C03-01 and TEC2014-51940-C2-1-R) are acknowledged.

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Supramolecular gelation of non linear optically-active compounds

CO-3

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The control of the supramolecular polymerization and gelation process for the modulation of desired properties have attracted a considerable interest.^[1] In this work, non linear optic (NLO)-active organogelators are used as internal probes to get insight on the critical parameters governing the formation of supramolecular objects able to gelate solvents. Moreover, Second Harmonic Generation (SHG) microscopy has been used for the first time for the study of achiral organogelators.

On one hand, the difference in the chemical structure between compounds 1 and 2 determines the participation of the functional groups in the supramolecular polymerization process. As a result, the implication of the secondary amine in 1 led to a distinct supramolecular organization compared to compound 2 which has a tertiary amine. As a consequence, compound 2 is able to generate gels in many solvents while compound 1 is not. On the other hand, the donor-acceptor character of the dye together with the non covalent forces involved in the supramolecular polymer of compound 2, allow for obtaining systems endowed with spontaneous SHG response. This study provides important clues for the design of new organogelators and underlines the potential of supramolecular gels as soft materials in the research field of photonics.

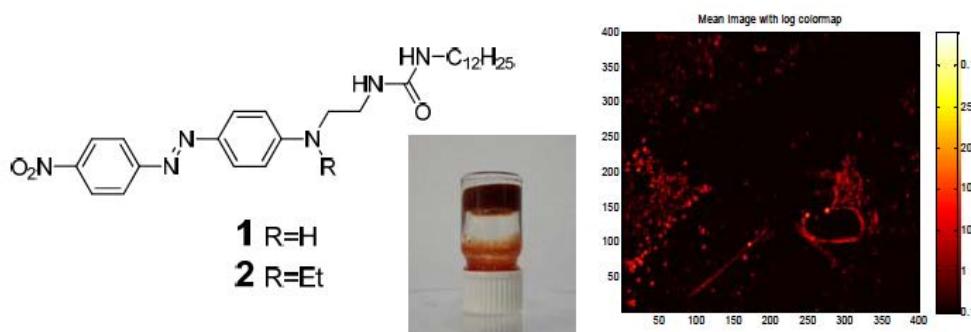


Fig. 1: Chemical structure of organogelators **1** and **2** (left), picture (centre) and SHG micrograph (right) of the gel formed by **2** from acetonitrile.

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Visible light reduction of ketones and aldehydes catalyzed by complexes based on Earth abundant elements and water as source of hydrogen atoms

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The development of alternative greener synthetic methods of high-value chemicals and energy carriers is a requirement for a more sustainable society. Among different opportunities to this end, the use of solar light-driven reactions has become one of the most ambitious and challenging approaches.¹ In this regard, during the last years a spectacular increase of efforts devoted to understand and mimic natural photosynthetic processes with the aim to generate solar fuels has been pursued.² Despite the significant advances on the reduction of organic substrates using homogeneous catalytic systems based on Ru, Rh, Ir, Fe or Co,³ the reduction of synthetic molecules using visible light as driving force and water as hydrogen source, has only rarely considered by using a combination of novel-metals and enzymes.⁴ Herein, we present, a new bio-inspired photocatalytic system based entirely on Earth-abundant elements that reduces ketones and aldehydes to alcohols with excellent yields (up to 1200 TON) making use of water as source of hydrogen atoms in aqueous phase. The same catalytic system can also be applied for the light-driven hydrogen production. Based on kinetic studies we showed that both reduction reactions, water to H₂ and carbonyls to alcohols are competing reactions, supporting strongly that both share a common well-defined intermediate. The reactivity toward H₂ or alcohol formation can be tuned simply by modulating the electronic nature of the ligand. The results based on reactivity, electronic effects and labelling studies exclude free radical mechanism, suggesting a cobalt hydride as intermediate responsible for the carbonyl reduction. This work opens up newer and greener avenues for the selective transformations of organic substrates by artificial photosynthetic schemes.

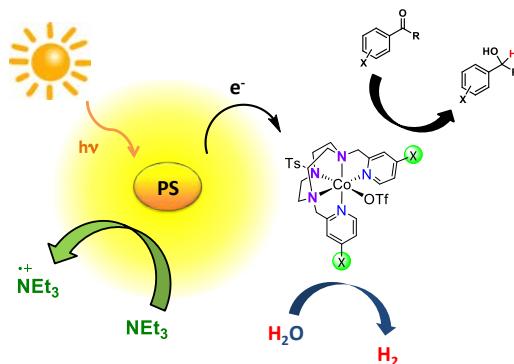


Figure 1. General scheme for the photochemical reduction of ketones and aldehydes using water as hydrogen source.

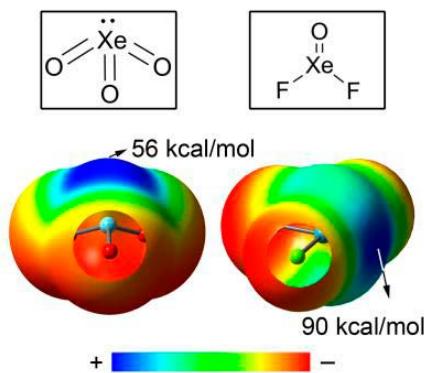
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Aerogen Bonding Interaction: A New Supramolecular Force?

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Supramolecular chemists rely on a depth comprehension of the noncovalent forces, which are the ground pillars of modern chemistry. A proper understanding and intelligent utilization of them is essential in order to achieve progress in fields such as supramolecular chemistry,[1] molecular recognition[2] and materials science.[3] In this context, one of the most known supramolecular forces that is ubiquitous in many chemical and biological systems is the hydrogen bonding. Moreover, σ -hole interactions involving tetrel, pnicogen, chalcogen and halogen atoms are also being recognized by the scientific community as powerful tools in supramolecular chemistry, crystal engineering and biochemistry. They refer to the interaction between group IV to VII bearing compounds (donor) and nucleophiles (acceptor). Their strength is moderately strong and they are highly directional due to the localization of a positive potential region on the extension of the covalent bonds (σ -hole) in the acceptor molecule. Very recently, a new supramolecular force has been put into scene, named aerogen bonding,[5] which implies an interaction between an aerogen bearing moiety and an electron rich entity. Very few examples are available in the CSD, due to the low reactivity of the aerogen element series. While its potential practical applications in the field of supramolecular chemistry are very limited, aerogen bonding interactions can be of great importance in Xenon chemistry.



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La espectroscopía de alta resolución en la química moderna

CO-6

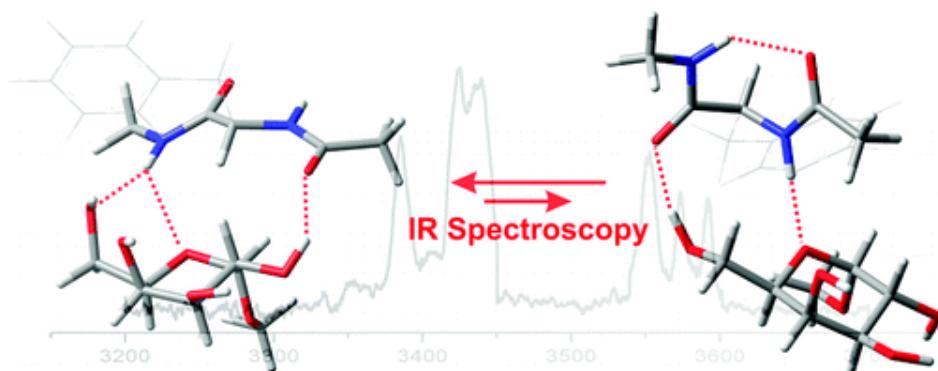
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La espectroscopía es la ciencia que estudia la interacción entre la radiación electromagnética y la materia. En este trabajo se presentan varios estudios estructurales sobre carbohidratos utilizando una estrategia experimental que combina espectroscopía de microondas (MW) y espectroscopía láser en alta resolución. Ambas espectroscopías presentan funcionalidades complementarias. Por una parte, la espectroscopía láser ofrece una alta sensibilidad lo que unido a la selectividad, hacen de ella la herramienta idónea para estudiar sistemas bioquímicos de tamaño mediano- grande[1-2]. Por otra parte, la espectroscopía de microondas proporciona una resolución mucho más alta y permite tener acceso a la estructura molecular a través de los momentos de inercia. Este enfoque combinado proporciona no sólo una visión química exacta sobre la conformación, estructura y propiedades moleculares, sino también permite evaluar la precisión de los cálculos teóricos. Con el fin de ilustrar las posibilidades de un enfoque combinado MW-láser se presentan los resultados de varios carbohidratos. Entre estos estudios incluimos la casuística de la D-ribosa,[3] la determinación estructural de la fructosa,[4] el reconocimiento molecular de los diferentes anómeros de un azúcar utilizando un péptido como sensor,[1,2] y la estructura de un pentasacárido que aparece en la mayoría de las N-glicoproteínas.[5]



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Activación Homolítica N–H de Amoníaco Promovida por Complejos de Iridio(I)

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La activación N–H de amoníaco mediada por metales de transición es una temática actual. Un inconveniente en este contexto es la formación de aductos estables de tipo Werner [$M-NH_3$], por lo que la naturaleza de complejos organometálicos de iridio resulta esencial para llevar a cabo la ruptura del enlace N–H de NH_3 , proceso que puede dar lugar a amido complejos [$M-NH_2$].¹ En este contexto, la utilización del complejo mononuclear $[Ir(cod)(dppe)Cl]$ ($dppe$ = difenilfosfanoetano) posibilita la adición oxidante de amoníaco a iridio, dando lugar a la formación del amido hidruro complejo dinuclear $\{[Ir(\mu-NH_2)(dppe)(NH_3)(H)\}_2[Cl]\}_2$.

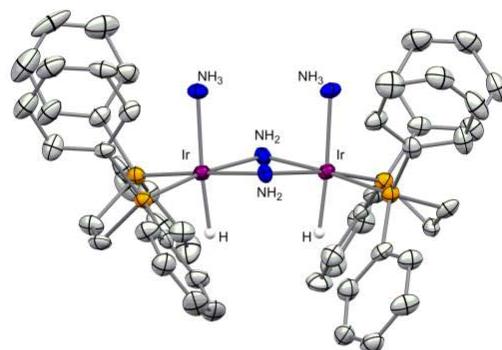


Figura 1. Estructura molecular de un amido hidruro complejo de iridio(III)

Este tipo de reactividad se ha extendido a complejos catiónicos análogos, que contienen difosfanos de diversa naturaleza. De esta manera, la reacción de los complejos $[Ir(cod)(P-P)]^+[BF_4]^-$ ($P-P$ = difenilfosfanopropano (dppp), difenilfosfanobutano (dppb)) con NH_3 gas ha permitido aislar los correspondientes complejos dicatiónicos dinucleares $\{[Ir(P-P)(NH_3)(H)](\mu-NH_2)\}_2[BF_4]_2$. Paralelamente, se han llevado a cabo estudios teóricos DFT que explican el mecanismo de activación homolítica N–H de amoníaco.

Agradecimientos: Proyecto CTQ2012-35665.

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Cyclic Oligosquaramide as Carrier for Cell Internalization of Alkylating Agents

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Chemotherapy is the main clinic treatment for cancer disease. Among others, alkylating agents are commonly used. Although in the last decades there has been a huge development of new chemotherapeutic agents, the main problem remains in their low selectivity for the target site and, consequently, their high toxicity.¹

Site directed drug delivery (SDDD) is based on the use of chemical agents that work as drug carriers. Thus, the drug is specifically carried to its target site, either a tumoral tissue or a cancer cell. Recently, cyclic oligosquaramide C2-BDP has proven to internalize across live cell membranes carrying a fluorophore (BODIPY).² Based on these results, here we present the design and synthesis of a carrier-alkylating agent conjugate to study the release of the drug by the hydrolysis reaction between both components.

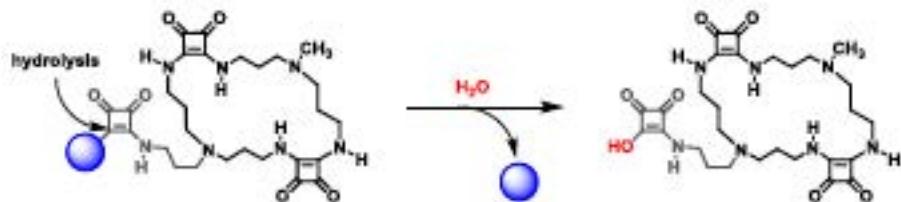


Fig.1. Release of alkylating agent (blue) by hydrolysis reaction

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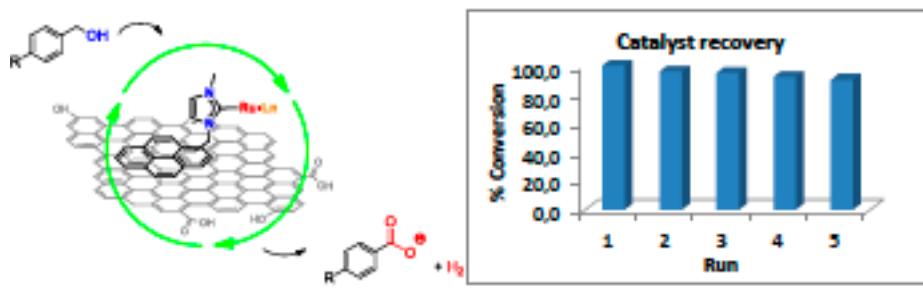
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Immobilization of ru-nhc complexes onto graphene: catalyst stabilization increases the catalytic activity

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Despite homogeneous catalysts are in general superior to heterogeneous catalysts in terms of activity and selectivity, their difficult separation from the products and subsequent reutilization is an important drawback that makes industries reluctant to use them in large scale processes. For these reasons several efforts are being carried out for the immobilization of known and highly active homogeneous catalysts onto solid supports. In this regard we have recently reported the immobilization of ruthenium and palladium organometallic compounds onto graphene-type materials by π -stacking interactions



Scheme 1

In this work we have synthesized three Ru-NHC complexes bearing different aromatic fragments that allow the immobilization of the complexes onto reduced graphene oxide by non-covalent interactions. The catalytic properties of the molecular complexes and the new hybrid-graphene materials were studied in the oxidative dehydrogenation of primary alcohols in water. The results showed that the hybrid materials improve the catalytic outcomes of the homogeneous complexes, and that the immobilization of the molecular entities onto reduced graphene oxide allows the recovery and reuse of the catalyst.

We thank the financial support from the “Generalitat Valenciana” (Project AICO/2015/039). The autors are grateful to the ‘Serveis Centrals d’Instrumentació científica (SCIC)’ of the universitat Jaume I.

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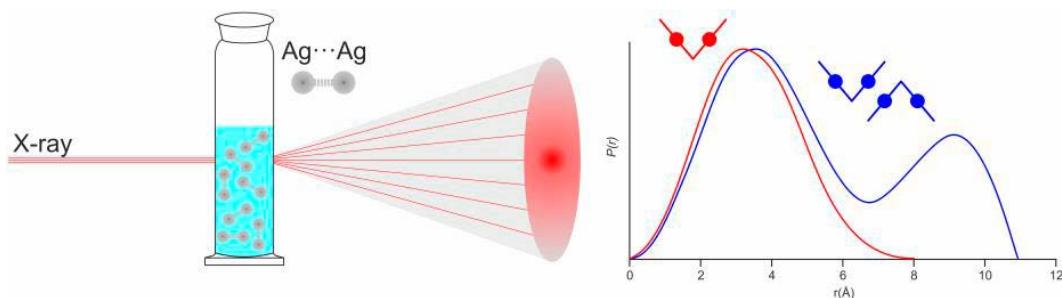
Dispersión de Rayos X en Disolución: Evidencia Directa de Interacciones Metal–Metal a Nivel Molecular

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Las interacciones metalofílicas han sido estudiadas tradicionalmente en disolución por métodos espectroscópicos (IR, Raman, UV/Vis, NMR, espectroscopía ESR), en estado sólido por cristalográfia de rayos X, y más recientemente los estudios computacionales han cobrado una gran importancia en el desarrollo de este campo. Estas interacciones juegan un papel fundamental de agregación en sistemas *host-guest*, nanopartículas, o materiales conductores, luminiscentes y ensamblados.

Recientemente observamos interacciones argentofílicas no soportadas en un sistema *host-guest* catión-catión $\text{Ag}^+ \subset [\text{Ag}_2(\text{bisNHC})_2]^{2+}$ (NHC = carbeno N-heterocíclico), en disolución y estado sólido, con la capacidad de formar agregados moleculares.^[1] La inesperada fortaleza observada en estos sistemas nos motivó a utilizar de manera pionera la técnica de *Small Angle X-ray Scattering* (SAXS), para la detección y estudio de interacciones metal-metal a nivel molecular (Esquema 1). En este trabajo postulamos además que las interacciones metalofílicas pueden superar los límites del radio de van der Waals si se involucran ligandos fuertemente dadores.^[2]



Esquema 1

Agradecemos la financiación al Ministerio de Economía y Competitividad de España (Programa “Ramon y Cajal” (P.J.S.M) y CTQ2011-27593).

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Enantioselective Synthesis of β -Aminophosphinic Acids: Biologically Significant Phosphorous Isosters of β -Amino Acids.

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Natural amino acids play a key role in life's chemistry as structural units of peptides, proteins and enzymes. Therefore the study of the chemistry and biologically activity of their synthetic analogues is of significant relevance. Namely, different studies have demonstrated that phosphorous derivatives can act as enzymatic inhibitors, antibacterial, anticancerous, antiviral or anti-AIDS, as well as having pesticide, insecticide or weed-killer properties.¹

In this sense, we have developed an enantioselective methodology in order to synthesize a new family of phosphorous analogues of amino acids with general structure **A** (figure 1). These compounds are considered to be bioisosters of amino acids with general structure **B** (figure 1) in which the carboxylic group has been substituted by a phosphinic acid fragment.

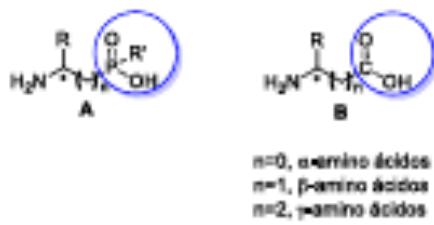


Figure 1.

These amino phosphinic acids are easily synthesized by the stereoselective addition of different methylphosphinates to diverse *N*-*tert*-butylsulfinylaldimines.² Moreover, both enantiomers of a specific amino phosphinic acid can be obtained in a stereoselective manner by selecting the nature of the starting methylphosphinate.

Acknowledgements: Financial supports from the "Ministerio de Ciencia e Innovación" (grant No. CTQ2013-49066-C2-1/2-R) and "Junta de Andalucía" (grant No.P11-FQM-8046).

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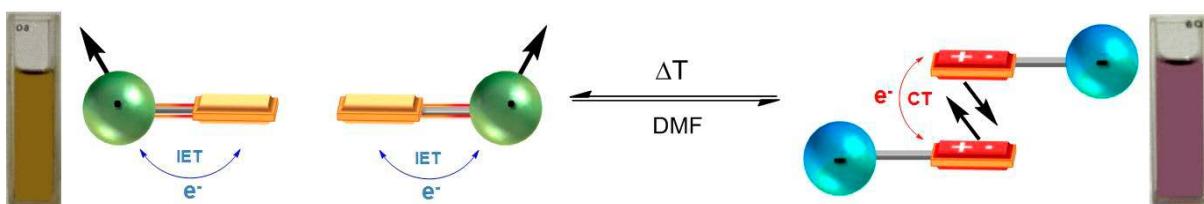
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Multifunctional switchable materials based on organic Donor-Acceptor systems

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The ability to control at the molecular level the physical properties (optical, magnetic and electrical) of advanced materials is an important goal for the realization of functional devices. Switchable molecular materials are characterized by multiple electronic states that can be accessed through variation of external stimuli such as temperature or light. Organic molecules formed by an electron donor (D) and an electron acceptor (A) units covalently linked by a π -conjugated bridge (D- π -A) are an interesting family of molecules widely investigated for several applications, ranging from organic light-emitting devices, non-linear optics, molecular electronics and photonics. When an external stimulus is applied, an electron transfer process can be induced with the movement of an electron from the donor to the acceptor and stabilize the zwitterionic state that exhibits different physical properties. We have reported a D-A system based on a tetrathiafulvalene (TTF) unit as electron donor connected to a polychlorotriphenylmethyl (PTM) radical as electron acceptor that exhibits bistability in solution through the application of external stimuli such as the polarity of the solvent or temperature. [1-3] Moreover, in order to exploit the magnetic and conducting properties in the solid state, we have designed a new dyad with a larger bridge to improve the self-assembly of the TTF moieties of the system. The crystal structure shows an interesting supramolecular architecture with segregated donor and acceptor units. [4] Finally, the studied systems have been functionalized with thiol groups and assembled into gold surfaces by means of covalent interactions to form Self-Assembled Monolayers (SAMs) in order to exploit their potential application as molecular switches or rectifiers.



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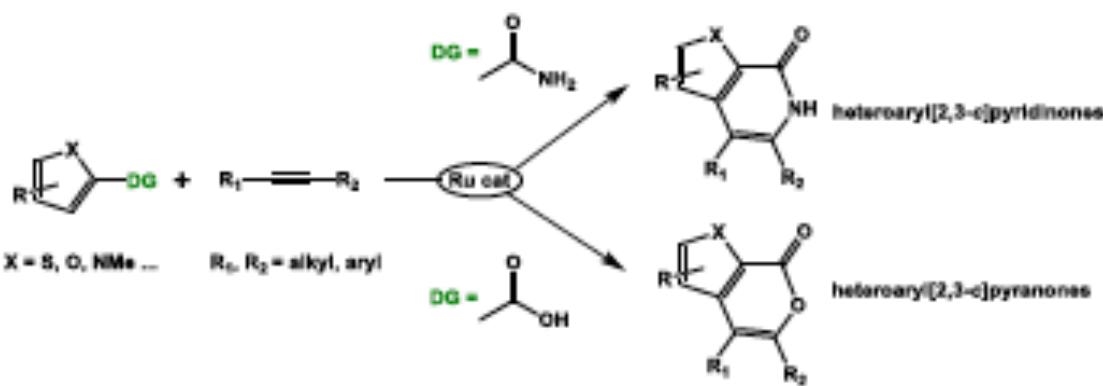
Ru-catalyzed coupling reactions for the synthesis of valuable fused heterocycles: primary amides and carboxylic acids as directing groups

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C-H bond activation is a unique tool for the synthesis of relevant molecules which are difficult to obtain by classic synthetic paths¹. Heterocyclic compounds can be obtained by metal-mediated reactions, often catalytically. Thanks to the presence of a directing group, the reaction proceeds with selectivity.¹ Many metals have been used for this purpose, including Pd, Rh and the less-expensive Ru.

Having previously obtained outstanding results using primary amines as directing groups in coupling reactions with alkynes,^{2,3} our group has moved on to explore the reactivity and synthetic possibilities of primary amides. They show some advantages over other directing groups: they are widely available and robust starting materials, and their use avoids the need of manufacturing more complicated groups prior to the C-H bond functionalization steps. In this way, we have synthesized new, previously unreported heteroarylpyridinones, which possess interesting biological activities. We have also applied this methodology to molecules with O-containing directing groups to obtain analogous structures. In this case, the coupling of heterocyclic carboxylic acids with internal alkynes yields heteroarylpyranones, which also show promising pharmaceutical activity.



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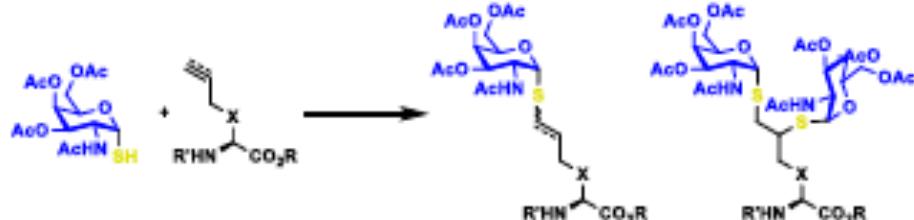
Síntesis de nuevos glicoaminoácidos miméticos al antígeno Tn a partir de reacciones Tiol-eno (TEC) o Tiol-ino (TYC)

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El antígeno Tn (α -O-GalNAc-Ser/Thr) está involucrado en el proceso de reconocimiento de células cancerosas. Esta simple estructura se puede encontrar en un gran número de epítopos de reconocimiento de glicoproteínas, por ejemplo, la mucina MUC1.¹ Por esta razón, la síntesis de nuevos miméticos de Tn está atrayendo el interés de los químicos.

En este sentido, nosotros hemos llevado a cabo la síntesis de distintos miméticos del antígeno Tn basados en azufre.² Cambiando el oxígeno por azufre, podemos proveer de distintas afinidades al antígeno Tn cuando se incluye en epítopos de glicopéptidos. La síntesis de los diferentes *building blocks* de sulfa-Tn se han logrado a través de una estrategia radicalaria, bien por hidrotiolación de alquenos (TEC) o por hidrotiolación de alquinos (TYC), partiendo de 3,4,6-tri-O-acetyl-2-acetamido-2-deoxy-1-tio- α -D-galactopiranosa y los correspondientes aminoácidos insaturados, convenientemente protegidos.



¹ A. Varki, *Glycobiology*, **1993**, 3, 97.

² C. Aydillo, I. Compañón, A. Avenoza, J. H. Busto, F. Corzana, J. M. Peregrina, M. M. Zurbano, *J. Am. Chem. Soc.*, **2014**, 136, 789.

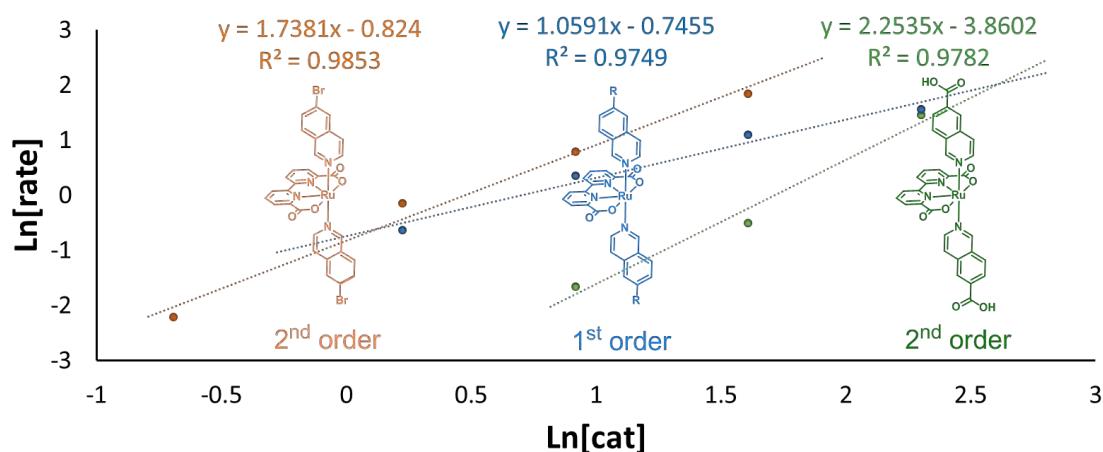
Same Catalyst, Different Rate Law

CO-15

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La investigación centrada en la catálisis de la oxidación del agua por complejos moleculares ha avanzado mucho en la última década. Un buen ejemplo de la efervescencia del campo es la evolución de los *Turnover Frequencies* (TOFs): desde el dímero de Ru-bpp de Llobet *et al* en 2004 (TOF *ca.* 0.0015 s^{-1}),¹ pasando por los complejos de Ru-bda de Sun *et al* en 2012 (TOF *ca.* 300 s^{-1}),² hasta el polyoxometalato de Hill *et al* en 2014 (TOF $>1000\text{ s}^{-1}$).³ Paralelamente al incremento de la velocidad, la estabilidad de los catalizadores también ha sido mejorada y actualmente existen catalizadores con ligandos orgánicos que pueden superar los 100,000 ciclos manteniendo su naturaleza intacta.⁴ En el presente trabajo han sido sintetizados una serie de Ru-bda complejos con distintos ligandos axiales.⁵ Mediante estudios electroquímicos y DFT, se ha demostrado que son las interacciones supramoleculares entre los ligandos axiales, y no los efectos electrónicos, quienes controlan la velocidad de generación de oxígeno en disoluciones homogéneas con CAN como oxidante a pH 1. Además, no solo se puede controlar la velocidad de la reacción sino también el orden de la reacción a través de pequeñas modificaciones en los ligandos axiales.



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- 4 L. Wang *et al.*, *Chem. Commun.*, **2014**, *50*, 12947
- 5 C. Richmond *et al.*, *Chem. Eur. J.*, **2014**, *20*, 17282

Elucidation of action mechanisms of lubricant additives

CO-16

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Lubricants play a crucial role in reducing wear, friction, oxidation and in heat removal in moving parts of all kinds of machinery. It also increases life of contact surfaces, saving millions of dollars in equipment and providing the required performance of moving parts in engines, gearboxes, shafts, bearings, etc. Modern lubricants consist of a base oil, that can be mineral or synthetic, and a number of additives, that are used to supplement the limitations of lubricants and to enhance the performance of base oils.

In this work, we are mainly studying three kinds of additives: friction modifiers (FM), anti-wear agents (AW) and extreme-pressure additives (EP). They are known as film forming additives. We are studying the nature of this film by several techniques, like XPS, SEM and TEM of abraded particles of the films, in order to elucidate the action mechanism of the additives.

The main elements involving the films are Fe (from the steel substrate), Mo, S and P. However, there are other elements in lower proportions: Ca, Mg, Na and B. The work consists in the tribological testing of the lubricants, including friction and wear evaluation, and characterizing the films formed (Figure 1). This information, along with the characterization of the fresh additives, will enlighten us about the action mechanism.



Figure 1. Left, SEM image (both SE and BSE) and right, XPS of P 2p edge of the film.

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Diseño y estudio de materiales avandazos autoorganizados basados en líquidos iónicos poliméricos

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La preparación y el desarrollo de materiales funcionalizados nanoestructurados es un área de investigación emergente en diferentes campos de aplicación. Recientemente, los líquidos iónicos poliméricos (LIPs) se han convertido en compuestos de gran interés para el diseño y la obtención de nuevos materiales multifuncionales y autoorganizados.^{1,2}

Los LIPs son estructuras macromoleculares formadas por repetición de unidades de líquidos iónicos (LIs) conectadas a través de un esqueleto polimérico por lo que presentan las propiedades y aplicaciones de los LIs y de los materiales poliméricos. La gran diversidad estructural según la naturaleza química del LI y el adecuado autoensamblaje de estos elementos estructurales permite el diseño de diferentes materiales con interesantes propiedades y aplicaciones.³

En este contexto, en esta comunicación se presentan las diferentes estrategias utilizadas para el diseño de nuevos materiales LIPs. En particular, el empleo de polímeros RAFT basados en *p*-clorometilestireno permite la preparación simple de LIPs mediante su modificación con unidades de imidazolio. Gracias a su elevada modularidad (anión, catión, etc...) se han obtenido LIPs con propiedades termosensibles con transiciones de fase tipo LCST.⁴ Además, son capaces de estabilizar AuNPs y estas AuNP-LIPs han demostrado ser sistemas multicatalíticos. También es posible su procesabilidad mediante electrospinning para obtener membranas de diferente polaridad con aplicación en procesos de separación.

Agradecimientos: Ministerio de Ciencia e Innovación (FPU12/00667), Generalitat Valenciana (GV- PROMETEO 2012/020) y UJI-P1-1B2013-37

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³ W. Xu, P.A. Ledin, V.V. Schevchenko, V.V. Tsukruk, *ACS Applied Materials and Interfaces*, **2015**, 7, 12570

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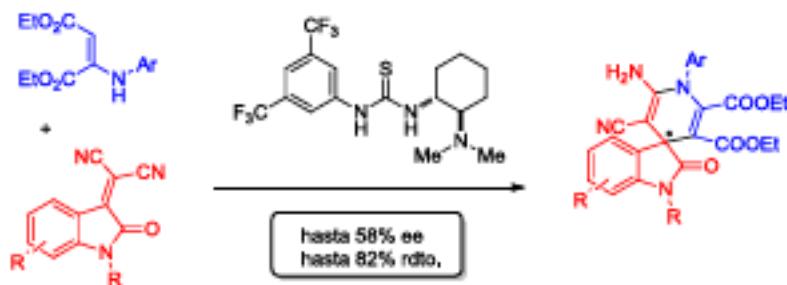
Síntesis organocatalítica de 2-oxoespiro-[indol-3,4'-(1',4'-dihidropiridinas)] quirales

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El desarrollo de nuevos procedimientos para la síntesis de derivados de espirooxindol ha suscitado recientemente un gran interés.¹ Estas estructuras de gran complejidad, se encuentran en muchos productos naturales con interesantes propiedades biológicas.² Además, los derivados de 1,4-dihidropiridina también están presentes en una gran variedad de productos naturales activos.³ Como es bien sabido, el control de la enantioselectividad en la síntesis de estos compuestos supone un reto que ha impulsado el desarrollo de numerosos proyectos dentro del campo de la investigación química. Todo esto unido a la creciente demanda de procesos químicos sostenibles, han inspirado el trabajo que se presenta en esta comunicación.

Así pues, el reto asumido en esta investigación ha sido desarrollar por primera vez, una síntesis organocatalítica y enantioselectiva de espirooxoindoles derivados de 1,4-dihidropiridina.⁴ Se han obtenido enantioselectividades prometedoras y buenos rendimientos, por lo que este trabajo supone un buen punto de partida para el estudio de estas interesantes moléculas, altamente funcionalizadas.



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Tailoring 2D Nanoporous Networks with Persistent Hydrogen-bonded Macrocycles

CO-19

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An innovative methodology^[1-3] based on **molecular self-assembly** for the nanostructuration of surfaces able to selectively recognize functional π-conjugated guest molecules will be presented. The synthesis of different DNA-based derivatives will be described.^[4] The self-assembly process undergone by such versatile molecular tectons into rectangular tetramer macrocycles *via* selective H-bonding between complementary nucleobases, at the solid-liquid interface,^[1] will be explained. These **2D porous monolayers**, as well as their ability to host appropriate guests, will be studied by Scanning Tunneling Microscopy (Figure 1).

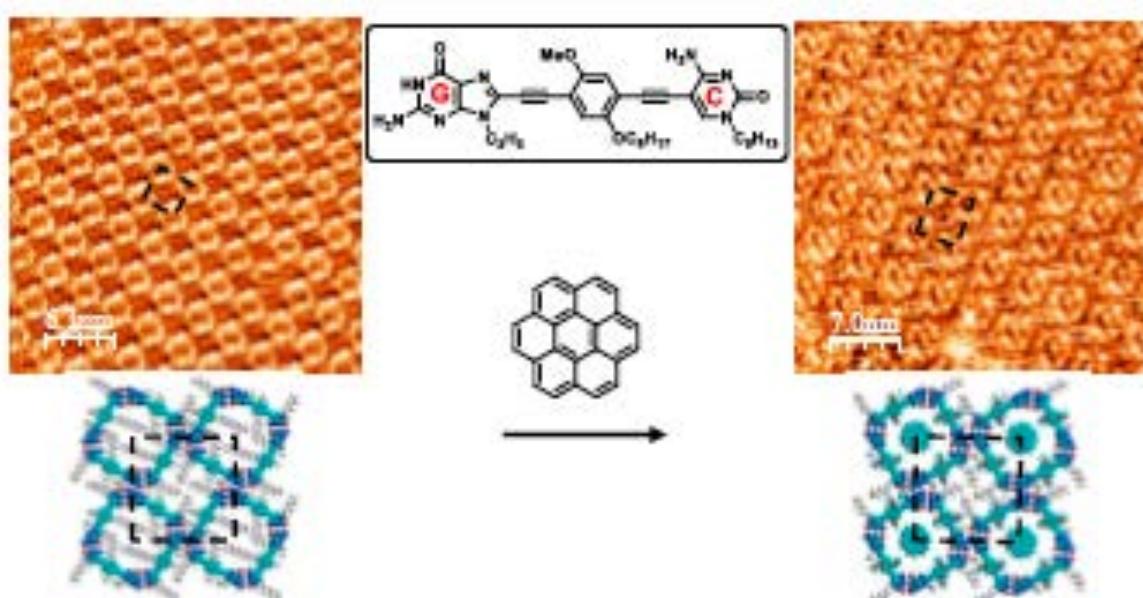


Figure 1: Self-assembled network of cyclic tetramers (left) and host-guest system (right) observed by Scanning Tunneling Microscopy at the octanoic acid/HOPG interface.

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- [2] C. Montoro-García, J. Camacho-García, A. M. López-Pérez, N. Bilbao, S. Romero-Pérez, M. J. Mayoral, D. González-Rodríguez, *Angew. Chem. Int. Ed.* **2015**, *54*, 6780–6784.
- [3] C. Montoro-García, J. Camacho-García, A. M. López-Pérez, M. J. Mayoral, N. Bilbao, D. González-Rodríguez, *Submitted*.
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Design, synthesis and development of potential antimalarial drugs from thiazole derivatives.

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Malaria is a disease caused by parasites of the *Plasmodium* genus and transmitted by the bite of the female *Anopheles* mosquito,¹ which affects nearly 40% of the global population. Although malaria has been widely eradicated in many parts of the world, the global number of cases continues rising, because the prevention and cure of this disease depends primarily on the administration of a small number of drugs, whose effectiveness is continuously threatened due to the rapid spread of malaria parasites that are resistant to antimalarial drugs, especially chloroquine and artemisinin which are by far the most effective and frequently used compounds.^{2,3}

The development of new drugs against malaria has been neglected since the 1970s, but in recent years, due in part to the support of public funding programs, the interest in the development of new antimalarial drugs has been renewed.

In this communication, we are describing a synthesis of thiazole derivatives in several steps. These compounds exhibit structural features and promising properties to potentially become drugs against this disease.⁴

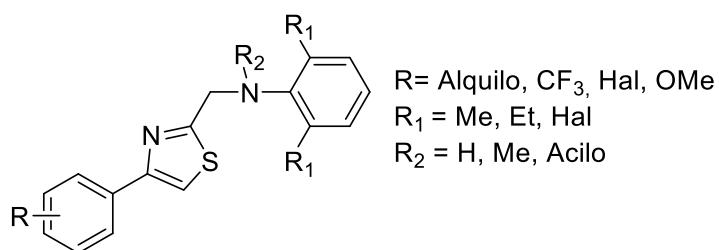


Figure 1: General structure of the synthesized compounds

This compound is a thiazole derivative, substituted mainly at carbon-2 and at carbon-4. It also allows functional modifications on carbon-5 of the heteroaromatic ring. This base structure meets Lipinski rules,⁵ has a suitable molecular weight and allows the introduction of structural variety easily.

Once we synthesized and characterized these compounds, we proceeded to evaluate their pharmacological activity in collaboration with the multinational pharmaceutical company GlaxoSmithKline. The results showed that they display antimalarial properties.

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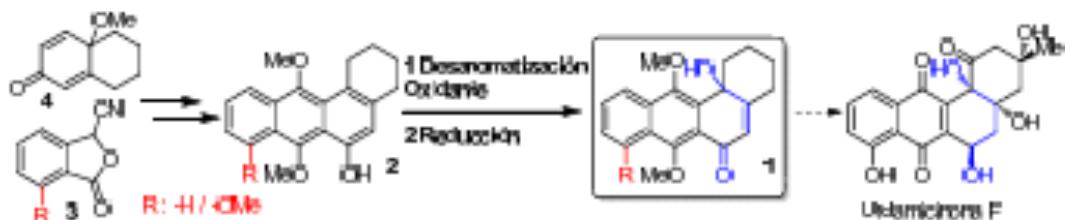
Aproximación a la síntesis de anguciclinonas con hidroxilos angulares mediante el uso de Oxono® como fuente de oxígeno singlete

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Las Anguciclinonas son un grupo de moléculas naturales que presentan un gran interés sintético ya que poseen un amplio rango de propiedades biológicas.¹ Dado que la síntesis de derivados que poseen –OH angulares ha sido poco estudiada,² nos planteamos abordar la síntesis de modelos tetracíclicos de este grupo de anguciclinonas usando la metodología de desaromatización oxidante de p-alquil fenoles mediante Oxono, desarrollada por nuestro grupo de investigación.³

Así, el esqueleto tetracíclico angular de benzo[*a*]antraquinona, característico de este tipo de moléculas, se obtuvo a partir de una anulación de Hauser⁴ entre las correspondientes cianofatlidas **3** y el quinol bicíclico **4**. Los *p*-quinoles objetivos **1** se consiguieron a través de una desaromatización oxidante con Oxono en medio básico, seguida de reducción del *p*-peroxiquinol intermedio.⁵ Una vez puesto a punto y optimizado el estudio modelo, se aplicará a , para completar la síntesis total de este producto natural.



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Light-driven Co-catalyzed reduction of olefins using water as a source of protons

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A prerequisite for a sustainable society is the development of new efficient, cheap and greener synthetic methods. Among all the possibilities, the use of sun light as a source of energy is envisioned as one of the most sustainable alternatives. Herein we report the expansion of the catalytic activity of cobalt complexes such as $[\text{Co}(\text{Py}_2^{\text{Ts}}\text{tacn})(\text{OTf})](\text{OTf})$, initially developed for the light-driven water reduction to hydrogen¹, in combination with photoredox catalysts and sacrificial electron donors towards new organic transformations using light as a source of energy and water as a source of protons. In addition, mechanistic studies are also performed to get more insights on the mechanism involved by characterisation of intermediates, kinetics and DFT studies.

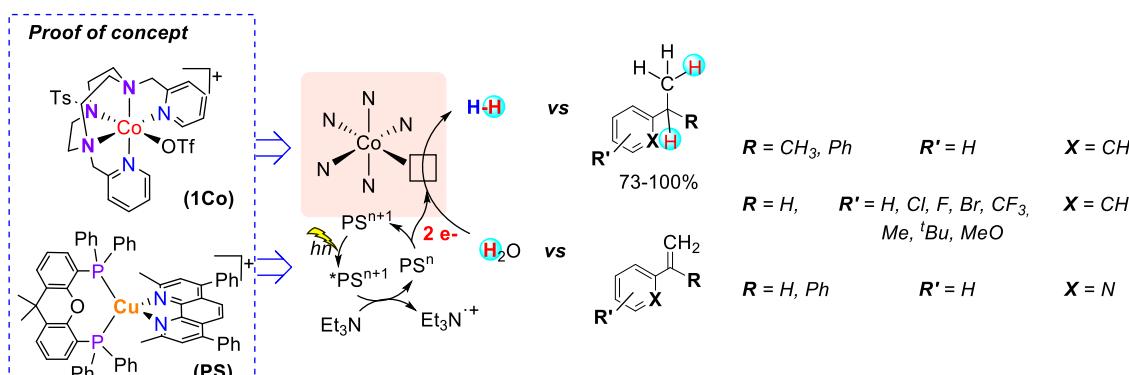


Figure 1. Expansion of the catalytic activity of $[\text{Co}(\text{Py}_2^{\text{Ts}}\text{tacn})(\text{OTf})](\text{OTf})$ (**1Co**).

We have been able to reduce a wide range of monosubstituted and disubstituted aromatic olefins with either electrowithdrawing and electrodonating groups to their corresponding alkanes, using $[\text{Co}(\text{Py}_2^{\text{Ts}}\text{tacn})(\text{OTf})](\text{OTf})$ as catalyst, $[\text{Cu}(\text{bathocuproine})(\text{Xantphos})](\text{OTf})$ as photosensitizer, Et_3N as a source of electrons, light as a source of energy and water as a source of protons. In addition, several modifications of the metal centre have shown different selectivity towards H_2 formation or olefin reduction.

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Paving the way to novel phosphorus-based architectures: a non-catalyzed protocol to access six-membered heterocycles

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Phosphorus-based materials exhibit properties that are inaccessible from other synthetic systems. The presence of phosphorus atoms into π -conjugated systems renders materials with electron-accepting properties,^{1a} a myriad of coordination reactions^{1b} and the possibility to keep control over the intermolecular interactions through phosphorus post-functionalization.¹ In the last years, these singular characteristics have particularly attracted the attention of the materials science community. Thus, recently reported phosphorus containing materials have demonstrated, for instance, great potential to access intriguing phenomena such as thermochromism,² electrochromism² and piezochromism.³ Currently however, this field of research requires accessing novel architectures to fully exploit the potential of phosphorus heterocycles and open up new research horizons.

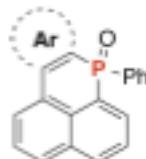


Fig. 1. Phosphaphenalene

In this communication, I present a new non-catalyzed protocol to access fused, six-membered heterocycles. The versatility of this reaction allows preparing novel phosphaphenalene derivatives with different aromatics in the periphery (Fig. 1). The unique aromaticity of the phosphorus-containing phenalene structures leads to unusual photophysical properties. Thus, I will furthermore discuss the structure/properties relationships. Altogether, the latter phosphorus-based architectures introduce new opportunities into the field of functional materials.

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**In solution and on surface studies of novel
polychlorotriphenylmethyl (PTM) radicals for molecular
electronics applications**

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Polychlorotriphenylmethyl (PTM) radicals are persistent organic radicals with appealing properties for molecular electronics and molecular spintronics. The central methyl sp^2 carbon is the spin bearing atom and the bulky substituents protect the paramagnetic centre from undesired reactions. Due to their high stability, these radicals can be easily functionalized, allowing tuning the properties of the final compound. Moreover, the neutral paramagnetic radical can be reversibly reduced or oxidized to two ionic diamagnetic species, the cation and the anion, respectively.¹ During the last years, PTM derivatives have been used in the preparation of self-assembled monolayers (SAMs) for the preparation of robust molecular memories.² In addition, with the aim of studying the charge transport through these radicals, thiolated PTM radical derivatives have been used to successfully functionalize gold surfaces. In molecular electronic devices where the active functional molecule is covalently grafted to the metal electrodes, the stability and directionality of the molecule-metal bond plays a crucial role. Recent studies have shown very promising results by exploiting the C-Au bond instead of the commonly used S-Au.³ For this, the synthesis of a new PTM radical derivative bearing a terminal alkyne group has been carried out. Stable SAMs based on this derivative and anchored to gold through the formation of a C-Au bond have been prepared and characterized by different surfaces techniques. In addition to these studies, the homocoupling reaction between two PTM-alkyne molecules and the reduction of one of the radical centres to the anion form has been carried out to give rise to a mixed-valence system. The aim of this second part of the work is to study in solution the intramolecular electron transfer (IET) between the donor and acceptor units through an olygoyne bridge. To perform these studies we have used the electron paramagnetic resonance (EPR) spectroscopy.

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Stereoselective direct aldol reaction of α -keto amides catalyzed by ureidopeptide-based Brønsted bases

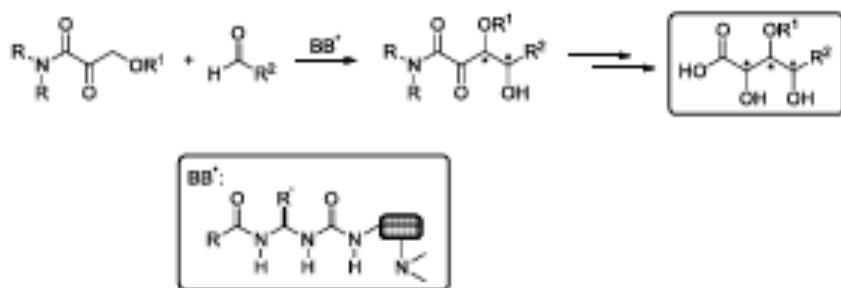
CO-25

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The aldol reaction constitutes one of the most powerful methods for the construction of α -hydroxy carbonyl units that are fundamental building blocks in the synthesis of biologically active and pharmaceutically important compounds.¹ Given their synthetic utility, a tremendous effort has been made to develop catalytic asymmetric direct aldol reactions since the first report by Shibasaki.² Nevertheless, scarce examples have been described employing poor acidic aldol donors, such those having a carboxylic oxidation state, to produce α -hydroxy carboxyl compounds. On the other hand, there are no examples of BBs catalyzed direct aldol reactions using enolizable aldehydes as aldol acceptor due to their tendency to produce self-condensation.

In this communication, we present an organocatalyzed direct aldol reaction of α -keto amides and enolizable aldehydes that provides polyoxygenated fragments which have not been prepared by means of catalytic and stereoselective aldol reactions yet.³ Main problems related to the stereoselective generation of the enolate, face shielding of the aldol acceptor, reactivity and prevention of the aldol condensation have been addressed by employing a new family of bifunctional BBs, recently described by our group.⁴



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Hybrid organic-inorganic materials for integrated optoelectronic devices

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Hybrid organic-inorganic optoelectronics are heralded as the next generation of lighting and photovoltaic technologies.¹ In this context, our efforts encompass three main actions, namely the development of suitable third generation of electroluminescent materials for ionic-based lighting devices, the application of nanocarbon-based hybrids in solar cells and lighting devices, and the development of bio-inspired components for lighting, energy conversion, and diagnostic applications.

Herein, the implementation of the third generation of materials – *i.e.*, lighting perovskite nanoparticles, small molecules, and copper(I) complexes – for light-emitting electrochemical cells (LECs) will be presented as new approaches to develop deep-red, blue, and white lighting sources.² Next, carbon nanohorns will be shown as new integrative components for preparing new nanocarbon-hybrid dye-sensitized solar cells (DSSCs), resulting in several breakthroughs, namely i) the enhancement of charge transport and collection in the electrodes, ii) the development of iodine-free, solid-state electrolytes, and iii) the fabrication of platinum-free counter electrodes.³ Finally, a new strategy to stabilize any type of bio-components – *i.e.*, enzymes, fluorescent proteins, etc. – in a rubber-like material was developed. As an example, the latter was applied to fabricate the first bio-inspired hybrid light-emitting diodes featuring a bottom-up energy transfer protein-based cascade coatings. The synergy between the excellent features of fluorescent proteins and the easily processed rubber produces bio-HLEDs with less than 10% loss in luminous efficiency over 100 hours.⁴ Currently, other applications like bio-reactors and ready-to-go-kits are under development in our laboratory.⁴

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Síntesis, caracterización estructural y magnética de un compuesto tetranuclear Zn₂Dy₂ con propiedades de molécula imán

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Los compuestos de coordinación con iones lantánidos han sido muy estudiados durante los últimos años debido a sus interesantes propiedades magnéticas y fotofísicas.¹ En concreto, estos sistemas han impulsado de forma determinante la investigación en el campo del magnetismo molecular debido a que muchos de ellos, particularmente de Dy, se comportan como moléculas imán. Estos nanoimanes presentan importantes aplicaciones en campos tales como la espintrónica molecular, el almacenamiento de información de ultra alta densidad y computación cuántica a nivel molecular.² Diversos resultados teóricos y experimentales han mostrado que una buena estrategia para obtener moléculas imán con propiedades mejoradas es la preparación de complejos heteronucleares Zn/Dy. En vista de ello, en la presente comunicación presentamos las propiedades magneto-estructurales del complejo tetranuclear [ZnDy(μ-L)(μ-CO₃)(Ac)]₂·2CH₃CN (Figura 1) que presenta propiedades de molécula imán (L is un ligando compartmental quirial que se obtiene por la condensación 1:2 del 1R,1R-diamino ciclohexano con la ortovanilina)

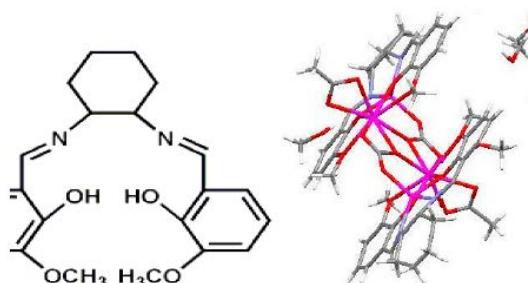


Figura 1

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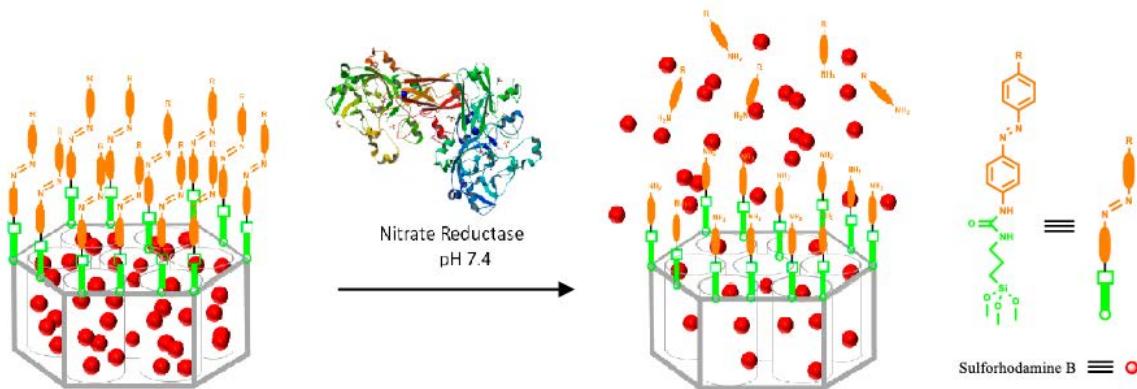
Mesoporous systems capped with an azoaniline derivative for transport and controlled delivery applications

CO-28

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Mesoporous silica (MS) has proven to be an excellent solid support owing to its superior properties such as good biocompatibility, high rigidity, chemical stability, high surface areas, uniform and tailored made morphologies and pore size, as well as facile functionalization as surfaces and pores.[1] Materials derived from the combination of MSs as solid supports and molecular gates as movable entities have emerged in the literature and play prominent roles in materials science nowadays.[2] In this work, we chose to synthesize a molecular gate, based on MSs whose surface is functionalized with a diazobenzene derivative. It is known that the azo bond is specifically cleaved by the action of the gut microbiota (azoreductases enzymes) in the large intestine so a molecular gate containing this functional group would be useful for controlled drug release in the colonic mucosa, for example treatment of Crohn's disease.[3] The molecular gate has been loaded with a dye (sulforhodamine B) in order to study the release under reducing conditions by UV-vis and fluorescence.



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Ruthenium (ii) 1,2,3-triazolylidene carbenes: synthesis, structure and catalytic activity

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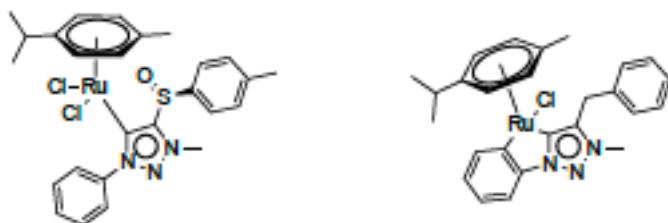
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N--Heterocyclic carbenes (NHCs) are currently powerful tools in different areas of Chemistry, such as ligands in catalysis.¹ Sulfinyl groups can either coordinate to the metal centre or create a vacant position for the catalytic process which make them a very interesting group. Despite this exceptional feature, there are not so many examples in literature of NHCs bearing a sulfoxide functionality.²

Herein, we describe the synthesis of new chiral ligands based on 1,2,3-triazole incorporating an enantiomeric pure *S*-*para* tolyl sulfinyl moiety on the C-4.

The ruthenium complexes containing the mentioned ligands have been tested in hydrogen transfer reactions.³ With the aim of proving a different behaviour due to the presence of the sulfoxide group, the catalytic activity of these new complexes has been compared with the analogous containing different groups in C-4.



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Towards new glycosyltransferase ligands

CO-30

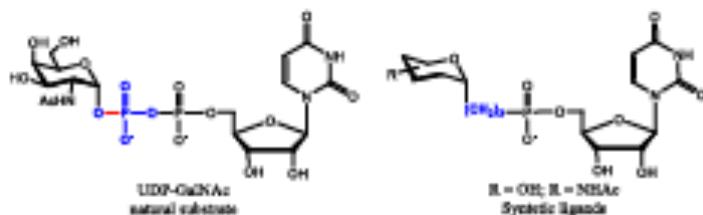
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GalNAc-T2 is an enzyme that catalyze the transfer of N-Acetylgalactosamine from the donor substrate UDP-GalNAc to the acceptor hydroxyl groups in mucine-type proteins. It belongs to a wide family of glycosyltransferase of which twenty isoforms are present in the human body. At the present time, despite the importance of this enzyme, involved in several metabolic disorders^[1]; very few binding substrates exists for this family of enzymes^[2] and no inhibitors have been reported.



Here, we propose a new method to generate a new family of α -C-glycoside ligands, based on the reactivity of the phosphonate group, miming the natural substrate but suppressing one phosphate function; leading to a new class of non-too polar and non-hydrolyzable compounds. We standardize the synthesis on a wide pool of different carbohydrates. Afterwards a docking study confirmed the binding capability of these new molecules with the GalNAc-T2 enzyme and a biological assay and a crystal structure validated the in-silico predicted binding capability.



This method can be efficiently used to synthesize a wide variety of new compounds, and is easily extendable to different class of molecules and nucleosides to find new glycosyltransferase ligands.

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Broad band Microcoils for inline/insitu reaction monitoring

CO-31

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Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful analytical technique employed in many areas of research. NMR spectroscopy provides both, qualitative and quantitative information from a reaction, and is a non-invasive analytical method, among other advantages. When dealing with small amount of material, there is a limitation in sensitivity in comparison with other techniques. The use of miniature NMR detectors, termed "microcoils", is an interesting approach to overcome this "weakness". Different microcoil geometries, planar, solenoidal, microslot and stripline can be used, allowing the analysis of mass-limited and volume-limited samples with an improvement of sensitivity compared to the conventional NMR probe [1]. Planar microcoils are easier to integrate in microfabrication processes allowing a precisely controlled geometry and an accurate coil sample positioning. Hence, planar microcoils can be integrated on top of a glass substrate defining a microfluidic NMR device called "NMR-chip".

We are focused on the use of NMR-chips for different applications. On one hand, we keep optimizing the concept of NMR-chip in terms of looking for the highest sensitivity and resolution to open a wider window of applications, and on the other hand, the different NMR-chip generations are hyphenated to alternate modes of heating/irradiating a reaction mixture for in-situ/ in-line reaction monitoring. These NMR-chips offer, among others, two fascinating aspects: In terms of NMR, the broad-band character for these planar microcoils has allowed us the acquisition of all kind of homo- and heteronuclear 1D & 2D NMR experiments and with a single non-tuned microcoil [2]. In relation with their properties as monitoring tools, the capability of the NMR chip of analysing very small volume of sample enables the acquisition of data in a rapid manner, allowing a fast determination of kinetic parameters within a single on-flow experiment and only using microliters of sample [3]. We will illustrate the latest developments in optimization of the NMR probe, i.e. with the incorporation of pulsed field gradients and its combination with broad- band character, and the hyphenation of these NMR detectors to other energy sources for activation of chemical reactions, i.e. a continuous-flow microreactor platform or UV-VIS devices for in-line and/or in-situ monitoring of different types of chemical reactions.

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Bodipy functionalised mesoionic NHC complexes: synthesis & fluorescence modulation

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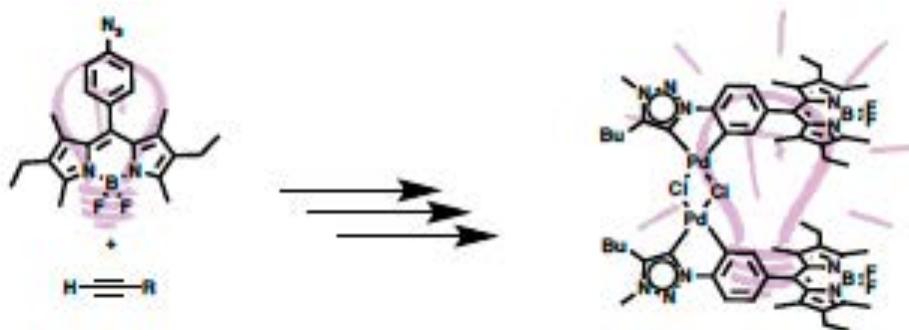
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Due to their excellent thermal and photochemical stability combined with their spectroscopic properties, boron-dipyrromethene (BODIPY) compounds have become valuable materials with numerous applications in materials science and medicinal biology, such as, building blocks for energy transfer cassettes, artificial light harvesting complexes, fluorescent switches, chemosensors and sensitizers for dye sensitized solar cells.^[1]

N-heterocyclic carbenes (NHCs) have had a huge impact on organometallic chemistry and homogeneous catalysis. Because of their exceptional donor properties and the ease of wingtip tunability, a vast range of metal--based catalysts have been prepared using NHC ligands.^[2]

Hence, we focused on combining a known BODIPY moiety with mesoionic NHCs^[3] to prepare transition metal complexes and study their new electronic properties. We did demonstrate that the BODIPY chromophore is an excellent probe for monitoring organometallic transformations at the NHC unit.



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Polycyclic aromatic hydrocarbons (PAHs) are receiving a great deal of attention because of their increasingly better performance in organic electronic applications. Among these, PAHs containing N atoms (N-PAHs) are particularly interesting since their electronic structure, stability, solubility, and supramolecular organization can be modulated by varying the number and position of N atoms.

In general, PAHs are planar structures but they can adopt twisted conformations as the result of the steric strain induced by overcrowding or congestion in key positions of the aromatic core. *twisted*-PAHs have shown enhanced solubility and unique optoelectronic and chiroptical properties as an effect of their distorted molecular structure.

We have developed a general strategy that provides access to a new family of *twisted*-N-PAHs (0D) with different twist angles by introducing silyl groups with different size and rigidity, providing direct experimental correlation between twist size and properties. In addition, this methodology has been successfully implemented in the preparation of low-dimensional materials (1D and 2D). The most recent advances of these materials including synthetic routes, optoelectronic properties, self-organising properties, and potential applications will be discussed.

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Chain walking of allylrhodium species towards esters during rhodium-catalyzed nucleophilic allylations of imines

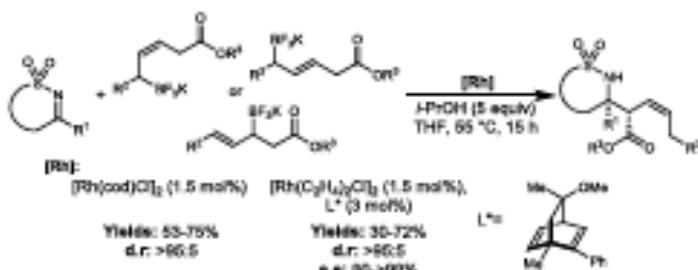
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As part of our interest in enantioselective Rh-catalyzed nucleophilic allylations with allylboron reagents¹ we discovered an isomerization of allylrhodium intermediates, resulting in more complex allylrhodium species that would otherwise be difficult to access.

Therefore, we present a family of isomeric ester containing potassium allyl trifluoroborates as the precursor of a common active allylrhodium intermediate that reacts, regioselectively α to the carbonyl, with cyclic imines in the corresponding allylation reactions. The obtained amines are isolated in good yields and excellent diastereoselectivities. It is also possible to perform a kinetic resolution of the starting racemic allyl trifluoroborates by employing a chiral diene ligand, occurring through a highly stereospecific reaction which produces the corresponding amines in good yields full diastereoselectivity and excellent levels of enantiopurity (Scheme 1).



Scheme 1

Moreover, we carried out mechanistic studies which evidence that allylrhodium intermediate isomerization occurs through a β -Hydride elimination-Hydrorhodation sequence allowing the allylation at the remote α to the carbonyl position.

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Selective recognition and sensing of succinate vs. other aliphatic dicarboxylates

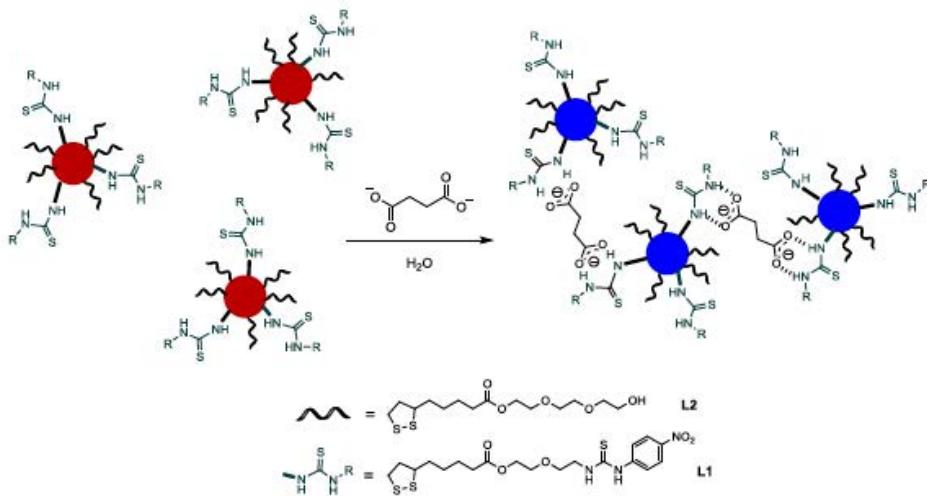
CO-35

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In recent years, functionalized gold nanoparticles (AuNPs) have attracted growing attention in colorimetric sensing in the chemical and biological sciences owing to their tunable photophysical properties.[1] The visual-sensing ability of AuNPs relies on changes in the surface plasmon resonance (SPR), which is dependent on the aggregation state and the surface morphology. Generally, the aggregation of AuNPs in solution through analyte-triggered interparticle cross-linking leads to a change in color from red to blue or purple, which is useful for observing molecular-recognition events. The interparticle cross-linking requires a “three-body” molecular-recognition event between a ditopic analyte and two nanoparticles.[2] Such molecular interactions can be dependent on the directionality of two interacting end groups of the analyte, and thus may be used for specific sensing purposes such as the selective sensing of organic compounds.

Dicarboxylate anions are biologically important molecules and their detection in aqueous media is of high interest.[3] We have synthesized gold nanoparticles functionalized with thiourea derivates as a colorimetric sensing system for dicarboxylate recognition in aqueous media. The sensing paradigm is depicted in the Figure.



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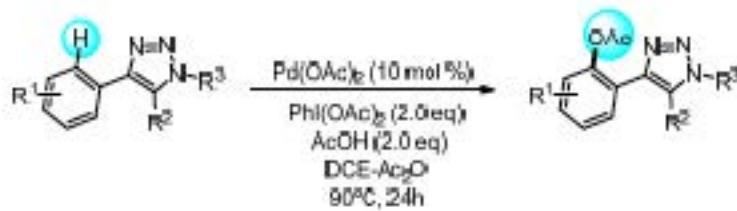
Palladium-catalyzed C(sp²)–H acetoxylation directed by 1,2,3-triazoles

CO-36

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Metal-catalyzed ligand-directed C–H functionalization has been widely exploited to convert proximal unactivated C–H bonds into new carbon–carbon and carbon–heteroatom bonds.¹ In particular, the development of C–O bond forming reactions remains a pressing challenge of prime interest for the assembly of complex molecules.² Although a number of coordinating functional groups have been used to assist such events, the use of 1,2,3-triazoles is comparatively unexplored.³ Owing to the prevalence of 1,2,3-triazole motif in a vast array of medicinally relevant compounds, its key use as directing group could provide a novel late-stage derivatization strategy for the preparation of heterocycle-containing compounds. Herein we describe the efficient Pd-catalyzed C(sp²)–H acetoxylation of a wide variety of 4-phenyl-1*H*-1,2,3-triazole derivatives featuring thus an unprecedented C–H oxygenation event assisted by the triazole ring (Scheme 1).



Scheme 1. Pd-catalyzed C(sp²)–H acetoxylation of 4-phenyl-1*H*-1,2,3-triazoles.

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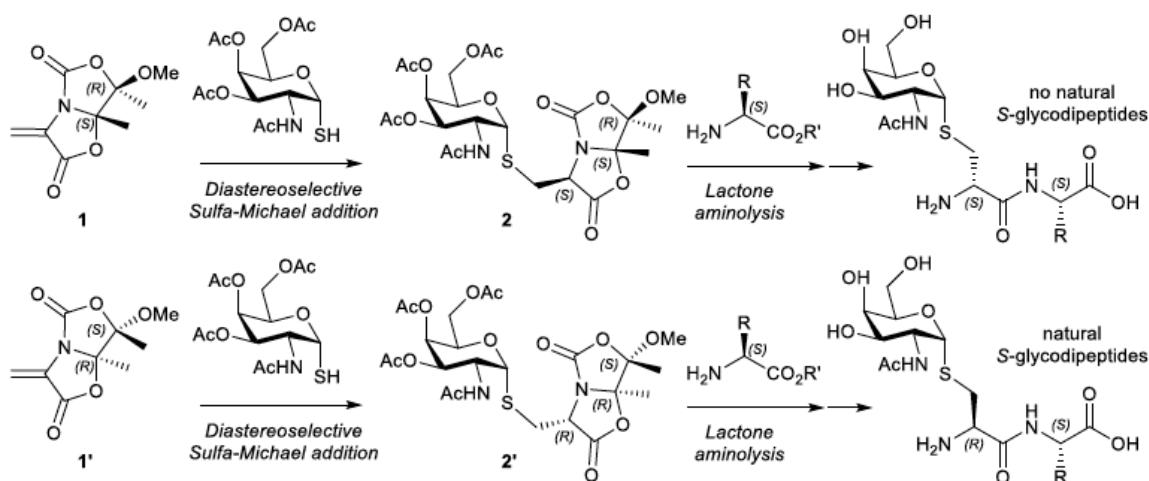
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Synthesis of S-glycodipeptides through sulfa-michael addition and lactone aminolysis sequence

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The importance of S-glycopeptides has been rising during last years. S-glycosylation can be regarded as a new post-translational modification of peptides, key in their biological activities.¹ We recently reported new chiral dehydroamino acid derivatives which presented high yields and stereoselectivities in sulfa-Michael additions.² These chiral derivatives could undergo stereoselective sulfa-Michael reactions with the appropriate protected thiocarbohydrates, as well.³ In order to extend this methodology, we designed new chiral bicyclic acrylate derivatives (**1** and **1'**). These new compounds presents the same reactivity and stereoselectivity of previously reported precursors.³ This fact was shown when compounds **1** and **1'** were reacted with tri-O-acetyl-2- acetamido-2-deoxy-1-thio- α -D-galactose affording the corresponding S-Michael adducts **2** and **2'**. The protection of the carboxylic acid as a lactone opens up new possibilities of nucleophilic attacks. We reacted **2** and **2'** with several amino ester derivatives opening the lactone ring and yielding the respective amides. Therefore, the corresponding free S-glycodipeptides were obtained by this methodology, after acidic hydrolysis.



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Polymolecular assemblies for electronic applications

CO-38

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Organic semiconductors have awakened considerable research interest in the development of electronic devices on account of their great potential. They offer the advantage to be processed by solution methods lowering the production costs, plus the fabrication of light weight, flexible and large area devices in contrast with the actual inorganic counterparts, although their intrinsically lower mobility. Organic materials are based on π -conjugated molecules where the π delocalized electrons are the responsible of the conduction and even if the exact relationship between structure and efficiency is not completely understood, it is known that well-ordered structures and face to face packing of the aromatic moieties with significant intermolecular π -orbital overlap allows for enhanced charge transport properties.

Research in our group focuses on the design of new polycyclic aromatic hydrocarbons and on controlling their supramolecular organization for organic electronic applications [1-4]. We have designed a new method to obtain polymolecular organized assemblies of organic semiconductors based on polycyclic aromatic hydrocarbons like acenes and azaacenes able to recognize each other by supramolecular interactions with an optimal distance, between 3.5 Å and 4 Å, for the electrical conduction. The characterization of these systems was carried out in solution by NMR, UV-Vis and in solid state using X-ray diffraction that confirmed the desired packing of the supramolecular assemblies. Finally, these systems were used in the preparation of organic thin film transistors in order to study their semiconductive behavior.

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C-H bond functionalization of phenyl-substituted benzotriazole using trans-metal trapping chemistry

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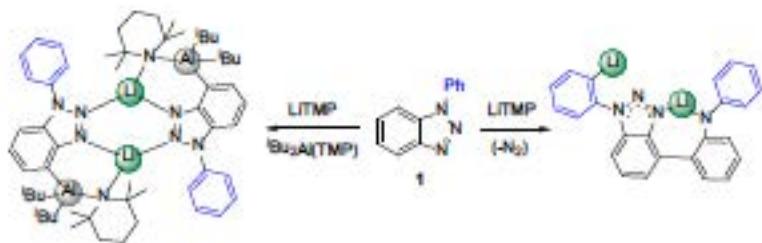
maria.fuentes-dominguez@strath.ac.uk

Previous work from our group has shown that lithium amide LiTMP (TMP = 2,2,6,6-tetramethylpiperidine) does not co-complex with alkyl-TMP-aluminium reagents acting as an effective trans-metal trapping bimetallic system. For instance, the benchmark substrate anisole can be metallated by LiTMP in very low yield (<5%) but in the presence of $^i\text{Bu}_2\text{Al}(\text{TMP})$ the deprotonation becomes near quantitative.¹

In this presentation, we report the extension of this methodology toward other aromatic substrates. Benzotriazole ring is a heterocyclic scaffold present in different interesting synthetic molecules. One of the challenges in this area is to bring about the regioselective functionalization of benzotriazoles.

Mongin recently reported the deproto-metallation of 1-aryl-1H-benzotriazoles using in situ mixtures of LiTMP and $\text{ZnCl}_2\cdot\text{TMEDA}$.² To gain insight into the intermediate organometallic chemistry behind such metallations, we have screened 1-phenyl-1H-benzotriazole **1** with the bimetallic base mixtures LiTMP/ $\text{ZnCl}_2\cdot\text{TMEDA}$ and LiTMP/ $^i\text{Bu}_2\text{Al}(\text{TMP})$. This investigation has revealed the first structurally characterised metallo derivatives of 1-aryl-1H-benzotriazoles.

We show that while reaction with the harsh base LiTMP leads to ring opening side reactions of the trinitrogen heterocycle, in contrast applying the kinetically fast combined LiTMP/ $^i\text{Bu}_2\text{Al}(\text{TMP})$ trapping protocol leads to stabilised, ring-intact luminated products which can smoothly undergo quenching with electrophiles.



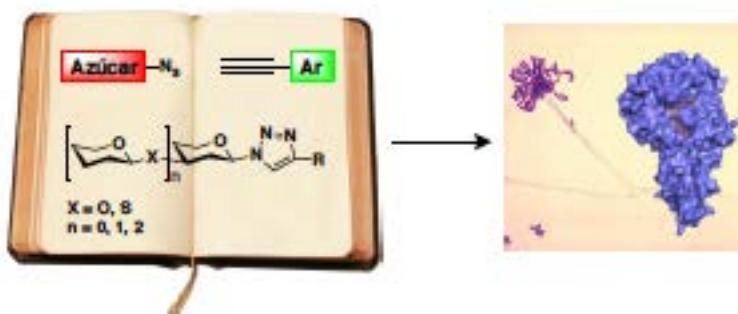
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Obtención de nuevos inhibidores enzimáticos para transglicosilasas de *Aspergillus fumigatus* mediante click-chemistry.

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Se estima que alrededor de 1.200 millones de personas en todo el mundo han sufrido alguna infección fúngica. La mayor parte son poco invasivas, pero algunas especies de *Candida* o *Aspergillus* son más peligrosas y llegan a matar entre 1,5 y 2 millones de personas al año (más que la malaria o la tuberculosis).[1]

Proponemos un diseño racional de glicomiméticos que tendrían como diana transglicosilasas de la pared celular del hongo. Hasta ahora hemos desarrollado compuestos que funcionan como inhibidores de *Saccharomyces cerevisiae* Gas2 (ScGas2).[2]

Recientemente, se han preparado azidas de $\beta(1\rightarrow 3)$ oligosacáridos y varios alquinos con residuos aromáticos. Mediante reacciones click catalizadas por cobre se ha sintetizado una biblioteca de oligosacáridos modificados que han sido estudiados mediante diversas técnicas (STD-RMN, inhibición enzimática, fluorescencia, cristalográfia) tanto en ScGas2 como en enzimas de *Aspergillus fumigatus*.

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A mechanistic approach to the overpotential control in Cu-based water oxidation catalysis.

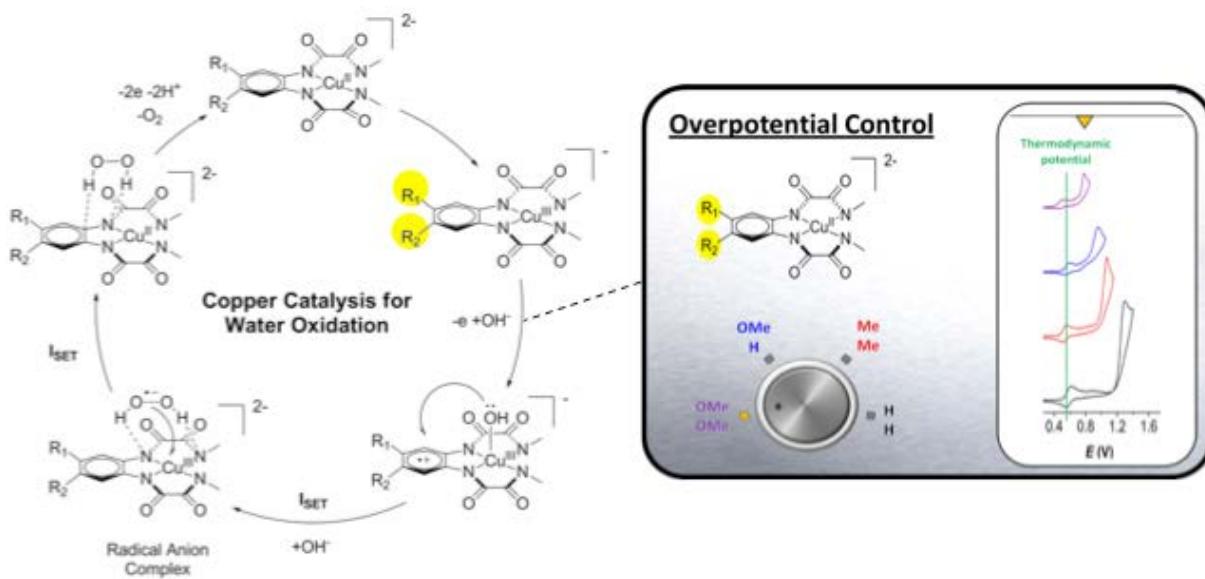
CO-41

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Water splitting is one of the most promising ways for solving the energetic problem because with the appropriated technology, sunlight could be used to produce oxygen and hydrogen (the cleanest fuel) from water. The development of greener, cheaper and more efficient water oxidation catalyst (WOCs) is still a challenge. First row transition metals are promising candidates for this reaction but too many factors must be controlled such as the solubility in water, the stability and the overpotential needed for the water oxidation. For this reason, a mechanistic understanding of the reaction could be very useful for the rational design of new WOC.

Herein, we present a new group of mononuclear copper catalysts based on redox non-innocent ligands.¹ We explored the mechanism of this reaction, and we confirm the involvement of the ligand in the oxidation of the catalyst. We designed *in silico* modifications of the ligand that were checked experimentally. Including donor substituents that stabilized the ligand centered radical allowed us to reduce the water oxidation overpotential by more than 500 mV, reaching a record low overpotential of 170 mV. The theoretical study also showed the important role of the copper center as a single electron transfer catalyst.



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Approaches to the synthesis of tripartin

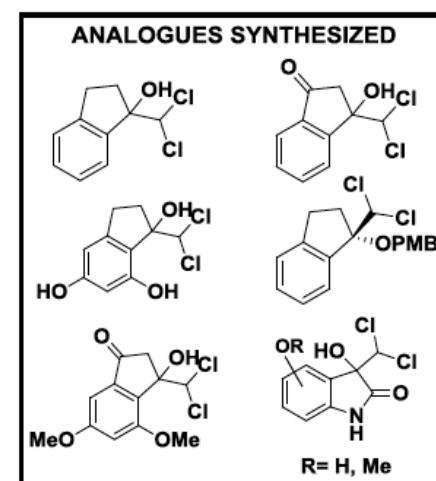
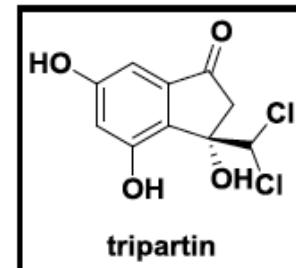
CO-42

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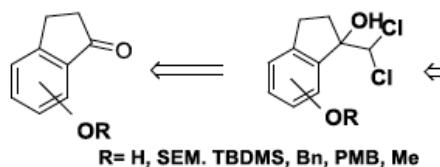
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Histone methylation is one of the most expressed epigenetic modifications in diseases with high impact on society such as leukemia, breast and prostate cancers and inflammation. This process is responsible for regulating transcription, maintaining genomic integrity and contributing to epigenetic effects. The methylation of specific lysine residues is regulated by the competing action of two enzymes: histone methyltransferases (HMTs) and histone demethylases (KDMs). Nowadays only a few KDM selective inhibitors have been identified as potential therapeutic targets. The natural product tripartin, a selective inhibitor of histone demethylase KDM4 in HeLa cells, has been isolated from a culture of *Streptomyces sp.* associated with a larva of the dung beetle *Copris tripartitus* Waterhouse.¹

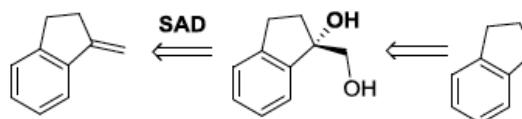
It is considered that the dichloromethylhydroxyindanone group is essential for the biological activity of tripartin. As this functionality could mimic the 2OG cofactor of KDMs we have addressed the synthesis, following different strategies, of racemic and enantiopure tripartin and analogues with similar structures whose biological activity as histone demethylase inhibitors is under evaluation. The synthesis of the indanone moiety will be presented, as well as an enantioselective alternative based on the Sharpless Asymmetric Dihydroxylation (SAD).



RACEMIC:



ENANTIOSELECTIVE:



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Luminescent NHC gold complexes from propargyl functionalised imidazolium salts

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Allenyl-gold complexes derived from propargyl functionalised phosphonium salts are a novel class of organometallic compounds which were recently found to be stable and isolable, displaying an interesting regioselectivity[1]. N-heterocyclic carbene (NHC) complexes of gold have attracted a lot of attention due to their diverse catalytic, biological, medicinal and optical properties[2-4]. Incorporation of the propargyl fragment into imidazolium salts allows the formation of a series of NHC precursors which also have the capability to form allenyl complexes giving rise to the formation of polynuclear complexes with enhanced optical and biological properties.

A series of propargyl functionalised mono and bis-imidazolium salts have been prepared and from these the corresponding NHC gold complexes have been prepared and characterised. A new method for the preparation of NHC-AuCl complexes using acetylacetone precursors has been developed (Figure 1).

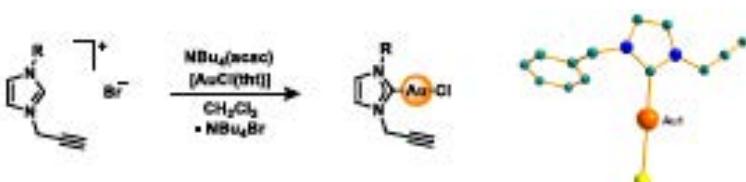


Figure 1. Formation of NHC-AuCl complexes

Studies of the reactivity of the complexes in both the central carbene functionality and the propargyl side arms together with the emissive and biological properties of the complexes have been carried out.

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Charge transport in Metal-Organic Framework ultrathin films

CO-44

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In the last decade, applications for Metal-Organic Frameworks (MOFs) have been found in gas storage, separations, sensing and catalysis. Recently, there is a growing interest in MOFs' optical and electrical properties. However, research regarding their integration in optoelectronic devices is yet to fully blossom.^[1] Although the general insulating character of MOFs has limited development, in the last year electrical conductivity has been reported for MOF thick films.^[2-4]

Investigation of the electrical conductivity of MOF thin films at the nanoscale (<100 nm) remains still a challenge due to the synthetic difficulties in producing smooth films with homogenous coverage and low roughness with nanometric accuracy. We report the fabrication of high-quality films of NAFS-1^[5] (below 10 nm) by using a hybrid approach that involves sequential transfer by using the Langmuir-Blodgett (LB) technique of pre-assembled 2D nanosheets to substrates modified with a Self-assembled Monolayer (SAM) of alkylphosphonic acid molecules.^[6] Our Hg-drop electrode junction studies are indicative of moderate electrical conductivity in ultrathin MOF films for the first time and suggest hopping mechanism as the most likely origin.

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Comunicaciones Flash Póster

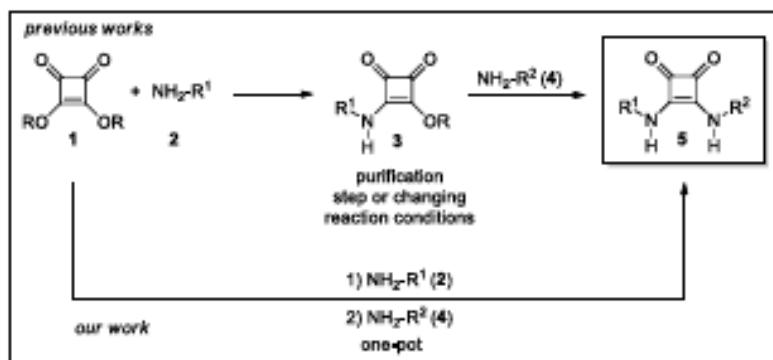
One-pot synthesis of unsymmetrical squaramides and their application in organocatalytic Henry reactions

FP-1

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In this work, we developed the first one-pot synthesis of unsymmetrical squaramides. Following this methodology, we prepared the most common bifunctional squaramide-based organocatalysts, obtaining in most cases better yields compared to those obtained in the analogous step-by-step syntheses (Scheme 1).[1] Also, we developed additional syntheses of squaramides that have been used in other areas besides catalysis, such as biologically active squaramides in medicinal chemistry. This new synthetic approach could make the use of squaramides more appealing for different industrial processes. Furthermore, using this one-pot approach, we synthesized new chiral squaramides that were employed in the asymmetric Henry reaction.[2] Diverse enantiomerically enriched nitroaldol products were obtained in good yields and enantioselectivities (up to 94% ee) under mild conditions and using a low catalyst loading of 0.25–2.5 mol%. This represents the lowest catalyst loading that has been used for this type of reaction in the organocatalytic field up to date.



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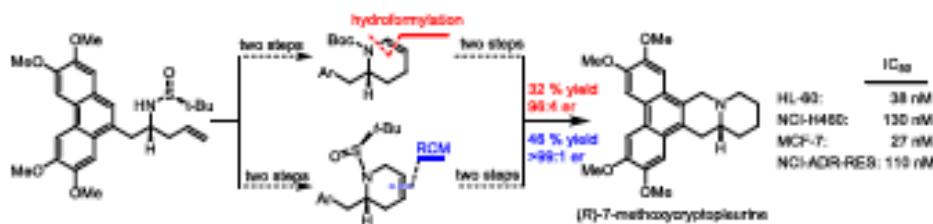
2. *In preparation.*

Syntheses and Cytotoxicity of (*R*)- and (*S*)- 7-Methoxycryptopleurine

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The phenanthroquinolizidines are a family of plants-derived alkaloids with significant therapeutic potential. These compounds exhibit a range of promising biological activities, from which their extremely high cytotoxicity ($IC_{50} \sim 10$ nM) against different cancer cell lines [1] has attracted the attention of medicinal chemists. In this context, robust methods have been developed that allow the rapid construction of the required enantioenriched phenanthroquinolizidine scaffold. Herein two efficient protocols are described for the transformation of a key chiral homoallylic sulfinamine intermediate [2] in four steps into enantioenriched 7-methoxycryptopleurine. While one of the protocols relied on a rhodium catalyzed linear hydroformylation process,[3] the alternative approach was based on a ring-closing metathesis from the corresponding N-allyl-sulfinamine. The cytotoxic evaluation of both enantiomers of the target compound demonstrated that the (*R*)-compound is much more potent than its antipode against the four cancer cell lines examined.[4]



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Enantioselective synthetic approach to the marine alkaloids of the madangamine group

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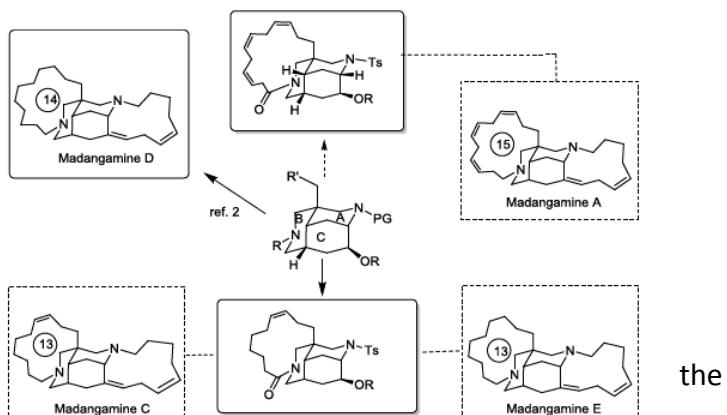
Madangamine alkaloids constitute a small group (six members isolated so far) of complex pentacyclic natural products, which are structurally characterized by a diazatricyclic core (ABC rings), unprecedented among natural products, and two linear carbon bridges. The peripheral macrocyclic ring D is different in each madangamine, in size as well as in degree and position of unsaturation, whereas ring E is identical in madangamines A-E.¹

In the context of our studies on the enantioselective synthesis of complex piperidine-containing natural products

from phenylglycinol-derived bicyclic lactams, we have developed a unified strategy to access the variety of alkaloids of this group, in which the formation of the macrocyclic rings would take place after the construction of the highly functionalized central core.

Recently, we have accomplished enantioselective synthesis of madangamine D, which

represents the first total synthesis of an alkaloid of the madangamine group,² and we are currently studying the construction of the D-ring of more complex members of this family, madangamines A, C and E. By the final assembly of the macrocyclic ring E, we could complete the enantioselective synthesis of other members of this group of alkaloids.



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Acknowledgment: Financial support from the MICINN, Spain (CTQ2012-35250). Thanks are also due to PharmaMar S.A. (Madrid) for the cytotoxicity assays.

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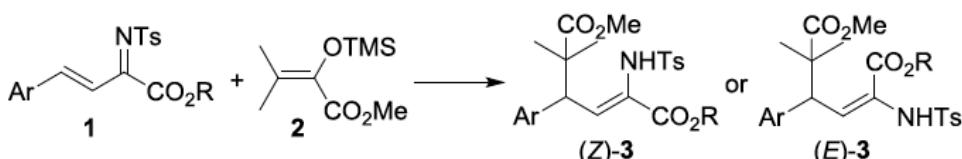
E,Z-stereodivergent synthesis of *N*-tosyl α,β -dehydroamino esters via a Mukaiyama-Michael addition

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α,β -Dehydroamino acid derivatives are non-proteinogenic amino acids often found as structural subunits in natural products and play an important role in the biosynthesis of D-aminoacids and other non-proteinogenic amino acids.^[1] Some of these compounds shown antibiotic and other intriguing biological activities. These properties are affected by the *E/Z* configuration of the double bond of the dehydroamino acid moiety.^[2] Accordingly, much synthetic effort has been devoted to the preparation of dehydroamino acids and their derivatives with a defined double bond geometry. Recently, the stereoselective synthesis of (*Z*)- α,β -dehydroamino acids based on the nucleophilic conjugate addition to imines derived from β,γ -unsaturated α -keto esters has been reported.^[3] However, a procedure based on this approach that leads stereoselectively to the *E* or *Z* dehydroamino esters starting from a same set of reactants has no been reported so far.

In this communication we report our preliminary results in the *E/Z* stereodivergent synthesis of α,β -dehydroamino esters **3** via a Mukaiyama-Michael addition of silylketene acetals **2** to *N*-tosyl imines of β,γ -unsaturated α -keto esters **1**.



Financial support from MINECO (CTQ2013-47949-P) and Generalitat Valenciana (ISIC2012/001 and predocctoral grant to M.E.) is acknowledged.

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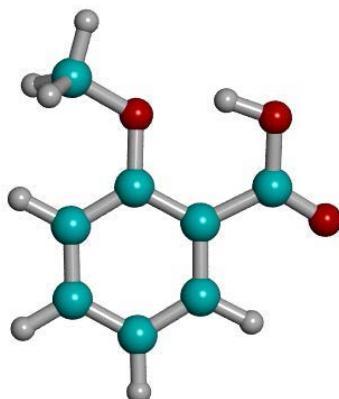
The structure of *o*-anisic acid by microwave spectroscopy

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Intramolecular interactions between different functional groups could affect to molecular structure. The carboxylic group is an interesting example, due to its double character as hydrogen bond donor-acceptor. The formation of hydrogen bonds with other functional groups makes possible the stabilization of the *trans*-COOH isomer which is normally less stable than the *cis*-COOH one. In the present study we have chosen *o*-anisic acid (see Figure) to analyze this stabilizing effect. A conformational study was first done by *ab initio* methods and then the microwave spectrum in the range 4-16 GHz was recorded using Molecular Beam Fourier Transform Microwave Spectroscopy (MB-FTMW). We observed only one rotamer, which was assigned to the calculated minimum energy conformation. Furthermore, we measured the spectra of the eight monosubstituted ^{13}C isotopologues. The rotational constants obtained, allowed us calculate the molecular structure of *o*-anisic acid, which presents a planar framework and an intramolecular hydrogen bond O-H \cdots O, which stabilizes the *trans*-carboxyl group isomer.



Polar Self-assembled Subphthalocyanine Columnar Stacks

FP-6

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Subphthalocyanines^[1] (SubPcs), the lowest homologues of phthalocyanines, are versatile non-planar aromatic macrocycles with excellent optoelectronic properties. In the last decades they have been studied as promising light-harvesting and/or donor materials for photovoltaic and light-emitting applications. We thought that controlling organization of these cone-shape molecules could be interesting in order to improve their efficiency in these sorts of devices. Moreover, we were interested in studying if SubPcs are able to form columnar stacks both in solution and liquid crystalline phases because we could be able to obtain, among others, materials with permanent polarization. The organization of these unique molecules in columns constitutes in itself a challenging enterprise due to the fact that they always bear an axial ligand. We have already forced the formation of these aggregates providing SubPcs with aromatic amides in the peripheral positions to promote hydrogen bonding and π - π stacking interactions all along the column, long alkyl chains to increase the solubility of the stacks and using the smallest axial substituent possible: fluorine.^[2]

A new family of SubPcs has been synthesized to carry out an extensive study of the mechanism of aggregation in solution, as well as their liquid crystalline phases. We have noticed that two different kind of aggregates can be formed as a function of temperature, concentration and solvent as seen in Figure 1c. On the other hand, oriented columns have been obtained in the presence of an electric field when cooling from the isotropic phase to the mesophase.^[3]

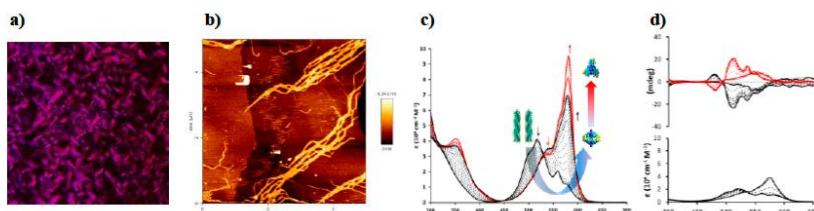


Figure 1. a) POM image of the columnar mesophase; b) AFM image of a drop-casted MCH solution; c) Absorption changes as a function of the volume fraction of toluene and subsequently dioxane; d) CD changes as a function of temperature in MCH of α and β enantiomers.

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Nanopartículas de óxido de hierro funcionalizadas con ácidos nucleicos y péptidonucleicos para la liberación controlada mediante hipertermia

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En la actualidad, las nanopartículas magnéticas son objeto de estudio gracias a sus interesantes propiedades y amplio rango de aplicaciones en diferentes áreas de investigación. Una de las áreas donde mayor desarrollo se está produciendo es el uso de nanopartículas magnéticas como sistemas portadores para la liberación controlada de fármacos.

En el presente trabajo se aprovecha la propiedad de las nanopartículas de óxido de hierro (IONPs, por sus siglas en inglés) de generar calor cuando están sometidas a un campo magnético alterno. El calor generado puede provocar la desnaturización de los ácido nucleicos (ADN) y péptidonucleicos (APN) conjugados en la superficie en dichas nanopartículas de una forma controlada¹.

Se ha desarrollado un sistema de IONPs esféricas de 12 nm funcionalizadas con glucosa² y diferentes grupos carboxílicos de un polímero anfifílico que recubre la superficie de las IONPs. En un paso posterior las cadenas de ADN y APN fueron sometidas a hibridación con su hebra complementaria marcada con un fluoróforo (FAM o Dy490). Finalmente, la cantidad de ADN-FAM complementario desnaturizado en medio básico se utilizó para estimar el grado de funcionalización de las IONPs mediante espectroscopia de fluorescencia. Los resultados obtenidos indicaron que la proporción óptima de ADN/APN para la funcionalización de las IONPs era 50/50. A continuación, se llevaron a cabo estudios de estabilidad de las IONPs en medio de cultivo celular, observándose que únicamente las IONPs funcionalizadas con glucosa tenían una estabilidad satisfactoria, a diferencia de las IONPs que carecían de glucosa.

Actualmente se está trabajando en la optimización de la temperatura adecuada para la liberación controlada de este sistema, así como la incorporación de diferentes biomoléculas con cadena de ADN complementaria a este sistema.

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Textile-metal-organic framework composites for Personal Protection

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The persistent threat of terrorist attacks with chemical warfare agents (CWAs) prompts the research on new protective materials capable of fighting their poisoning effects. Specifically, this kind of materials must be able to remove toxic chemicals at ambient temperature and humidity conditions.¹ In this context, metal-organic frameworks (MOFs) arise as an alternative class of porous materials characterized by its rational design, high surface areas, thermal stability and catalytic activity.¹

In the present communication, we report different routes to improve the phosphotriesterase like catalytic activity of the highly robust metal-organic framework $[Zr_6O_4(OH)_4(bdc)_6]$ (bdc = benzene-1,4-dicarboxylate), named UiO-66, for its application as self-detoxifying adsorbent of chemical warfare agents both as microcrystalline powder and integrated into silk fibroin fabrics. Specifically, we have studied the impact of the introduction of missing linker defects and/or acidic and basic sites on the UiO-66 framework on its catalytic activity. Noteworthy, the insertion of lithium tert-butoxide in the Zr_6O_6 clusters of the activated UiO-66 framework gives rise to a basic catalyst $[Zr_6O_6(bdc)_6(LiO^tBu)]$ ($[UiO-66@LiO^tBu]$) which is highly efficient for the hydrolytic degradation of the model nerve agent diisopropylfluorophosphate (DIFP) with a half-life of 5 minutes only. Moreover, while the catalytic activity of pristine UiO-66 is poisoned by the degradation products of chemical warfare agents (CWAs) (i.e. methylphosphonic acid, phosphoric acid) the catalytic activity of $[UiO-66@LiO^tBu]$ is unaffected, proving the positive effect of LiOR insertion on its self-detoxifying properties. Finally, we also demonstrate that it is possible to integrate these materials on the surface of silk fibroin fibers leading to self-detoxifying protective textiles, which complement air permeation with catalytic degradation properties.

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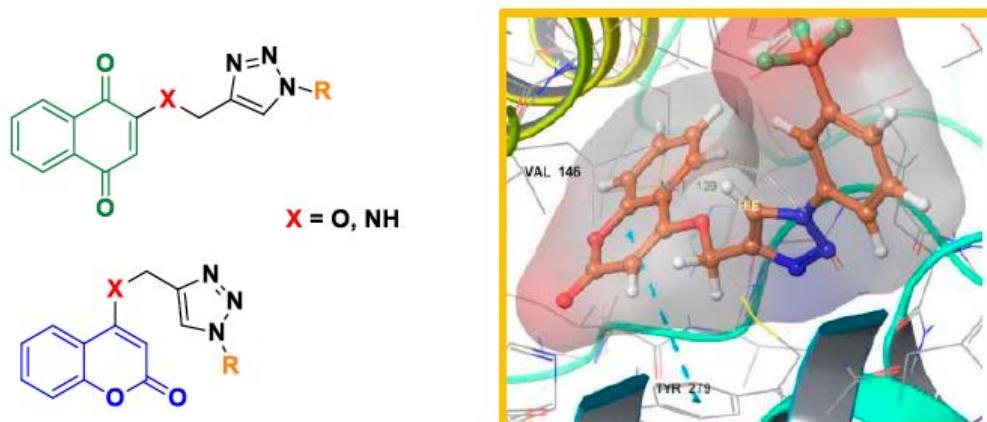
Síntesis y estudios *in silico* de derivados 1,2,3-triazolil naftoquinónicos y cumarínicos con potencial actividad antimalárica

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La malaria es una enfermedad producida por parásitos del género *Plasmodium* y representa una importante causa de morbilidad y mortalidad en los países menos desarrollados, especialmente en África. La falta de eficacia de los tratamientos actuales y la resistencia a los tratamientos clásicos, hacen necesario la búsqueda y el desarrollo de nuevos agentes antimaláricos.

En este trabajo se han realizado estudios *in silico* de modelización molecular tipo Docking sobre una diana terapéutica de malaria, el citocromo bc₁. En base a ello, se han sintetizado cuatro familias de compuestos potencialmente bioactivos basados en estructuras privilegiadas y que contienen el agrupamiento 1,2,3-triazolil. Para ello se han utilizado reacciones de cicloadición 1,3-dipolar catalizadas por cobre entre alquinos y azidas para generar 1,2,3-triazoles-1,4-sustituidos utilizando dos naftoquinonas y dos cumarinas propargiladas y diversas azidas preparadas a partir de ácidos borónicos y haluros de alquilo o arilo.



Agradecimientos: Al MINECO (SAF2012-37344-CO3-01) y EU ResearchPotential (FP7-REGPOT-2012-CT2012-31G37-IMBRAIN) por la financiación concedida.

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Modulación de propiedades antibióticas por luz

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En este trabajo se desarrolla la síntesis y el estudio fotoquímico de nuevos interruptores moleculares con isomería Z/E. Dichos interruptores están basados en estructuras de origen natural como la hidantoína o el cromóforo del fitocromo. Además otra parte de su estructura está inspirada en dos agentes antibacterianos pertenecientes al grupo de las quinolonas, el ácido nalidíxico y el ciprofloxacino. De esta forma, se espera que las moléculas sintetizadas presenten actividad bactericida cuya capacidad pueda ser regulada mediante el estímulo de la luz.

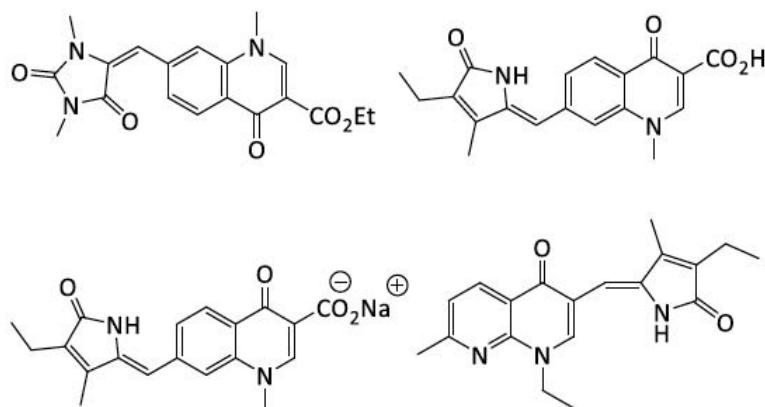


Figura 1. Interruptores moleculares con estructura basada en ciprofloxacino y ácido nalidíxico.

Tras llevar a cabo la síntesis de los nuevos compuestos, se ha realizado un análisis de su comportamiento fotoquímico mediante la irradiación de los mismos, alcanzándose en cada caso sus distintos estados fotoestacionarios. Este hecho confirma que las moléculas sintetizadas poseen comportamiento de interruptor. Finalmente se han estudiado sus propiedades bactericidas con el objetivo de conocer si existe una diferencia de actividad entre los dos isómeros, para ello se han analizado dos parámetros: concentración mínima inhibitoria (CMI) y concentración mínima bactericida (CMB). Por un lado se ha estudiado el estado fotoestacionario y por otro el isómero térmicamente estable, encontrándose diferencias en dos de los casos, lo que pone de manifiesto que la luz puede emplearse con el fin de regular la capacidad antibacteriana.

Molecular switches based on interlocked di(acylamino)pyridines

FP-11

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Herein we present the synthesis of a tailor-made switchable polyamide-based molecular shuttle, bearing a di(acylamino)pyridine (DAP) and an amide group as binding sites, separated by an alkyl chain. Due to the versatile chemical properties of the DAP moiety, the control of the translational motion of the macrocycle along the thread can be achieved by different means (Fig. 1). Hence, the application of external stimuli, such as chemical transformations (redox reactions and pH variations), molecular recognition events with small molecules¹ or electrochemical processes, allows us to control the statistical distribution of the macrocycle over the two binding sites, giving rise to a fully controllable switch.²

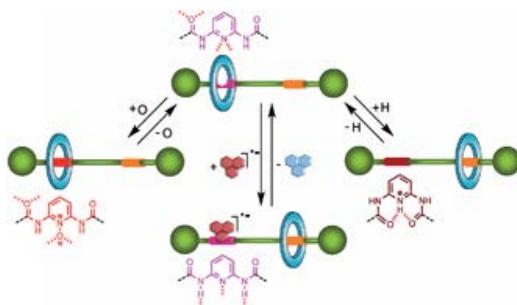


Figure 1. Versatile control of the translational motion of the macrocycle in DAP-based shuttles by different stimuli.

This work was supported by the MINECO (CTQ2009-12216/BQU and CTQ2014-56887-P) and Fundacion Seneca-CARM (Project 19240/PI/14). A.M.-C. thanks the Marie Curie COFUND and U-IMPACT programs (Grant Agreement 267143) and the MINECO (Contract Nº. FPDI-2013-16623) for the postdoctoral contracts.

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Dual mode self-assembly of discotic cone-shaped molecules

FP-12

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Subphthalocyanines (SubPcs) are versatile non-planar aromatic macrocycles with excellent optoelectronic properties, which make them powerful competitors in a wide variety of emerging applied fields such light-harvesting and/or donor materials for photovoltaic and light-emitting applications. Controlling the organization of these cone-shaped molecules constitutes in itself a challenging enterprise due to the fact that they always bear an axial ligand.¹ We have already proved that tetrahedral-shaped molecules such as SubPcs can be polymerized in solution to form self-assembled non-centrosymmetric columnar nanostructures.² Herein we show an extensive study of the mechanism of aggregation of SubPcs **1** and **2** in solution (Fig. 1a). We have noticed that two different kind of aggregates can be formed as a function of temperature, concentration and solvent as seen in Fig. 1b. From these observations we propose that each solvent media promotes a different supramolecular regime (Fig. 1c), and thus the prevalence of one particular supramolecular species. In dioxane, both compounds are fully dissociated and the monomer is the dominant species in solution. In toluene, a non-polar solvent but a good solvating agent for π -surfaces, tail-to-tail H-bonded dimerization takes place for both compounds (Regime A). On the contrary, in MCH, an apolar non-aromatic solvent, SubPc-1 aggregates head-to-tail to form columnar stacks (Regime B) whereas SubPc-2 remains in the tail-to-tail dimeric form, since head-to-tail supramolecular polymerization cannot occur due to obvious steric hindrance.

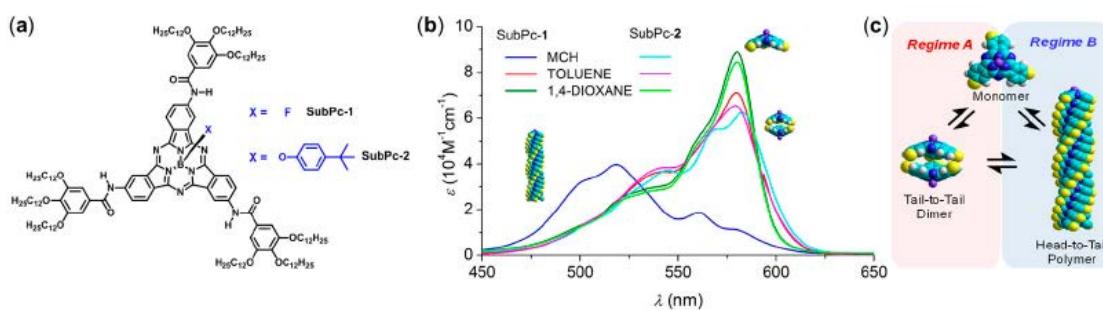


Fig. 1. (a) Subphthalocyanines **1** and **2**. (b) Absorption changes as a function of the solvent. (c) Model of the different self-assembly regimes

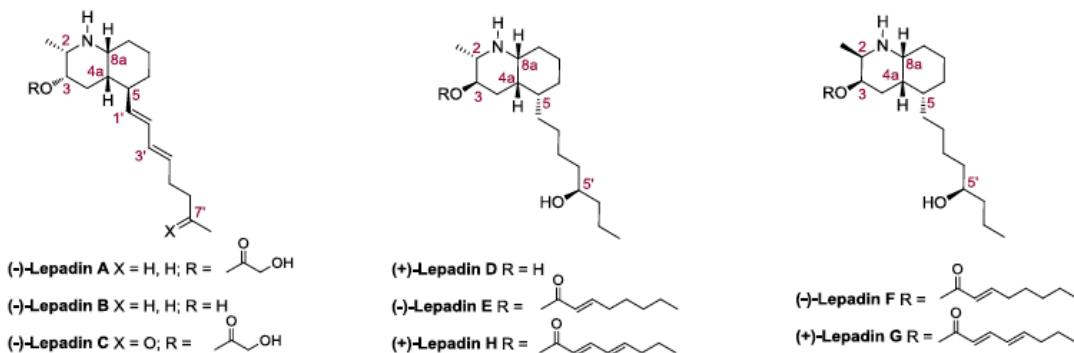
¹J. Guilleme, L. Martínez-Fernández, D. González-Rodríguez, I. Corral, M. Yáñez, T. Torres, *J. Am. Chem. Soc.* **2014**, *136*, 14289; ²J. Guilleme, M. J. Mayoral, J. Calbo, J. Aragó, P. M. Viruela, E. Ortí, T. Torres, D. González-Rodríguez, *Angew. Chem. Int. Ed.* **2015**, *54*, 2543.

Enantioselective total synthesis of (-)-lepadin A-C and (+)-lepadin D

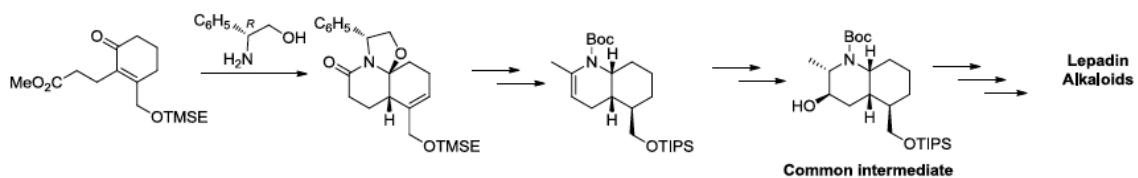
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The lepadin alkaloids, comprising eight *cis*-decahydroquinoline members, were identified from 1991 to 2002 from different marine sources such as the tunicate *Clavelina lepadiformis*, flatworm *Prostheceraeus villatus*, tropical marine tunicate *Didemnum* sp., and Australian Great Barrier Reef ascidian *Aplidium tabascum*.^[1] Lepadins A and B have been shown to exhibit significant *in vitro* cytotoxicity against several human cancer cell lines.^[1a,b] In addition, lepadin B is a potent blocker for neuronal nicotinic acetylcholine receptors (nAChR's). Lepadins D-F have low cytotoxicity but significant and selective antiplasmoidal and antitrypanosomal activity.^[1c]



In the context of our studies^[2] on the use of phenylglycinol-derived chiral tricyclic lactams for the enantioselective synthesis of alkaloids, we will present our studies on the synthesis of the lepadin family of alkaloids, which have culminated in the syntheses of (-)-lepadins A-C^[3] and (+)-lepadin D.



Acknowledgment: Financial support from the MICINN, Spain (CTQ 2012-35250), and the AGAUR, Generalitat de Catalunya (2014-SGR-0155).

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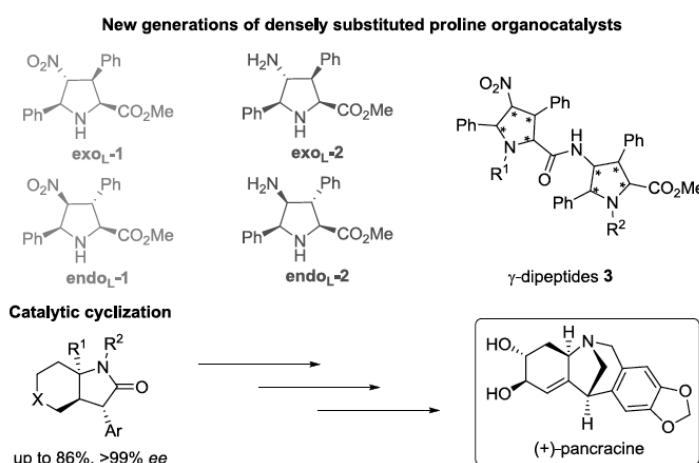
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New organocatalytic properties of densely substituted 4-nitropyrrolidines

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Recently, our group has developed an efficient methodology via (3+2) cycloaddition,¹ hydrolysis, hydrogenation and peptide coupling to synthesize densely substituted unnatural L- and D-Proline derivatives **1**, **2** and **3**. Encouraged by the efficiency of Proline-based organocatalysts in several C-C bond transformations, these novel densely substituted pyrrolidines have been used as organocatalysts in aldol, Michael reactions.² Aside these previously known reactions, we have discovered a catalytic cyclization promoted by several organocatalysts **1** and **3**. In this communication, we present our results on this new organocatalytic reaction and its usefulness in total synthesis of (+)-pancracine.³



Financial support by the Ministerio de Economía y Competitividad (MINECO) of Spain (project CTQ2010-16959) and from the Basque Government (Grupos Consolidados IT673-13) is acknowledged.

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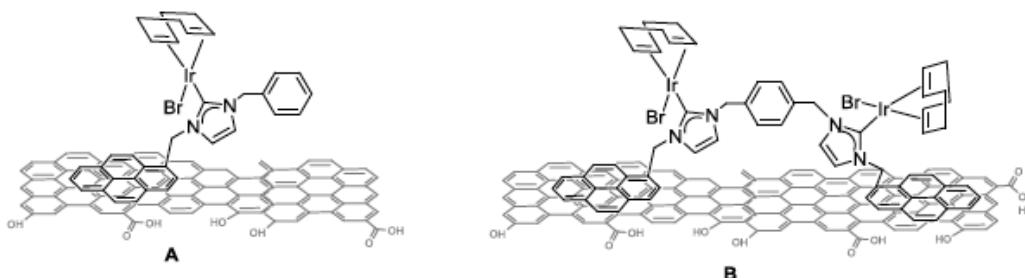
Unveiling the Importance of π -Stacking in Borrowing-Hydrogen Processes Catalysed by Iridium Complexes with Pyrene Tags

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The synthesis and design of new ligands that could facilitate the interaction between catalyst and substrate due to non-covalent interactions, have demonstrated to be a promising tool in a wide range of applications. We have recently shown that NHC-based ligands that contain polyaromatic systems have provided benefits in homogenous catalysis.¹⁻³ Besides, polyaromatic tags such as pyrene could be useful for the immobilization of the complexes by non-covalent interaction onto a grapheme surface. Chemically derived graphenes (CDGs) such as graphene oxide (GO) and reduced graphene oxide (rGO), are excellent candidates for catalyst immobilization due to its inertness, large surface area, stability and availability.^{4,5}

This work describes the preparation of a series of pyrene-tagged N-heterocyclic carbene complexes of iridium, and their use in two benchmark borrowing hydrogen reactions: the reduction of ketones by transfer hydrogenation and the β -alkylation of secondary alcohols with primary alcohols.⁶ The detailed study of these homogeneously catalysed reactions reveals several important implications regarding the strong influence of the pyrene tags in the catalysts regarding the reaction order respect the concentration of the substrate and the concentration of the catalyst and how the addition of an aromatic compound such as pyrene affect to the final reaction yield. Finally, two pyrene-tagged catalysts were supported onto



reduced-graphene oxide (rGO), and used as heterogeneous catalysts.

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How pyridine interacts with freons: π or σ intermolecular bonds?

FP-16

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Pyridine (Py) is a heterocyclic aromatic system with many industrial, chemical and pharmacological applications. We have studied the intermolecular interactions in pyridine clusters Py...B using different partner molecules, interacting either through the π electron system or with the basic nitrogen atom. Depending on the nature of the chemical species, π - or σ - type complexes have been observed. Here we present the different results obtained for the complexes formed when Py interacts with different halomethanes ($B = CH_2F_2^1$, CH_3F^2 and CH_4^3) using microwave spectroscopy (FTMW) in a jet expansion. All molecules interact through the nitrogen atom, except methane, which gives a T-shape complex. The experimental results are also compared with the theoretical ab initio and DFT studies performed for these adducts.

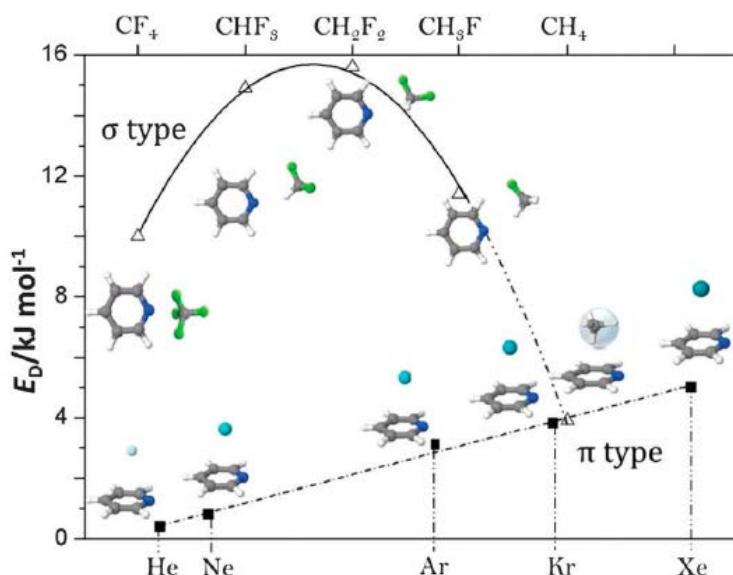


Figure 1.- The dissociation energies and the topologies of the Py...CF_nH_{n-4} complexes (n=0 to 4) are compared to the clusters with inert gases.

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3. Q. Gou, L. Spada, M. Vallejo-López, A. Lesarri, E. J. Cocinero, W. Caminati, *Phys. Chem. Chem. Phys.*, **2014**, *16*, 13041

Comunicaciones Escritas-Pósteres

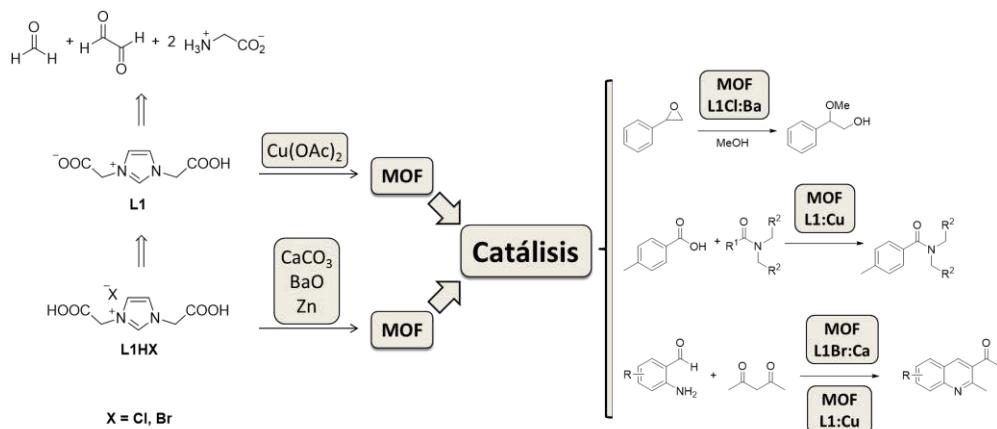
1,3-bis(carboximetil)imidazol como ligando en estructuras metal-orgánicas con actividad catalítica

PO-1

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Las estructuras metal-orgánicas (MOFs), formadas por un ligando orgánico y un precursor metálico, dan lugar a materiales porosos con diversas aplicaciones, entre las que destaca su uso en catálisis.¹ El ligando 1,3-bis(carboximetil)imidazol (**L1**), así como sus sales de bromuro (**L1HBr**) y cloruro (**L1HCl**), presentan una excelente coordinación a centros metálicos debido a su carácter multidentado.² Por ello se han utilizado en los últimos años para la preparación de MOFs en combinación con diversos metales, tales como calcio,² bario,² zinc³ y cobre.⁴ Sin embargo, dichas estructuras no han sido evaluadas hasta la fecha en estudios sistemáticos en catálisis. En este trabajo se han sintetizado MOFs mediante métodos descritos en la bibliografía utilizando los ligandos **L1**, **L1HCl** y **L1HBr**, y se han evaluado en diferentes reacciones, habiéndose demostrado su actividad catalítica en algunas transformaciones orgánicas de interés como son la apertura de óxido de estireno, el acoplamiento oxidativo entre ácidos y amidas y la síntesis de quinolinas mediante la reacción de Friedländer. Además, se ha estudiado la influencia de diversos parámetros implicados en dichas transformaciones.



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³ Z. Fei, W. H. Ang, T. J. Geldbach, R. Scopelliti and P. J. Dyson, *Chem. Eur. J.*, **2006**, *12*, 4014.

⁴ B. F. Abrahams, H. E. Maynard-Casely, R. Robson and K. F. White, *CrystEngComm*, **2013**, *15*, 9729.

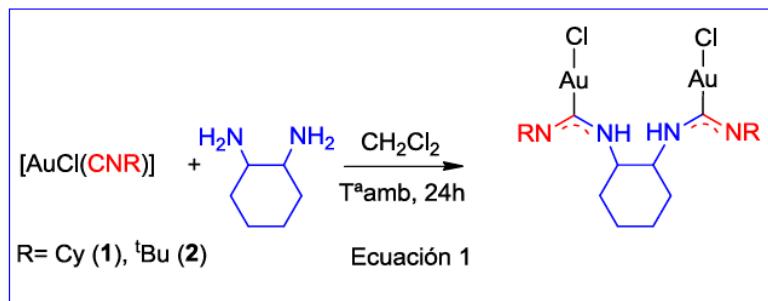
Síntesis de catalizadores de oro(I) y su estudio en reacciones multi-componente

PO-2

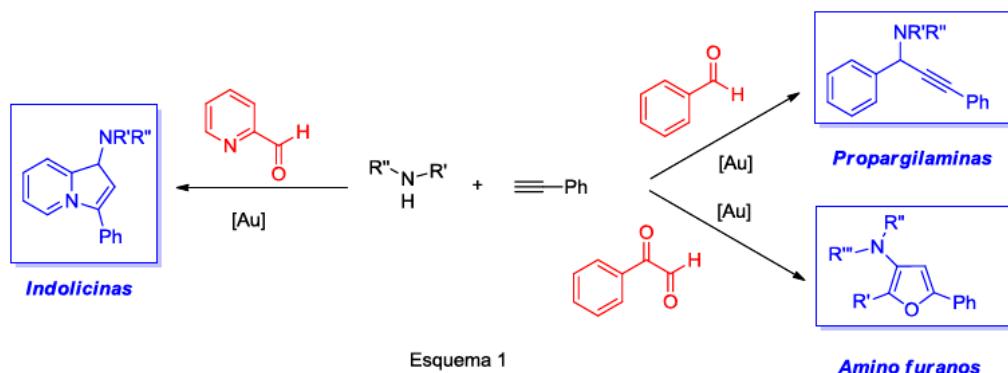
M. Aliaga Lavrijsen, M. Dolores Villacampa, M. Concepción Gimeno

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Los complejos de oro(I) con ligandos aminocarbeno N-acíclicos están mostrando una interesante actividad catalítica en diversos tipos de reacciones.¹ Estos derivados son fácilmente accesibles a través de la reacción de complejos de oro con isocianuro con diferentes aminas. Así, se han preparado los complejos **1** y **2** por reacción de $[\text{AuCl}(\text{CNR})]$ ($\text{R} = \text{Cy}$ o tBu) y la mezcla racémica de la amina *trans*-2-diaminociclohexano (Ecuación 1). Se ha investigado la actividad catalítica de los derivados **1** y **2** en diversas reacciones multi-componente para la obtención de indolicinas, propargilaminas y furanos (Esquema 1).



Los mejores resultados se han obtenido en ausencia de disolvente, en presencia de AgOTf y a una temperatura de 60 °C, con rendimientos de hasta el 99% con un 1% de catalizador.



[1] L. M. Slaughter, *ACS Catalysis*, **2012**, 2, 1802-1816

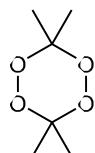
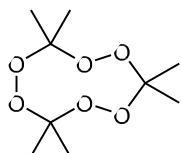
Fluorescence sensing of diacetonediperoxide (DADP)

PO-3

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Nowadays, there is an increased interest in detecting peroxides explosives that might be used in terrorist attacks. The present work focuses on the design and synthesis of a chemosensor sensitive to peroxides explosives such as triacetonetriperoxide (TATP) and diacetonediperoxide (DADP) (Figure 1). The main difficulty for the direct optical detection of these explosives is the fact that they don't present any characteristic band in their UV or fluorescence spectra. In the literature only indirect methods can be found, based mainly on the detection of the hydrogen peroxide generated through the acidic decomposition of these peroxides.¹



1

Figure 1: Structures of peroxides explosives TATP **1** and DADP **2**

Our detection strategy takes advantage of the host-guest properties of the cyclodextrins in aqueous media. Cyclodextrins (CDs) are cyclic oligosaccharides consisting of 6, 7 or 8 D-glucose monomer units (α -, β - and γ -CD respectively). They possess a central cavity with a hydrophobic interior, which allows them to include suitable lipophilic guest molecules into the cavity in water solutions. β -CD has the appropriate size to house inside polar aromatic fluorophores such as a dansyl group. We have carried out the synthesis of two dansyl-functionalized β -cyclodextrins (figure 2).²

These compounds in aqueous solution, when exposed to increasing concentrations of DADP, show a quenching of their fluorescence as a result of the inclusion of the DADP in the CD's cavity. The sensing mechanism is depicted in the figure 3.

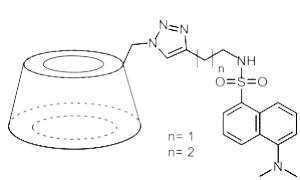


Figure 2: Sensor molecules

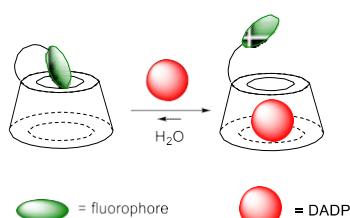


Figure 3: Sensing mechanism.

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² T. Ogoshi, A. Harada, *Sensors*, **2008**, 8, 4961

Silyl-thioether Multidentate Ligands: Synthesis of Rh(III) Complexes via Rh(I)/Rh(III) Mixed Valence and Cyclooctenyl Intermediates

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Previous work has shown that the silyl group can be stabilized onto a metal center via chelation with bidentate¹, tridentate (pincer)² or tetradentate ligands³. Most of these previous studies on silyl multidentate ligand have been performed using pendant phosphane or amine functionalities and, to the best of our knowledge, silyl ligands with thioether moieties have been scarcely studied.

This contribution will deal with the synthesis of various rhodium complexes supported by SSi and SSiS ligands. Through reaction of the thioether-silane SiMe₂H(*o*-C₆H₄SMe) (**L1**) with [Rh(cod)Cl]₂, complex {Rh[SiMe₂(*o*-C₆H₄SMe)]₂Cl}₂ (**1**) was obtained. The mixed valence Rh(I)/Rh(III) complex {(cod)Rh(μ-Cl)₂Rh[SiMe₂(*o*-C₆H₄SMe)]₂} (**2**), which is an intermediate in the formation of **1**, has been isolated. The reaction of formation of **1** was monitored by ¹H NMR spectroscopy revealing the formation of cyclooctenyl intermediates. The tridentate proligand SiMeH(*o*-C₆H₄SMe)₂ (**L2**) reacts with [Rh(cod)Cl]₂ to yield a robust cyclooctenyl Rh(III) complex, {Rh(*n*³-cyclooctenyl)[SiMe(*o*-C₆H₄SMe)₂]Cl} (**3**). Bringing our observations together allows a mechanism for the formation of **1** to be proposed.

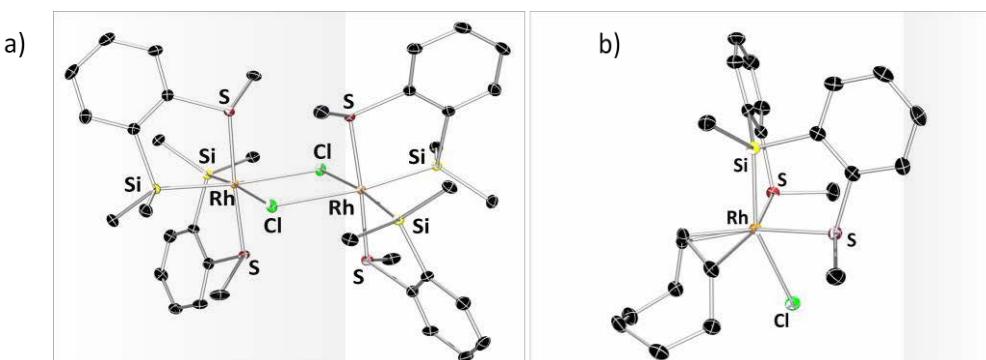


Figure 1: a) Molecular structure of **1**. b) Molecular structure of **3**.

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Enantioselective Direct Michael Addition of Cyanoacetates to α' -Oxy Enones

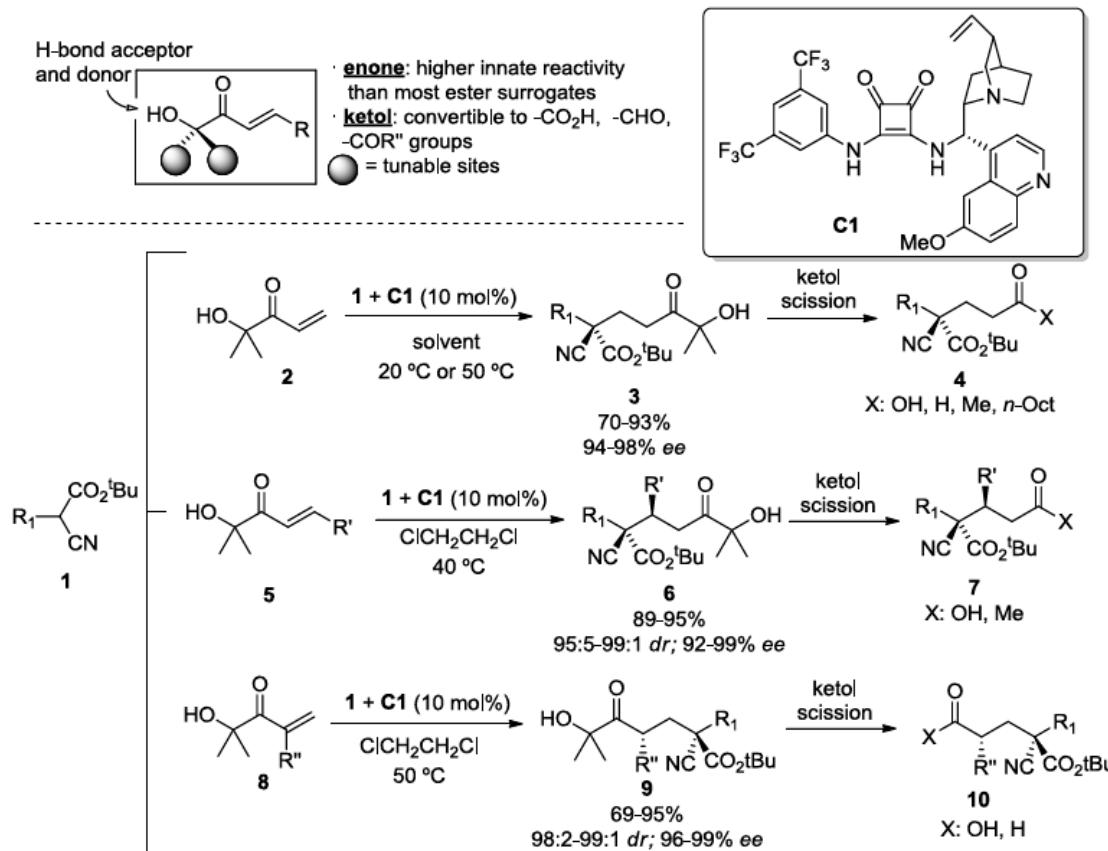
PO-6

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Studies in our group have shown that α' -oxy enones react in the presence of Brønsted base catalysts with cyanoesters to give the corresponding 1,5-dicarbonyl Michael adducts with a fully substituted carbon center in high enantioselectivity¹. The Michael addition of cyanoesters **1** to non-substituted enone **2** is efficiently promoted by catalyst **C1**. The reaction has also been found to be efficient with α - and β -substituted α' -hydroxy enones of type **5** and **8** in the presence of the same catalyst.

Besides their utility for the installation of aldehyde and ketone functionality, α' -oxy enones, act as α,β -unsaturated carboxylic acid surrogates (through simple oxidative cleavage of the ketol moiety in the resulting adducts), for which successful methodologies are notably deficient.



¹ E. Badiola, B. Fiser, E. Gómez-Bengoa, A. Mielgo, I. Olaizola, I. Urruzuno, J. M. García, J. M. Odriozola, J. Razkin, M. Oiarbide, C. Palomo, *J. Am. Chem. Soc.*, **2014**, *136*, 17869-17881.

Modificación personalizada de superficies reactivas con nanopartículas funcionales: presente y futuro

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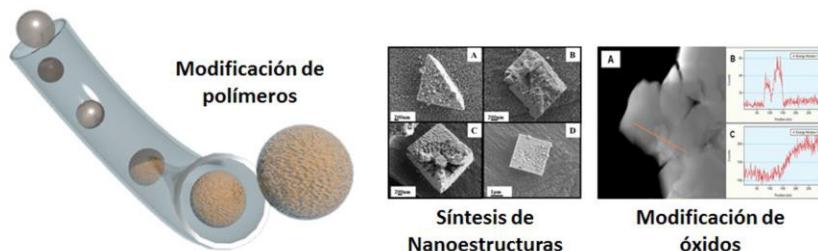
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² Fundació CTM Centre Tecnològic, Plaça de la Ciència 2. 08240 Manresa, Spain.
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El efecto de los materiales nanoestructurados sobre el medio ambiente es uno de los temas más importantes de la tecnología en los últimos años. Dado su alto grado de desarrollo, producción, difusión y aplicación, las mayores preocupaciones asociadas a los Nanomateriales (NMs) incluyen: a) la elevada reactividad y toxicidad de muchos NMs en comparación con sus análogos macroscópicos, b) la ausencia de técnicas analíticas adecuadas para su determinación en el medio ambiente y c) la ausencia de una legislación efectiva que regularice los niveles permitidos de varios NMs en suelo, agua y aire. Por ello es primordial la seguridad y estabilidad de los NMs mediante metodologías efectivas y ambientalmente amigables de nanopartículas.

La bifuncionalidad es determinada por las propiedades propias de la superficie en la que las NPs metálicas (MNPs) son sintetizadas (por ejemplo polímeros de intercambio iónico, óxidos) y por las propiedades respectivas de las MNPs (magnetismo, actividad bactericida, nanocatalizadores). La preparación de MNPs se puede llevar a cabo aprovechando las propiedades de la matriz reactiva a modificar (grupos funcionales, tamaño de poro); y así determinar la ruta sintética más adecuada para la distribución más favorable de las MNPs en función de su aplicación final.

De esta manera, se presenta la preparación materiales de valor añadido con aplicaciones en el campo de tratamiento de agua, catálisis heterogénea y electrocatálisis. Así mismo, puede doparse óxidos (e.g. óxido de uranio (IV)) con Pd- NPs para simular y estudiar la cinética posibles condiciones las reacciones de oxidación que pueden afectar el combustible nuclear después de mil años de almacenamiento geológico profundo.



Nuevos métodos colorimétricos para la detección de fitato: Características y aplicabilidad de sistemas metal-indicador para la determinación de fitato urinario

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El fitato es una sustancia natural presente en la orina y en los fluidos biológicos con efectos beneficiosos para la salud^{1,2}. Los métodos existentes para la detección y la cuantificación de fitato no son aplicables por su complejidad para la determinación en orina en los laboratorios clínicos de rutina.

En este poster se describe un nuevo método para la medida del fitato urinario. Tras un proceso de purificación y preconcentración de la muestra mediante extracción en fase sólida, el fitato se cuantifica colorimétricamente utilizando Al(III)-lumogalión o Al(III)-violeta de pirocatecol. El método Al(III)-lumogalión es lineal entre 0-15 µM de fitato, con un límite de detección de 0.183 µM. Por otro lado, el método Al(III)-violeta de pirocatecol es lineal en el rango 0-10 µM, con un límite de detección de 0.010 µM considerando el proceso de preconcentración. Ambos métodos son simples, rápidos, precisos, reproducibles y sensibles.

Las comparaciones realizadas con el método de referencia Al(III)-naranja de xilenol³ utilizando orina sintética y humana demuestra que el método Al(III)-violeta de pirocatecol es una buena alternativa para la medida del fitato urinario.

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Uso del fitato solo o en combinación con vitámeros B6 para la prevención de la formación de productos de glicación avanzada

PO-9

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La diabetes mellitus (DM) es una patología que conlleva el desarrollo de diversos trastornos metabólicos como la nefropatía o la cardiopatía diabética. Estos trastornos son inducidos por la hiperglucemia mediante la interacción química inespecífica entre azúcares reductores y diferentes macromoléculas biológicas en un proceso llamado glicación no enzimática. Este proceso conduce a la formación de los productos finales de glicación avanzada (AGEs) que presentan un deterioro estructural y funcional respecto a la molécula inicial.

Por ello, se estudió el efecto sobre la formación de AGEs del fitato¹, un compuesto de origen natural capaz de controlar los niveles de azúcar en sangre, tanto en solitario como en combinación con la piridoxamina¹ (PM), un vitámero de la vitamina B6 efectivo en la reducción de la formación de AGEs.

En un primer ensayo se administró diariamente fitato por vía oral a 33 pacientes diabéticos durante 3 meses, periodo tras el cual se observó un descenso tanto de la homoglobina glicada (HbA1c) (3,9%, p=0,017) como de los AGEs (25,1%, p<0,001). Tras 3 meses de blanqueo, sin consumo de fitato, los niveles plasmáticos de HbA1c y de AGEs se incrementaron hasta los niveles basales observados antes de iniciar el estudio.

En un segundo ensayo *in vitro* se comparó el efecto inhibidor en la formación de AGEs del fitato solo o en combinación con la PM. Así, el fitato a concentraciones fisiológicas, 1 µM y 2 µM, inhibió la formación de AGEs en un 12,7% y 19,9% mientras que la PM inhibió en un 17,5% y 28,2% cuando su concentración era 1 µM y 2,5 µM, respectivamente. Sin embargo, el uso combinado de 1 µM de fitato con 1 µM o 2,5 µM de PM provocó una inhibición del 29,0% y del 36,3%, del mismo modo que la combinación de 2 µM de fitato con 1 µM o 2,5 µM de PM disminuyó la formación de AGEs en un 31,6% y un 41,9%. Estos modelos demuestran que el fitato junto con la vitamina B6 puede utilizarse para el tratamiento de patologías generadas por la acumulación de AGEs en el organismo.

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Control del tamaño y la morfología de las partículas de MOFs. Influencia en la incorporación de metalofármacos.

PO-11

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La búsqueda de tratamientos médicos más eficientes hace necesario el desarrollo de nuevos métodos de administración de moléculas bioactivas que controlen su velocidad de liberación. En este contexto, los polímeros de coordinación porosos (PCPs o MOFs) son considerados como sistemas de transporte/liberación de fármacos alternativos debido a la diversidad de estructuras que presentan, así como a la posibilidad de funcionalizar sus poros, lo que favorecería la formación de interacciones más específicas entre la matriz porosa y las moléculas huésped. Además de la biocompatibilidad de las matrices utilizadas, parámetros como la morfología o tamaño de partícula son de gran importancia puesto que pueden influir tanto en la cantidad de fármaco encapsulada como en la estabilidad del sistema en medio fisiológico.

En esta comunicación, se muestra que haciendo uso del *coordination modulation method*, es posible controlar la morfología y el tamaño de partícula del polímero de coordinación poroso CYCU-3 ($[Al(OH)(4,4'-estilbenodicarboxilato)]_n$). Dependiendo de las condiciones de síntesis, se ha conseguido aislar desde materiales amorfos en el rango nanométrico a agujas cristalinas micrométricas. Además, se ha investigado la incorporación del compuesto liberador de CO, ALF794, ($(Mo(CO)_3(CNCMe_2CO_2H)_3$) en los distintos materiales aislados. Estudios preliminares muestran que tanto la capacidad de adsorción de la matriz porosa como la estabilidad de los sistemas híbridos obtenidos se ven afectadas por la cristalinidad y el tamaño de partícula.

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Chemical Coating of Metal-Organic Frameworks for Enhanced Water Stability

PO-12

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Metal-Organic Frameworks (MOFs) are porous, crystalline solids built from the assembly of metal nodes and organic linkers. Built upon their remarkably high surface areas, they have found application in areas like gas storage and separation, catalysis, sensing or drug delivery among others¹. However, incorporation of MOFs into applications that demand high chemical stability is severely limited by weak coordination bonds that hydrolyse under humid conditions or undergo chemical decomposition in the presence of acid or base. Only a minimum fraction of the MOFs reported in the last decade are hydrolytically stable.

This problem can be circumvented by introduction of hydrophobic moieties to the aromatic linkers, either before MOF assembly or post-synthetically, but this also comes at expense of a drastic reduction of the porosity as result of the introduction of bulkier substituents in the empty space². Here, we introduce an alternative strategy for improving the hydrolytical stability of MOFs with minimal loss of surface area. Our approach relies on coating the surface of the MOF crystals with functionalized catechols, which have already demonstrated their versatility in tuning the hydrophobicity of metal nanoparticles and textile fibers³.

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Fluor-containing pseudopeptidic tripodal small cages

PO-13

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Simple open chain and macrocyclic pseudopeptides have revealed to be an interesting class of supramolecular building blocks, being able to participate in different molecular recognition and self-assembling processes. Thus, a new pseudopeptidic molecular cage derived from tripodal precursors with C₃ symmetry has been synthesized with the aim of studying its potential properties as receptor for biologically relevant anions.¹

These cage-like hosts are synthesised by the triple SN₂ reaction between tripodal tris(amido amines) and several 1,3,5-tris(bromomethyl)benzene electrophiles. Previous studies have shown that the cages derived from an aromatic electrophile with triple substitution in the ring (Me or Et) increase the chloride binding.

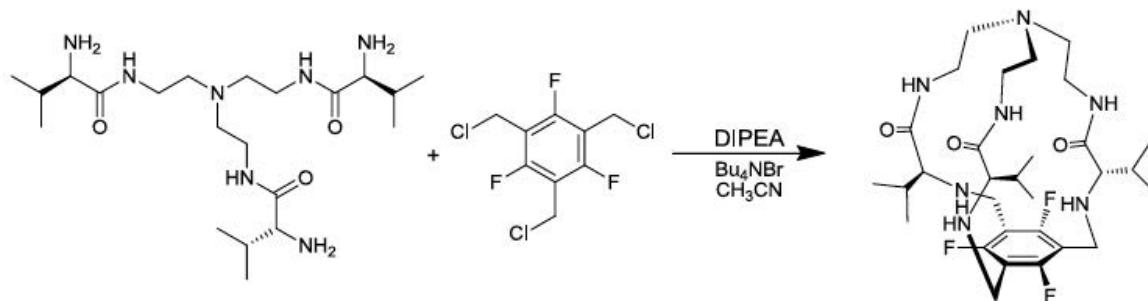


Figure 1. Macrocyllation for the synthesis of the pseudopeptidic cages.

In this work, we have introduced specifically electronegative groups (fluorine) in the triple substitution of the ring,² which is expected to modify its electronic density, and to provide the potential for an increased anion-π interaction inside the cage (see Figure 1).

Acknowledgements:

Financial support by GV-PROMETEO/2012/020, UJI P1·1B2013-38, CTQ2012-38543-C03-01 MINECO and ACOMP/2015/15I252.01/1 are acknowledged.

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Síntesis de heterociclos a través de reacciones de ciclación de [3]-cumulenoles

PO-14

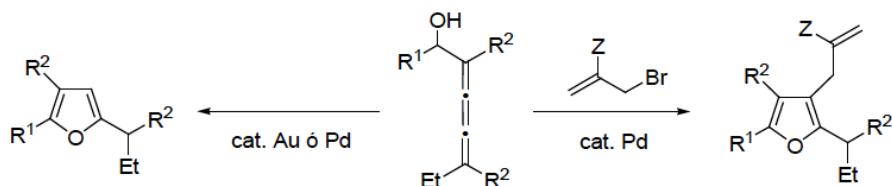
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Los cumulenos han despertado un gran interés en los últimos años debido a sus potenciales aplicaciones en el diseño de fármacos antitumorales¹ así como a sus importantes propiedades eléctricas y fotofísicas.² Además, los cumulenos representan intermedios sintéticos muy versátiles en Síntesis Orgánica.³ Entre los derivados de cumulenos, los 2,3-dien-1-oles se han estudiado ampliamente,⁴ mientras que existen muy pocos ejemplos de reactividad de 2,3,4-trien-1-oles.⁵ La falta de estudios sobre estos compuestos se debe probablemente a la dificultad en la preparación de los materiales de partida y a la posibilidad de obtener un gran número de isómeros frente al aducto deseado. Sin embargo, la adición catalítica intramolecular de un nucleófilo a un cumuleno puede representar un método muy eficaz y de gran economía atómica. Por ello, y continuando con nuestro estudio sobre alenos y cumulenos, se describe la influencia de diferentes metales en reacciones de cicloeterificación de 2,3,4-trien-1-oles, llevadas a cabo de forma totalmente controlada y a través de diferentes modos de reacción.



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⁴ Para una revisión de química de alenos, véase: *Progress in Allene Chemistry* (Eds.: B. Alcaide, P. Almendros): *Chem. Soc. Rev.*, **2014**, *43*, 2879.

⁵ Una vez comenzada nuestra investigación, el grupo de Fensterbank describió una síntesis de furanos y dieninos catalizada por oro a partir de [3]-cumulenoles: L. Ferrand, N. Das Neves, M. Malacria, V. Mourès-Mansuy, C. Ollivier, L. Fensterbank, *J. Organomet. Chem.*, **2015**, *795*, 53.

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Light emission from ionic NHC-cycloplatinated compounds

PO-15

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The use of $[\{Pt(\mu\text{-Cl})(\eta^3\text{-2-Me-C}_3\text{H}_4)\}_2]$ as starting material allowed to accomplish a step by step cyclometallation of the NHCs^[1] through the intermediate carbene complexes $[PtCl(\eta^3\text{-2-Me-C}_3\text{H}_4)(HC^*\text{-}\kappa C^*)]$ (**1A**, $HC^*\text{-}\kappa C^*=1\text{-}(4\text{-cyanophenyl})\text{-3-methyl-1}H\text{-imidazol-2-ylidene}$ (**A**); **1B**, $HC^*\text{-}\kappa C^*=3\text{-methyl-1-(naphthalen-2-yl)-1}H\text{-imidazol-2-ylidene}$ (**B**)), to give two new NHC-cyclometallated compounds, $[\{Pt(\mu\text{-Cl})(C^*)\}_2]$ ($HC^*\text{-}\kappa C^*=$ **A** (**2A**), **B** (**2B**)). Compounds **2A/2B** were used as precursors to get the highly luminescent compounds $(NBu_4)[Pt(C^*)(CN)_2]$ ($HC^*\text{-}\kappa C^*=$ **A** (**3A**) (see **Figure 1**), **B** (**3B**)) and $[Pt(C^*)(CNR)_2]PF_6$ ($HC^*\text{-}\kappa C^*=$ **A**, R = 2,6-dimethylphenyl (**4A**), tBu (**5A**); **B**, R = 2,6-dimethylphenyl (**4B**), tBu (**5B**)).

Differences in the luminescent behavior of **3A/B-5A/B** were found by modification of both the NHC and the ancillary ligands. To see, solid samples of compounds **3A** and **3B** show blue and yellow intense phosphorescence respectively ($F \approx 60\%$) (**Figure 2**) upon excitation at $\lambda_{exc} = 365$ nm. On the other hand, the color modulation can be achieved by changing the ancillary ligands, as shown for compounds **4A/B-5A/B** (**Figure 3**). TD-DFT calculations for a better insight in the optical properties of these derivatives have been performed.



Figure 1. X-ray crystal structure of **3A**.

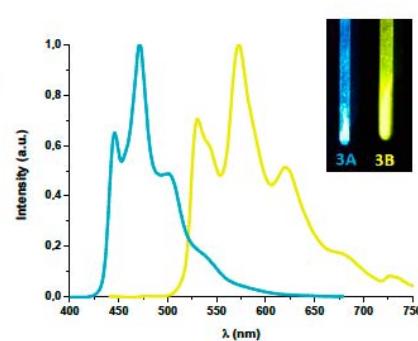


Figure 2. Normalized emission spectra of **3A** and **3B** in solid state at 298 K.

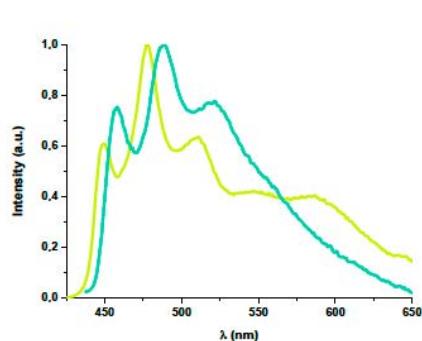


Figure 3. Normalized emission spectra of **4A** (green) and **5A** (yellow) in solid state at 298 K.

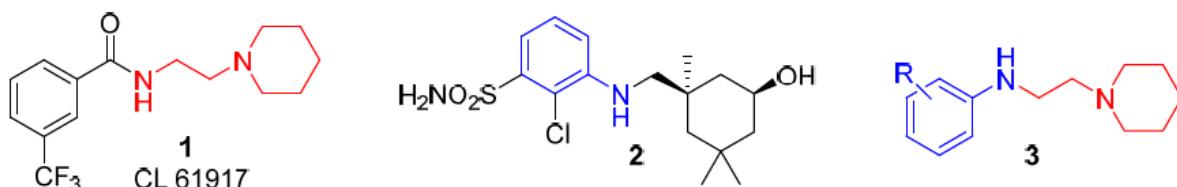
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Synthesis of novel anilines with anti - influenza activity

PO-16

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Influenza A viruses are a major global concern because of the high medical and socioeconomic burden that causes the flu. So far, only two of the eight viral proteins have been exploited as validated targets: the M2 proton channel and the neuraminidase. Alarmingly, M2 channel blockers are obsolete and significant resistance to neuraminidase inhibitors has also been observed in some Influenza A strains.¹ Thus, there is an urgent need for developing new and effective drugs to fight the flu, preferably with novel mechanism of action. Few years ago, Wyeth and Roche reported anti-influenza activity for **1** (CL 61917) and aniline **2**, respectively.² Of note, the mechanism of action of both compounds was neither related to M2 nor with neuraminidase, but with another viral protein, hemagglutinin. Taking into account the structure of both series of compounds and the interest of our group in the synthesis of novel anti-influenza drugs,³ we envisaged a novel series of compounds of general structure **3**, sharing structural elements from the previous compounds.



From *N*-(2-chloroethyl)piperidine and several anilines we have synthesized a broad range of compounds, diversely substituted in the aromatic ring. Interestingly, several of them displayed low micromolar inhibitory activity against some H1N1 influenza A strains, while not being cytotoxic. The mechanism of action of this new family of anti- influenza agents is currently under study.

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Diseño de nuevos materiales mesoporosos de titanio y su aplicación en procesos de polimerización por apertura de anillo de ϵ -caprolactona

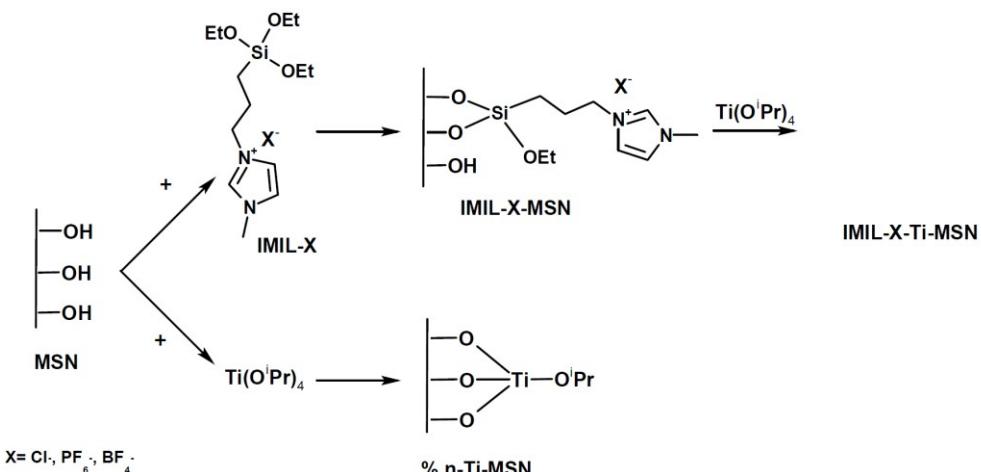
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Poli- ϵ -caprolactona es un polímero biodegradable, cualidad que lo hace un excelente material para sustituir a los actuales plásticos. Debido a su biocompatibilidad presenta excepcionales propiedades como biomaterial para implantes y sistemas de liberación de medicamentos¹. Uno de los métodos de obtención de este biopolímero es mediante polimerización por apertura de anillo de ϵ -caprolactona.

Este trabajo pretende aportar una mejora en la obtención de este demandado polímero. Para ello, se sintetizaron nuevos catalizadores heterogéneos que permiten una fácil separación del medio de reacción y su posterior reutilización. En el diseño de los materiales se emplearon soportes silíceos con dimensiones de nanoscalas que presentan una elevada área superficial.

La utilización de estos catalizadores en el proceso de polimerización de ϵ -caprolactona demuestra que el método sintético, el empleo de diferentes soportes y la presencia de



Esquema 1. Preparación de materiales de Titanio.

1 S. Martinez-Diaz et al. *Am. J. Sports Med.*, 2010, 38, 3509

Síntesis y caracterización estructural de nuevas moléculas imán basadas en compuestos de coordinación de iones lantánidos

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Una de las áreas de investigación más activas en el campo del magnetismo molecular es la preparación y estudio de moléculas imán, MI (moléculas que presentan histéresis magnética por debajo de una temperatura que se conoce como de bloqueo TB). El interés por este tipo de sistemas se debe a sus importantes aplicaciones potenciales en espintrónica molecular, en dispositivos de almacenamiento de información de ultra alta densidad y en computación cuántica a nivel molecular[1]. En esta comunicación se expondrán los resultados de la síntesis y caracterización estructural de complejos mono- y dinucleares derivados del ligando del 5-methyl-[2,2'-bipyrimidine] 1-oxide (mbpymo) e iones lantánidos que presentan comportamiento de MI.

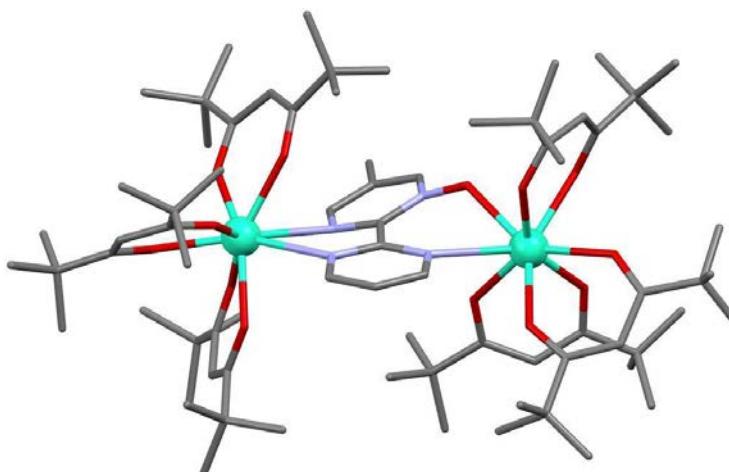


Figura 1. Estructura cristalina del complejo dinuclear [(Dy(tmh)₃)₂(μ-mbpymo)]

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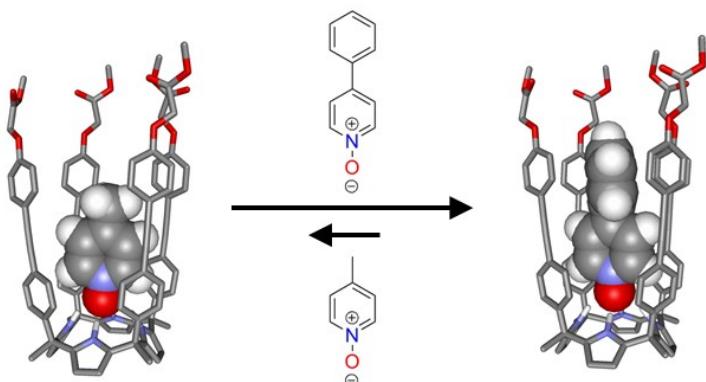
Synthesis and Binding Studies of Super Aryl-Extended Calix[4]pyrroles

PO-19

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Aryl-extended calix[4]pyrroles are macrocyclic compounds able to recognize anions and electron-rich neutral molecules by a combination of hydrogen bonding, π - π and CH- π interactions.^[1,2,3,4] We envisaged that the extension of the aromatic surfaces provided by the a,a,a,a-isomer of meso-methylphenyl calix[4]pyrrole (aryl-extended calix[4]pyrrole) receptor could enhance its binding properties by establishing additional interactions with the included guest molecules. The deeper aromatic cavity displayed by super-extended calix[4]pyrrole in comparison to the aryl-extended counterpart may also increase their selectivity in the recognition of certain substrates. The basic aryl- extended calix[4]pyrrole core was synthetized by the acid-catalyzed condensation of pyrrole and 4-iodophenylmethyl ketone. The extension of the aromatic surfaces was achieved by Sonogashira cross-coupling reactions. The receptor was characterized by a set of high resolution spectra and X-ray diffraction analysis. We studied the binding properties of this unprecedented receptor using two pyridine N-oxide derivatives of different size. The obtained results demonstrated the relevance of additional interactions with the upper aromatic cavity in enhancing the binding affinity with the larger guest.



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Materiales híbridos titania/organometálico mesoporosos fotoactivos bajo luz visible

PO-20

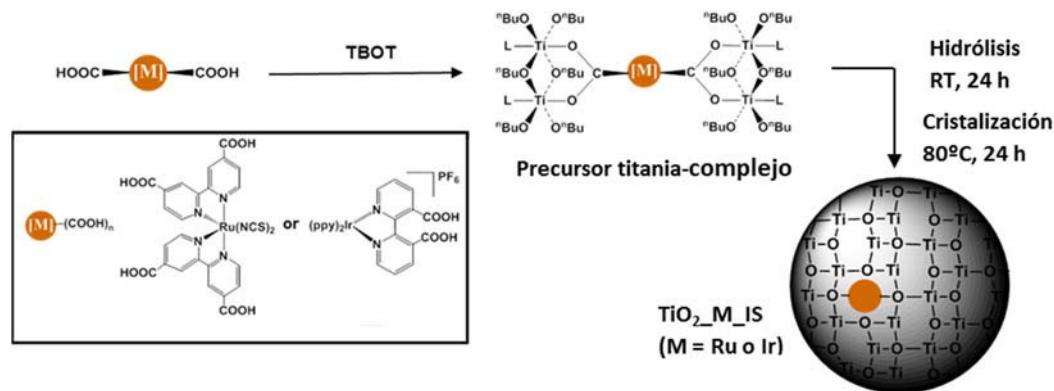
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La titania (TiO_2) se ha convertido en uno de los semiconductores más empleados en el diseño de sistemas fotoactivos para el aprovechamiento de luz solar. Sin embargo, su elevado salto electrónico (3.2 eV) hace que sólo pueda recoger, aproximadamente, el 4% de los fotones del espectro solar (UV). Para habilitar la absorción en el rango del visible, es frecuente recurrir a la adsorción o a la unión covalente de cromóforos en su superficie. Recientemente, nuestro grupo de investigación ha diseñado un nuevo método sintético, basado en la química de tipo Sol-Gel, para la preparación de organotitanias híbridas activas en el visible. Este método, no explorado hasta la fecha, permite la integración de cromóforos orgánicos dentro de la red anatasa de la titania.[1] En esta comunicación se presenta la incorporación de complejos neutros y catiónicos de Ru(II) e Ir(III) a la red cristalina de la titania, lo que ha dado lugar a nuevos materiales semiconductores híbridos de alta estabilidad, activos bajo luz visible, con aplicaciones photocatalíticas y en celdas solares.



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Phthalocyanine-Ferrocene hybrids as components of donor-acceptor ensembles

PO-21

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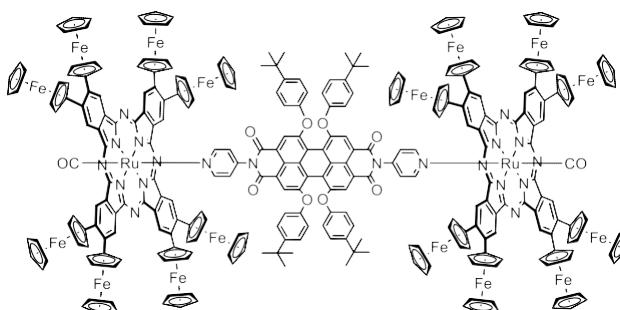
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Phthalocyanines (Pcs)¹ are versatile compounds that have been widely used in artificial photosynthesis due to their optimal optoelectronic and redox properties. These properties can be tuned by functionalization at their periphery and/or on the axial position, along with the possible introduction of a metal atom in the internal cavity of the macrocycle. Thus, functionalization of Pcs with electron donor groups is a common strategy to construct phthalocyanines exhibiting reducing behaviour.

Owing to its stability and well defined electrochemistry, Ferrocene (Fc) has been used sometimes to construct multicomponent systems with porphyrins and phthalocyanines², but there is only one example in which it has been directly linked to a free-base Pc^{2d} . We have synthesized both Zinc(II) and Ruthenium(II) Pcs directly substituted with 4 and 8 units of Fc and studied its optical and redox properties.

In addition, we have also used these Pcs as the reducing components of donor-acceptor hybrids, with perylenediimide (PDI) as the acceptor unit, as it can be seen in Figure 1. In a referable Pc-PDI-Pc hybrid photoexcitation of either the Pc or the PDI leads to a radical ion pair with a long lifetime³. We expect that a second donor moiety, i.e. the Fc, should stabilize the Pc radical cation, leading to longer lifetimes of the charge separation state.



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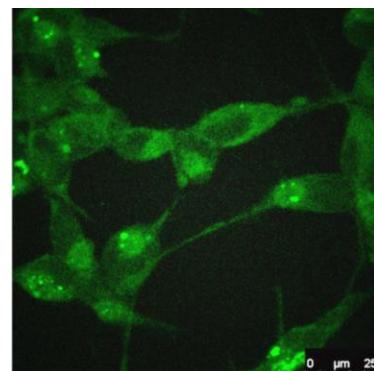
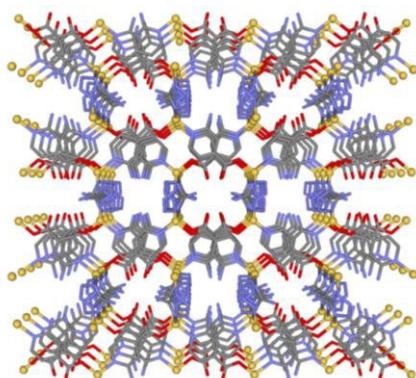
Highly Active Anti-Diabetic Metal-Organic Framework

PO-22

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Diabetes mellitus is a chronic disease occurring when the pancreas does not produce enough insulin (type I) or when the body cannot effectively use the insulin (type II). Hyperglycaemia, is a common effect of uncontrolled diabetes and over time leads to serious damage of the body system. Zinc has shown insulin-like effects by supporting the signal transduction of insulin and by reducing the production of cytokines, which lead to beta-cell death during the inflammatory process in the pancreas in the course of the disease. We have designed and synthesized a novel zinc metal-organic-framework (MOF) under mild hydrothermal routes using 5-aminotetrazole and methyl-2-amino-4- isonicotinate anionic ligands. The MOF exhibits a three-dimensional structure with intense blue-greenish photoluminescence emission at room temperature in the solid state. The luminescence, porosity and adsorption capacity for CO₂ and H₂ of the Zn- based MOF has been fully determined using a combination of computational methods and experimental techniques. The Zn-based compound designed in this study exhibited a remarkable *in vivo* antidiabetic activity and low *in vitro* cell toxicity.



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Bioorthogonal “click” functionalization of magnetic nanoparticles

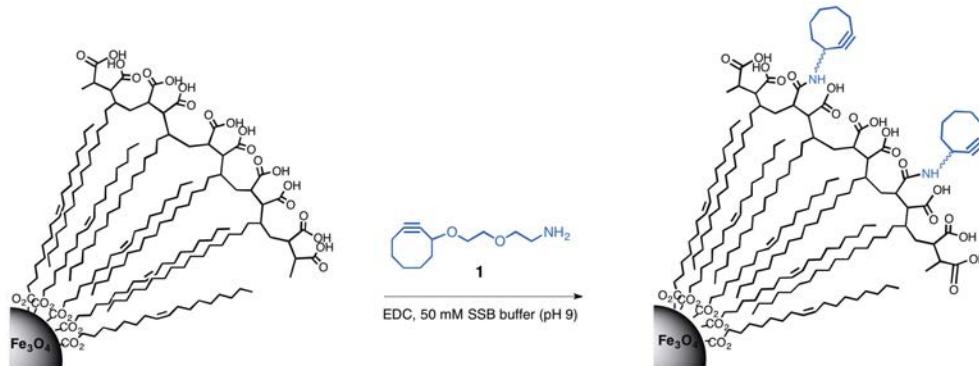
PO-23

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We propose the use of bioorthogonal strain-promoted “click” [3 + 2] azide-alkyne cycloaddition (SPAAC) as a tool to immobilize magnetic nanoparticles (MNPs) on cell surfaces for magnetic hyperthermia studies. The SPAAC reaction uses the ring strain to activate the alkyne, thus avoiding the use of the cytotoxic Cu(I) catalyst.¹ In this work, we present our preliminary results concerning the functionalization of MNPs with strained alkynes. The cyclooctynyl amine derivative **1** was prepared in three steps and 56 % overall yield starting from 8,8-dibromobicyclo-[5.1.0]-octane and following a chromatographic purification-free method adapted from the literature.² Hydrophobic 12 nm iron oxide MNPs were synthesized following a seed-mediated thermal decomposition methodology and transferred to water by coating with an amphiphilic polymer - poly(maleic anhydride-alt-1-octadecene), PMAO.³ Hydrolysis of the maleic anhydride moieties yields carboxyl groups that can be used for the covalent attachment of the amine **1** under standard amide coupling conditions.



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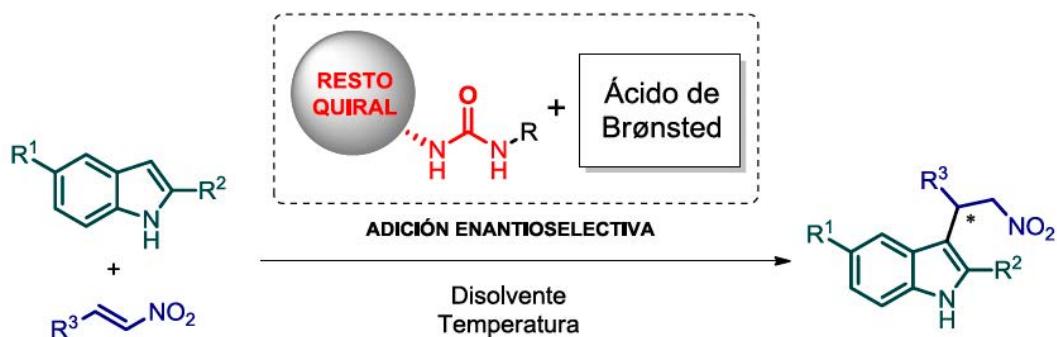
Activación de organocatalizadores urea por ácidos de Brønsted externos y su empleo en la reacción de Friedel-Crafts

PO-24

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En algo más de una década, la organocatálisis se ha consolidado como una nueva y poderosa herramienta para la síntesis de compuestos enantiopuros.¹ Asimismo, es ampliamente conocido el papel del indol como núcleo estructural de multitud de compuestos de interés.² Anteriores investigaciones en el seno de nuestro grupo han demostrado la eficacia de catalizadores tiourea en la síntesis de derivados indólicos enantioméricamente enriquecidos, obteniéndose mejores resultados de rendimiento y enantioselectividad tras adición de un ácido de Brønsted externo.³ En el presente trabajo se estudia el empleo de catalizadores urea en la activación de reacciones de tipo Friedel-Crafts y se explora el uso de aditivos ácidos de Brønsted en la misma. Los catalizadores urea presentan en general, menor acidez y mayor autoasociación que sus homólogos de tipo tiourea. Se cree que un posible efecto cooperativo entre el catalizador y el aditivo puede corregir estos inconvenientes.



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³ E. Marqués-López, A. Alcaine, T. Tejero, R. P. Herrera, *Eur. J. Org. Chem.*, 2011, 3700.

Síntesis, y reactividad de benzamiduro complejos de Pt(II)

PO-25

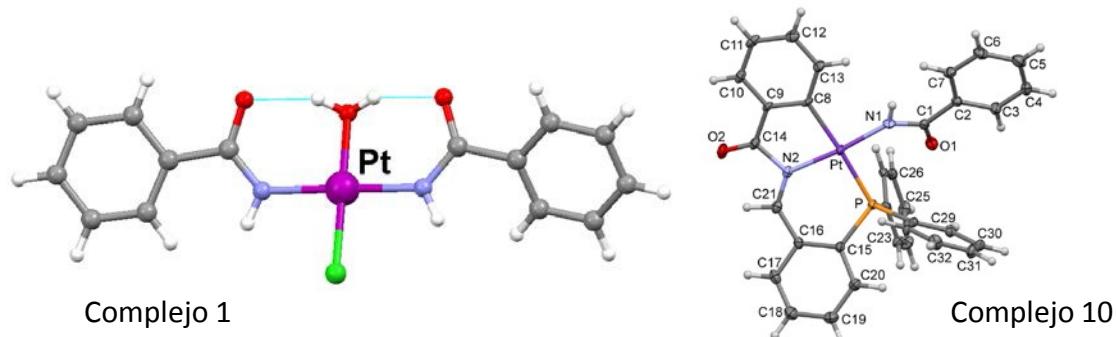
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La síntesis de amiduro complejos del tipo $[NBu_4][trans\text{-}PtCl(NH(CO)R)_2(H_2O)]$ ($R= Ph$ (1), $C_6H_4CH_3$ (2), $C(CH_3)_3$ (3)) puede realizarse por ataque nucleofílico del grupo OH^- al carbono del nitrilocomplejo de platino $[PtCl_2(NCR)_2]$ y transcurre con sustitución de un ligando cloro por una molécula de agua presente en el medio que se estabiliza por formación de puentes de hidrógeno intramoleculares.¹

El estudio de la reactividad del complejo 1 frente a fosfanos indica que se produce siempre la doble sustitución del ligando cloro y agua. En el caso de fosfanos monodentados se obtienen los complejos $[trans\text{-}Pt(NHC(O)Ph)_2L_2]$ ($L= PPh_3$ (4), PBz_3 (5),etc.), incluso si la reacción se realiza en relación complejo de Pt:L 1:1, en cuyo caso queda el 50% del complejo 1 sin reaccionar. La reactividad de 1 frente a ligandos bidentados como dppm(6), dppa(7), y dpCy(8) da lugar al mismo tipo de complejos que con ligandos monodentados, coordinándose uno solo de los átomos dadores. El incremento del número de átomos en la cadena entre los átomos de fósforo (ej. dppe) favorece la isomerización y formación del complejo quelato $[cis\text{-}Pt(NHC(O)Ph)_2(2dppe)]$ (9).¹

Por otro lado, cuando el fosfano posee grupos funcionales como en el ligando $P(Ph)_2(C_6H_4CHO)$, además de la sustitución de los ligandos cloro y agua por el fosfano, se produce la condensación del grupo aldehído de un fosfano con un benzamiduro y la metalación del fenilo de éste con liberación del otro fosfano dando lugar a un complejo tipo pincer² (PNC) $[Pt(NHC(O)Ph)(P(Ph)_2C_6H_4CH=NC(O)C_6H_4)]$ (10). Este complejo posee varios centros y enlaces con características básicas por lo que se ha ensayado la reactividad frente a especies ácidas como HCl y $[Me_3O]BF_4$.



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Direct determination of minor and major elements in biological micro-samples using solid sampling high-resolution continuum source graphite furnace atomic absorption spectrometry

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The control of essential and toxic element levels in many biological materials is an issue of particular interest in forensic and clinical analysis, and in the context of biomedical research. In these cases, usually a tiny and limited amount of sample is available, so sample treatments and the full analysis must be carried out only using very few micrograms of the sample. Analytical methodologies that provide accurate and precise results with adequate sensitivity directly from the solid sample are efficient and reliable alternatives for these purposes. These strategies are simple, increase the speed of analysis and reduce the risk of contamination and/or loss of analytes compared to traditional methods based on wet digestion of the samples.

High-resolution continuum source atomic absorption spectrometry (HR-CS AAS) provides significant advantages in comparison with traditional line source AAS (LS AAS). This new instrumental concept offers improved capabilities to the detection and correction of spectral interferences from the matrix sample, so it can be considered more suitable than LS AAS to direct analysis of solid samples. Moreover, it is feasible to choose secondary absorption lines in order to reduce sensitivity for the determination of major elements. In addition, the possibility of measuring only at the wings of the atomic absorption line for quantification purposes allows expanding the linear working range of an element to the required levels for any set of experimental conditions without the need to carry out additional measurements [1-3].

This work aims to explore the possibilities of solid sampling HR-CS GFAAS for the direct analysis of biological micro-samples. The capabilities of HR-CS GFAAS to direct analysis of complex samples using straightforward calibration with aqueous standards, and the possibility of using main or secondary analytical lines for the quantification of minor or major elements has been evaluated.

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Potent and selective inhibitors of re-emerging chikungunya virus replication

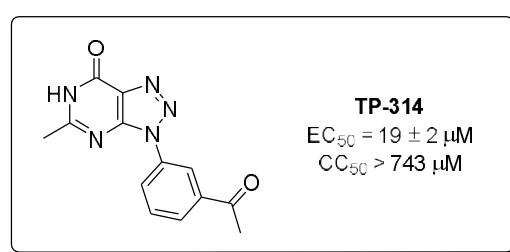
Asier Gómez-SanJuan,¹ Ana M. Gamo,¹ Alba Gigante,¹ Oskía Bueno,¹ Leen Delang,² Pieter Leyssen,² Johan Neyts,² María-José Camarasa,¹ Eva-María Priego¹ and María-Jesús Pérez-Pérez¹

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Despite the great advances performed in the development of drugs against viral epidemics, there is a growing number of diseases, some of them with a global impact, that are due to a viral infection. One of the viruses that have reached the category of re-emerging virus is Chikungunya virus (CHIKV), which is transmitted to humans by *Aedes aegypti* mosquito. Although traditionally restricted to Africa and Asia, the adaptation of the virus to *Aedes albopictus*, a mosquito species with an almost worldwide distribution, has contributed to the geographical spread of this virus in the past decade.¹

Screening against CHIKV replication of a chemical library constructed from our historical collections led us to identify a sample coded **TP-314** as an inhibitor of CHIKV-replication ($EC_{50} = 19 \mu M$) at non-toxic concentrations ($CC_{50} > 743 \mu M$).² We have now undertaken the synthesis and anti-CHIKV evaluation of novel series of compounds whereas additional substitutions have been performed at the aryl ring and at the triazolopyrimidine moiety, in many cases through microwave-assisted chemistry. The impact of such substitutions on the anti-CHIKV activity will be presented.



Acknowledgements: A. Gigante acknowledges the FSE and the CSIC for a JAE Pre contract. Financial support from SAF2012-39760-C02-01 is also acknowledged.

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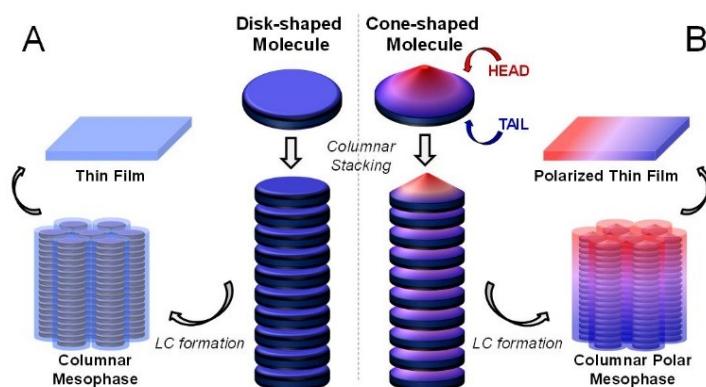
Polar Self-assembled Molecular Materials

PO-28

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Columnar nanostructures and liquid crystals are an important class of self-assembled organic materials that are making great impact in several optoelectronic technologies like transistors, solar cells, ferroelectric switches or light-emitting diodes. These materials are typically produced by the ordered stacking of functional molecules with a discotic shape (Fig. 1A). We have here studied related assemblies from a unique class of molecules, Subphthalocyanines,[1] having instead a rigid conical shape and a strong axial dipole moment (Fig. 1B).[2] In condensed phases, the generation of liquid crystalline materials[3] that can be efficiently aligned in the presence of electric fields and that exhibit permanent or switchable net polarization is observed. This is a novel and appealing attribute that may have important implications in, for instance, technologies that require an efficient directional transport of charges or memory devices combining ferroelectric and semiconducting properties.



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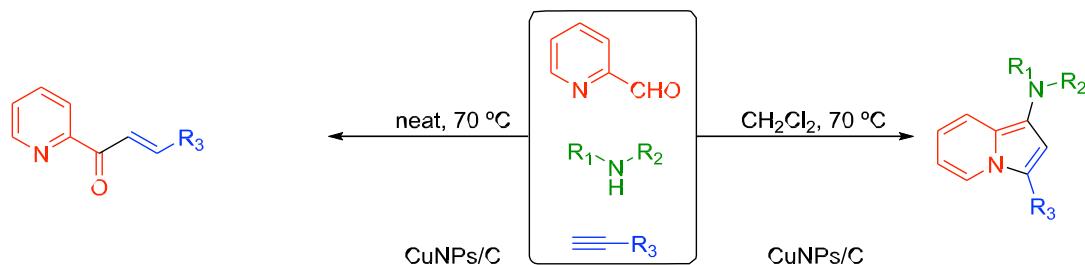
[3] a) J. Guilleme, J. Aragó, E. Ortí, E. Cavero, T. Sierra, J. Ortega, C. L. Folcia, J. Etxebarria, D. González-Rodríguez, T. Torres, *J. Mater. Chem. C*, **2015**, *3*, 985. b) J. Guilleme, E. Cavero, T. Sierra, J. Ortega, C. L. Folcia, J. Etxebarria, T. Torres, D. González-Rodríguez, *Adv. Mater.* **2015**, *27*, 4280. c) A. V. Gorbunov, M. García Iglesias, J. Guilleme, W. S. C. Roelofs, T. Torres, D. González-Rodríguez, E. W. Meijer, M. Kemerink, *Submitted*.

Synthetic and mechanistic studies on the solvent-dependent copper-catalyzed formation of indolizines and chalcones

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Indolizines [1] and chalcones [2] share a large variety of pharmacological activities, including anticancer, antibacterial, antifungal, anti-inflammatory, anti-tubercular, antioxidant or analgesic activity, among others. The multicomponent synthesis of a series of indolizines and pyrrolo[1,2-*a*]quinolines has been effectively accomplished from pyridine-2-carbaldehyde derivatives, secondary amines and alkynes using CuNPs/C as catalyst in dichloromethane [3, 4] (Scheme 1). The methodology has been applicable to a variety of amines and alkynes, with the latter including aryl alkynes (bearing electron-neutral, -releasing and -withdrawing groups) as well as aliphatic alkynes (42–93%). Interestingly, the same procedure, when applied in the absence of solvent using piperidine as the secondary amine, has led to heterocyclic chalcones as major products in modest-to-good yields (40–77%) and exclusive *E* stereochemistry. In both processes, the catalyst was shown to be superior to some commercially available copper catalysts and it could be reused in the chalcone synthesis over four cycles with a decrease in activity (85–64% conversion). Reaction mechanisms have been proposed for the indolizine and chalcone formation, based on the strong experimental evidence of participation of propargyl amines as intermediates in both cases. Based on leaching studies, both the indolizine and chalcone syntheses are suggested to proceed under heterogeneous catalysis.



Scheme 1

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4. M. J. Albaladejo, F. Alonso, M. J. González, *ACS Catal.*, **2015**, *5*, 3446

New pseudopeptidic ligands: synthesis and metal recognition behavior

PO-30

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Metal chelation is involved in many biological processes and metal-based drugs have gained much importance in the medicinal field nowadays. They are in use, as medicines for the treatment of diabetes, cancer, anti-inflammatory, antimicrobial and cardiovascular disease.¹ Among the various ligands explored in co-ordination chemistry,² the inclusion of amino acid residues in the ligand structure is one of the most common strategies, not only due to their strong coordinating ability for a variety of metal ions, but also because they provide coordination environments of the metal ions similar to those found in metalloproteins with multiple binding sites.³

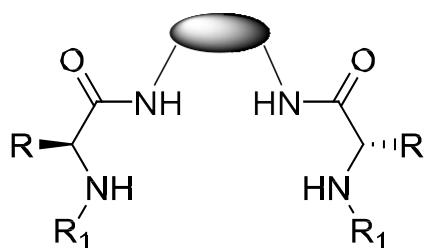


Figure 1. General structure of the pseudopeptidic ligands

Regarding metal complexation, recently our group has studied the coordination ability of some C₂ symmetrical bis(amino amides) derived from amino acids towards Cu(II) and Zn(II) ions.⁴ In this work, we present the synthesis of new bis(amino amide) ligands derived from *L*-valine and *L*-phenylalanine with the general structure shown in figure 1, as well as the analysis of their binding ability towards different M(II) species.

Acknowledgements

CTQ2012-38543-C03-01, PROMETEO2012/020, UJI P1·1B2013-38 and ACOMP/2015/111 are gratefully acknowledged. LG thanks GV for Santiago Grisolia fellowship.

- 1 R.R. Crichton, D.T. Dexter, R.J. Ward, *Coord. Chem. Rev.*, **2008**, 252, 1189–1199.
- 2 Supramolecular Chemistry. Concepts and Perspectives, VCH, Weinheim, Germany, **1995**.
- 3 J. Dong, Y. Wang, Q. Xiang, X. Lv, W. Weng and Q. Zeng, *Adv. Synth. Catal.* **2013**, 355, 692-696.
- 4 a) S. Blasco, M. I. Burguete, M. P. Clares, E. García-España, J. Escorihuela and S. V. Luis, *Inorg. Chem.* **2010**, 49, 7841-7852. (b) E. Faggi, R. Gavara, M. Bolte, L. Fajari, L. Julia, L. Rodríguez, I. Alfonso, *Dalton Trans.* **2015**, 44, 12700-12710.

Síntesis y Propiedades Fotocrómicas de (*SFC,SS*)-*p*-Sulfinil Ferrocenil Azobencenos Enantiopuros

PO-31

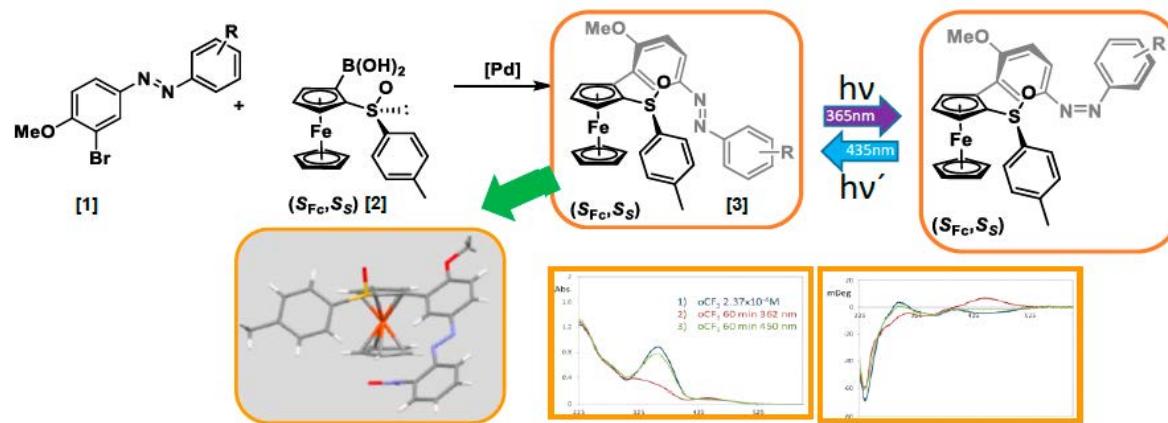
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El control del movimiento molecular representa unos de los objetivos más importantes en la química moderna. Los azobencenos ^[1] son unos excelentes candidatos debido a que pueden existir en dos formas, *cis* (*Z*) y *trans* (*E*), las cuales se pueden interconvertir entre sí fotoquímica- (mediante la radiación adecuada) y térmicamente. Esta interconversión induce un movimiento molecular y un cambio significativo en su geometría, por ello el esqueleto de azobenceno es un excelente candidato para la síntesis de dispositivos moleculares dinámicos.

En este trabajo se presenta la síntesis y el estudio de las propiedades fotocrómicas de una nueva familia de azobencenos **3** ^[2], los cuales presentan tanto quiralidad central como planar, gracias a un resto de sulfinilferroceno. El paso clave para la síntesis de estos nuevos interruptores moleculares es una reacción de acoplamiento cruzado tipo Suzuki entre el bromoazobenceno **1** y el ácido ferrocenilborónico **2**. ^[3]

Las propiedades fotocrómicas y quirópticas de estos compuestos se han determinado mediante espectroscopia de UV, RMN, DC, HPLC y medidas de rotación óptica. La fotoisomerización *trans* \leftrightarrow *cis* se llevado a cabo irradiando una lámpara de alta presión de Hg empleando un filtro de 365nm (*trans* \rightarrow *cis*) y un filtro de 435 nm para reisomerización (*cis* \rightarrow *trans*).



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[2] A. Sakamoto, A. Hirooka, K. Namiki, M. Kurihara, M. Murata, M. Sugimoto, H. Nishihara, Inorg. Chem. 2005, 44, 7547

[3] J. F. Jensen, I. Søtofte, H. O. Sørensen, M. Johannsen, J. Org. Chem. 2003, 68, 1258.

Study of substitution flexible ligands on Iron Oxide nanoparticles by microwave assisted synthesis

PO-32

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A fast method of functionalization of magnetic nanoparticles has been developed. For this work *flexible metallic-organic frameworks* (FL-MOF's) has been tried in conjunction with magnetic nanoparticles to make soft porous crystals. These new functional materials, have fascinating properties may include magnetism, fluorescence, micro-porosity, and can even avoid leaching. These new multifunctional fluorescent magnetic nanoparticles results very useful and can have different applications such as, contrast agent in magnetic resonance imaging, nanoporous materials for VOCs adsorption and adsorption or identification of heavy metals [1, 2, 3, 4].

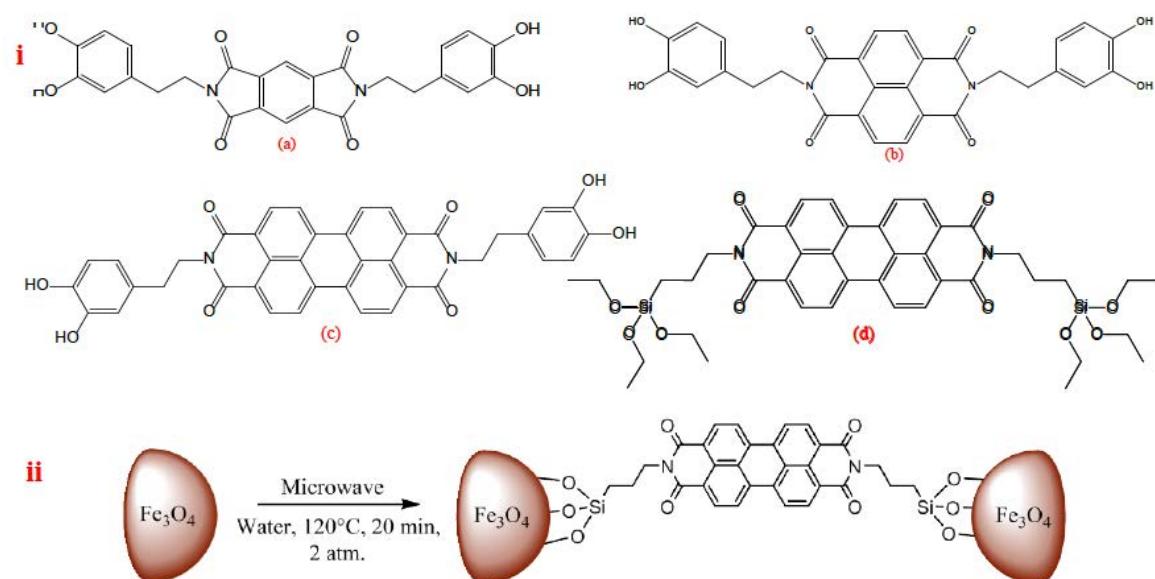


Fig 1. (i) The four different flexible molecules used to functionalize magnetic nanoparticles.
(ii) Example of magnetic nanoparticles functionalization assisted by microwave radiation.

¹ Zu-Jin Lin, Jian Lu, Maochun Hong and Rong Cao. *Chem. Soc. Rev.*, 2014, 43, 5867.

² Lu Yang, Huisheng Peng, Kun Huang, Joel T. Mague, Hexing Li, and Yunfeng Lu. *Adv. Funct. Mater.* 2008, 18, 1526–1535.

³ Devendra Singh and Jubraj B. Baruah. *Crystal Growth & Design*, 2011, 11, 768.

⁴ Kenia A. López, M. Nieves Piña, David Quiñonero, Pablo Ballester and Jeroni Morey. *J. Mater. Chem. A*, 2014, 2, 8796.

Chemical modulation of the CNHs and its applications

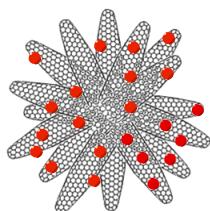
PO-33

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This communication focuses on the various chemical transformations used for selective modification of CNHs. Carbon nanohorns¹ (CNHs) are horn-shaped tubular structures (similar in structure to single-walled carbon nanotubes) capped with a conical tip. Individual nanohorns tend to cluster and form a globular structure between 80 and 100 nanometres in diameter with the tips of individual nanohorns projecting outward from the centre in all directions. The high purity and the lack of metal particles of produced CNHs is their major advantage compared to carbon nanotubes. These nanomaterials have interesting properties such as chemical and mechanical stability. These properties make them suitable for a high range of applications.



Functionalized material

The main handicap of these nanostructures is the lack of solubility, therefore in order to integrate them in different fields, they should be modified. Our group is focused on the design of very versatile new synthetic approaches² for the modification of CNHs. These methodologies allow us to modify the new materials in order to apply them in different fields such as catalysis, materials science, biomedicine....The different systems could be modulated in the search of a wide range of applications based on an appropriate surface modification. Future applications require a better understanding of the structure- property correlations. For this reason, a whole set of techniques such as AFM, TEM, TGA and NMR are often used in our group to characterize the structure of these ensembles. Therefore, in this communication we report our latest development on the functionalization of CNHs, with overview at the most important applications, such as materials and medicinal science.

[1] Iijima, S.; Yudasaka, M.; Yamada, R.; Bandow, S.; Suenaga, K.; Kokai, F.; Takahashi, K., *Chem. Phys. Lett.* **1999**, *309*, 165. [2] Rubio, N.; Herrero, M. A.; Meneghetti, M.; Díaz-Ortiz, A. Schiavon, M.; Prato, M.; Vázquez, E., *J. Mater. Chem.* **2009**, *19*, 4407.

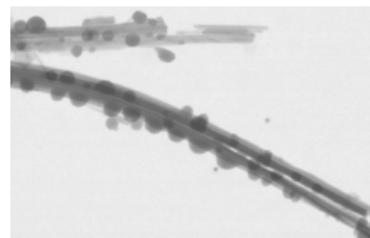
Modificación de Fibras de Sepiolita para la Preparación de Materiales Híbridos basados en Polifluoreno

PO-35

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Los materiales híbridos organo-inorgánicos son ejemplos dentro del campo emergente de la electrónica o fotónica híbrida encontrándose presentes en aplicaciones como placas solares, diodos emisores de luz o como bio-sensores o en bio-imagen mostrando unos excelentes resultados. La motivación de este trabajo es producir materiales avanzados donde las propiedades electrónicas se basan en estructuras no asociadas a las responsables de la buena procesabilidad del material, en otras palabras, diseñar adecuadamente materiales híbridos multiescala. En este trabajo se ha utilizado sepiolita, un filosilicato fibroso presente en la naturaleza en forma de agregados micrométricos con longitudes medias de 2-10 µm. Debido a su abundancia natural, el tamaño de las fibras desagregadas (10-12 nm) y la química superficial basada en grupos silanoles (Si-OH), la sepiolita es un excelente candidato para su modificación y su posterior aplicación. Las fibras de sepiolita se han modificado casi individualmente llevando a cabo una reacción en forma de gel en agua con una mezcla de metiltrimetoxisilano - MTMS/4-bromofeniltrimetoxisilano - BPTMS donde se han condensado nanoesferas las cuales reducen la superficie de contacto entre las fibras y evitan su reagregación. También se ha comprobado que la introducción del grupo funcional bromofenilo en la superficie de las nanoesferas ha permitido realizar la primera policondensación iniciada desde la superficie utilizando catalizadores de paladio portando ligandos tipo carbeno, (IPr)Pd(TEA)Cl₂, para injertar un semiconductor orgánico fluorescente, poli(9,9-dioctil)fluoreno. Con esta metodología se ha demostrado que la hidrofobización, desagregación y la incorporación de grupos funcionales en las nanoesferas de la superficie de las fibras de sepiolita ha permitido el injerto de poli(9,9--dioctil)fluoreno. De este trabajo se concluye que es posible la utilización de este silicato como portador de polímeros conjugados fluorescentes y aprovechar el comportamiento tixotrópico de la sepiolita en el procesado de estos materiales híbridos funcionales multiescala.



Agradecimientos

La investigación que lleva a estos resultados ha recibido financiación del programa People (Marie Curie Actions) del 7º Programa Marco de Investigación de la Unión Europea (FP7/2007-2013) en virtud del acuerdo de subvención nº PIIF-GA-2012-327563.

Activación pionera de tioureas quirales con complejos de Au

PO-36

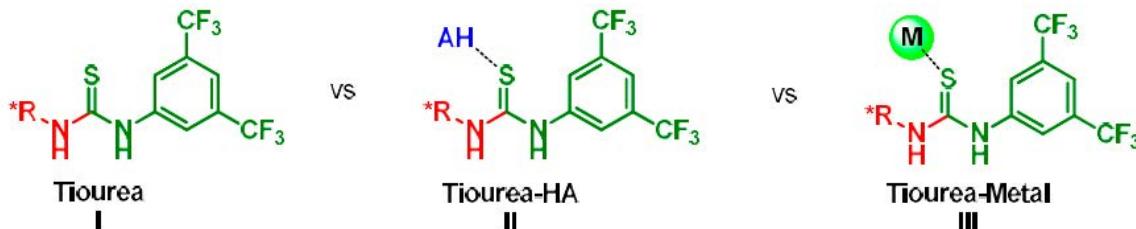
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Es bien conocido, que la organocatálisis ha experimentado un gran avance en el campo de la catálisis homogénea durante los últimos años, pero aún necesita superar algunos inconvenientes para conseguir emular los éxitos alcanzados con la catálisis enzimática o la metálica.

En este contexto, estudios previos han demostrado que la actividad de los organocatalizadores tiourea (I) puede verse modificada mediante la activación de los mismos con un ácido de Brønsted externo (II).¹ Basándonos en estos resultados, surgió la idea de que ese mismo efecto pudiera llevarse a cabo con un metal (III).

Así, en el presente trabajo, se muestran los primeros resultados obtenidos con una variedad de complejos catalíticos, en los que se combina una parte metálica (metal del grupo 11) con una tiourea quiral de forma sinérgica (III), con el objetivo de aprovechar las principales características que presenta cada una de estas especies por separado y unificarlas en un único complejo estable donde la tiourea sigue actuando como organocatalizador, viendo aumentada su capacidad catalítica.²



¹ Marqués-López, E.; Alcaine, A.; Tejero, T.; Herrera, R.P. Eur. J. Org. Chem., 2011, 3700-3705.

² Trabajo Final de Máster, Anabel Izaga Sebastián (2013-2014). Artículo en preparación.

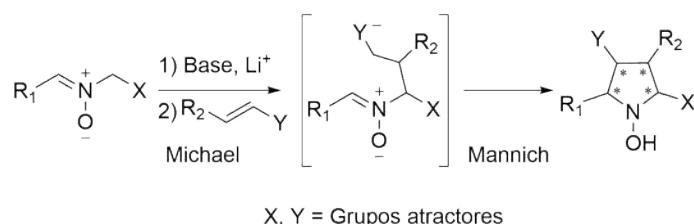
Síntesis de *N*-óxidos de 4,5-dihidroxazoles mediante reacciones de iluros de nitrona y aldehídos.

PO-37

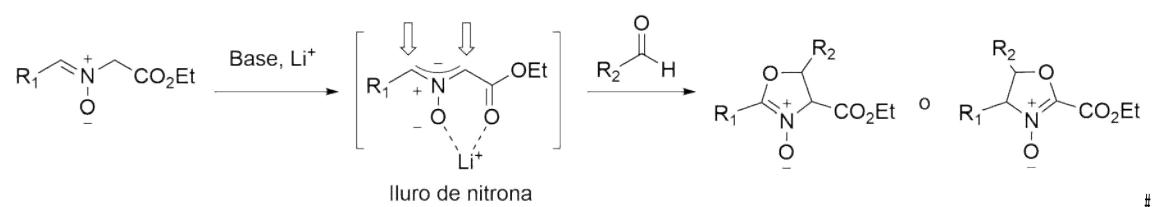
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La reacción de iluros de nitrona con olefinas deficientes en densidad electrónica ha sido estudiada en nuestro grupo de investigación.¹ Esta reacción transcurre a través de un mecanismo por pasos: reacción de adición Michael y posterior ciclación intramolecular de tipo Mannich para proporcionar *N*-hidroxipirrolidinas.



Con el fin de ampliar este estudio, se ha llevado a cabo la reacción con diversos aldehídos. En este caso, la regioselectividad de la reacción varía en función del sustituyente unido al grupo nitrona (R_1). Así, con R_1 =Arijo el ataque sobre el aldehído se produce a través del carbono del iluro unido al grupo éster, mientras que con R_1 =Alquilo, el ataque lo lleva a cabo el átomo de carbono del grupo nitrona.



En la comunicación se describen las experiencias realizadas y una propuesta para justificar la regioselectividad observada.

¹ P. Merino, T. Tejero, A. Díez-Martínez, *J. Org. Chem.*, **2014**, 79, 2189

Compuestos luminiscentes ciclometalados de Pt(II) y Pt(IV) basados en la unidad 2-fenilbenzotiazol

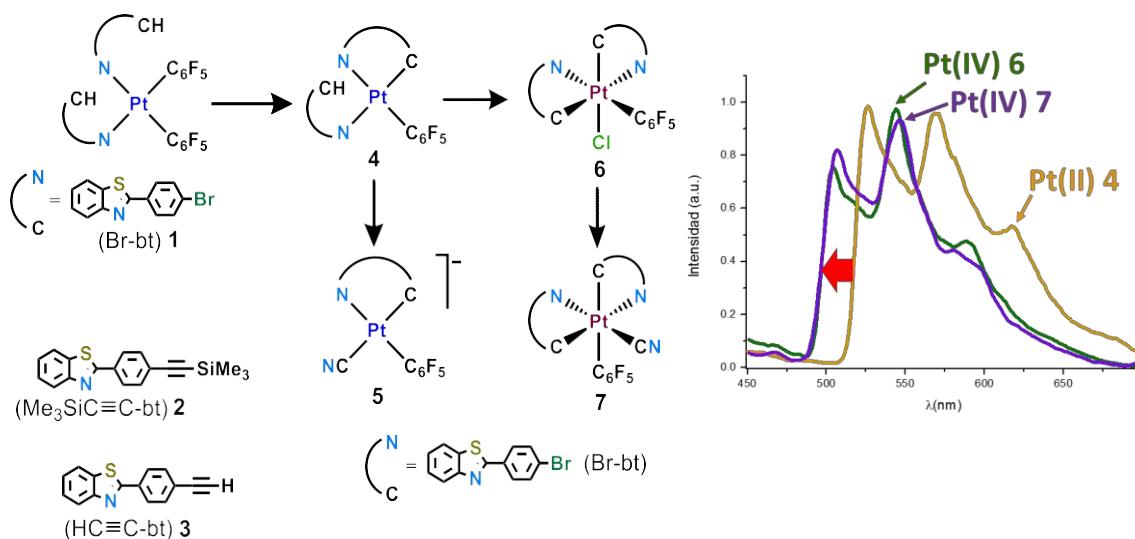
PO-38

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Los compuestos luminiscentes ciclometalados de Pt(II) han sido ampliamente estudiados debido al notable interés asociado a sus potenciales aplicaciones como dopantes en materiales electroluminiscentes, sensores, marcadores biológicos o fotocatálisis. Sin embargo, los estudios de las propiedades ópticas de derivados de Pt(IV) en general, y de compuestos ciclometalados de Pt(IV) en particular, son muy escasos.

En este trabajo se describe la síntesis y caracterización de derivados que contienen dos ligandos basados en la unidad 2-fenilbenzotiazol coordinados por el nitrógeno *cis*- [Pt(R-Hbt-*κN*)₂(C₆F₅)₂] (R = Br **1**, Me₃SiC≡C **2**, HC≡C **3**). El derivado **1** sufre activación de un ligando Br-Hbt para generar el compuesto ciclometalado [Pt(Br-bt-*κC,N*)(Br-Hbt-*κN*)(C₆F₅)] **4**, que puede ser oxidado con IPhCl₂ formando el derivado de Pt(IV) bis-cyclometalado [Pt(Br-bt-*κC,N*)₂(C₆F₅)Cl] **6**. Además, mediante reacciones de sustitución se han obtenido los derivados ciclometalados de Pt(II) (**5**) y Pt(IV) (**7**) con el ligando de campo fuerte CN⁻, lo que mejora notablemente las propiedades emisivas. Se han confirmado por difracción de Rayos X las estructuras cristalinas de algunos de estos derivados y se ha llevado a cabo un estudio detallado comparativo de las propiedades fotofísicas de estos compuestos.



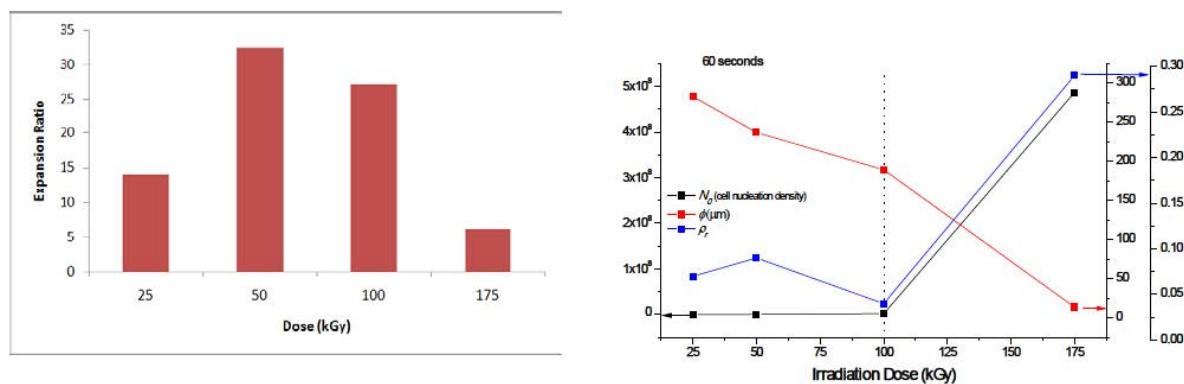
Study of the Cell Structure of LDPE foams Irradiated at Different Doses

PO-39

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Polyethylene foams have attracted much attention due to their excellent properties such as flexibility, high thermal stability or good mechanical properties. Crosslinking^{1,2} of the foam is essential in order to stabilize the cell structure of the foam. There are two ways to crosslink a polymer: chemically or physically³. A physical via (electron beaming) was used to crosslink a low density polyethylene (LDPE). Mixes of LDPE (85%) and azodicarbonamide (15%) (blowing agent) were irradiated at different doses (25, 50, 100 and 175kGy) in order to see how the dose affects the cellular structure of the foams. In this work we present some results related to variations in density, cell size and cell nucleation density when the dose increases. Lower density, smaller cell sizes and higher cell nucleation density is obtained when the irradiation is higher. These results are in agreement with a previous work carried out by this group for rubber foams⁴.



¹ H.J. Tai, J.B. Wang, *Journal of Cellular Plastics*, **1997**, 33, 304

² MA. Rodríguez-Pérez, *Advanced in Polymer Science*, **2005**, 184, 97

³ D.Batista, L.Gondim, *Radiation Physics and Chemistry*, **2007**, 76, 1696

⁴ L. Oliveira .2015. *Cinéticas de espumación y control de la estructura celular en materiales basados en caucho natural y poliolefinas*

Functionalization Of Aluminium Oxy-Hydroxide With Long-Chain
Amidosquaric Acids

PO-40

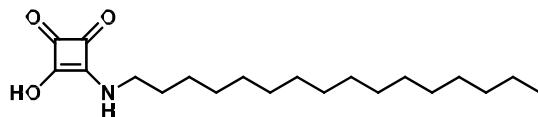
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We investigate the chemical adsorption of long-chain amidosquaric acids on an Al oxy-hydroxide surface. Such molecules exhibit strong acidity and low solubility in most solvents, and have not been used so far for attachment to solid surfaces. Thus, using AFM and SEM images, MALDI-TOF, XPS spectroscopy, contact angle measurement, solid-state UV spectroscopy and grazing angle infrared spectroscopy, the bonding process of the amidosquaric acids has been studied, proving its chemical nature. The results have been compared with those obtained with fatty acids, whose binding capacity on aluminium has been fully characterized previously¹. According to that, binding kinetics of adsorption of fatty acids has been proven to be faster. Nevertheless, amidosquaric acids show a greater stability, remaining attached to the surface after being rinsed with water and isopropanol.



Hexadecylamidosquaric acid

¹ I. Liascukiene, N. Aissaoui, S. J. Asadauskas, J. Landoulsi, J. Lambert, *Langmuir*, **2012**, 28, 5116

Síntesis de Compuestos Fotoprotectores

PO-41

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Parte de la radiación que nos llega del sol es dañina para los organismos vivos, por ello a parte de los mecanismos que posee la tierra para eliminarla, los organismos han ido perfeccionando sus sistemas de fotoprotección a lo largo de millones de años. En la actualidad se conocen varios tipos de metabolitos que presentan este rol biológico, como son las melaninas, la escitonemina,¹ los carotenos y las micosporinas.

Un caso singular son las micosporinas también conocidas como aminoácidos de tipo micosporina o MAAs. Estos metabolitos presentan unas propiedades físico-químicas² que unidas a sus propiedades fotoquímicas justifican su alta eficiencia como fotoprotectores.³ Estos compuestos se dividen en dos grandes grupos atendiendo a su estructura, las aminociclohexenonas y las aminociclohexeniminas, que presentan una fotoquímica que las hace candidatas a ser un excelente fotoprotector.



Esquema 1: Estructura genérica de aminociclohexenona y aminociclohexenmina presente en los MAAs.

En esta comunicación se presenta parcialmente la primera síntesis de análogos de los MAAs con estructura de aminociclohexenmina y las propiedades fotofísicas y fotoquímicas más relevantes de los análogos sintetizados.

¹ F. Garcia-Pichel, R. W. Castenholz, *J. Phycol.* **1991**, 27, 395-409.

² J. Favre-Bonvin, N. Arpin, C. Brevard, *Can. J. Chem.* **1976**, 54, 1105.

³ D. Sampedro, *Phys. Chem. Chem. Phys.* **2011**, 13, 5584-5586.

Nuevos organocatalizadores para la reducción enantioselectiva de iminas empleando Cl₃SiH como reductor

PO-42

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Las aminas que contienen un estereocentro en posición a respecto al átomo de nitrógeno son las que se encuentran con frecuencia en las moléculas bioactivas y en los productos naturales. Por ello, existe un gran interés en desarrollar métodos para su síntesis. La obtención de aminas quirales a partir de la reducción de cetonas proquirales empleando intermedios de imina representa una estrategia atractiva y sencilla para la obtención de estas aminas enantiopuras.¹

En esta comunicación se presentan una serie de organocatalizadores basados en estructuras de α,β -aminoamidas², para la reducción de iminas proquirales empleando Cl₃SiH como agente reductor:

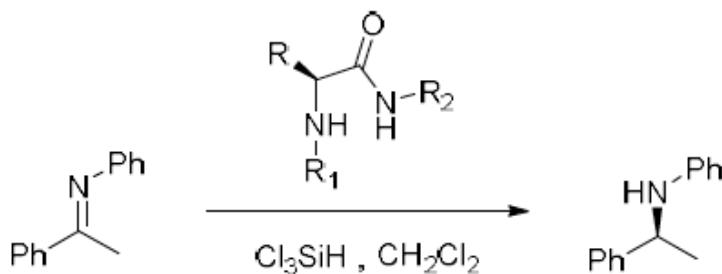


Figura 1: Reducción enantioselectiva de iminas.

Los estudios realizados demuestran que tanto la estructura del catalizador como su concentración son factores claves para conseguir aminas con buenas enantioselectividades.

AGRADECIMIENTOS: Financiado por GV-PROMETEO/2012/020 y UJI-P1-1B2013-37.

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Síntesis Asimétrica de APN's basada en una reacción dominó

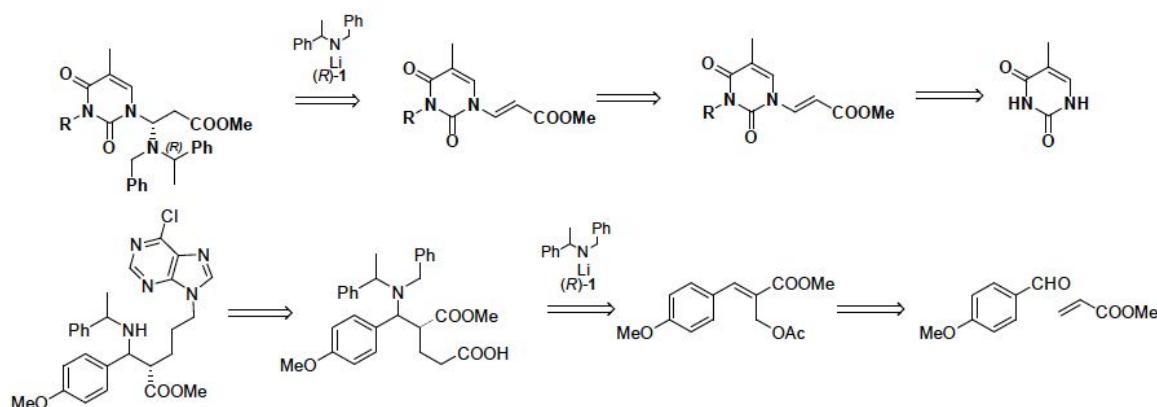
PO-43

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Los ácidos péptido nucleicos (APN) son una clase de ácidos nucleicos (xeno-homólogos de ácidos nucleicos no naturales) con aplicación en la terapéutica de genes, biosensores, o biomateriales. En los APN's la cadena ribosa-fosfato se reemplaza por una cadena de poliamida.^{1,2} De esta manera la secuenciación se determina en función de las bases nitrogenadas presentes en las cadenas laterales.

Nuestro grupo ha descrito las estrategias de una reacción dominó: que incluye los reordenamientos de acetato alílico y estereoselectivo de Ireland-Claisen seguidos de una adición asimétrica de Michael.³ Esta metodología nos permite obtener el δ aminoácidos directamente por tratamiento de aductos de Baylis-Hillman con el amiduro de litio quiral (*R*)-1.⁴ Además también hemos desarrollado estrategias que permiten la inserción de cadenas carbonadas en bases nitrogenadas y sus posterior derivatización. Con estas técnicas podemos obtener APN's enantioselectivamente.⁵



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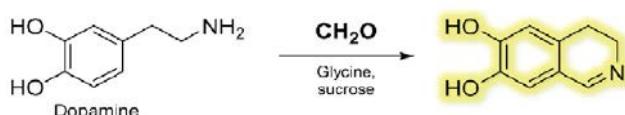
Dosimeter for detection of formaldehyde and future perspectives

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Formaldehyde is one of the most widely used compounds in the chemical industry. It is mainly found with urea, melamine or phenol, forming resins for the furniture and wood industry. Several agencies dedicated to the study of cancer, such as IARC or WHO catalog formaldehyde as an irritant and carcinogen. Current detection systems for this compound have the main disadvantage of low sensitivity and false positive in the presence of some interferences. This creates the need for systems capable of reliably detecting the presence of formaldehyde quickly.

In this work, dopamine in the presence of glycine and sucrose is capable to detect formaldehyde by Pictet-Spengler reaction. This reaction gives rise to isoquinolines, which are oxidized in situ to form the corresponding dihydroisoquinolin, which is colored and have fluorescent properties.



After verifying the effectiveness of the dosimeter in solution and determining its limits of detection, its sensing capability toward gaseous formaldehyde was studied in a solid support.



At present, the possibility of improving these results is being developed using "cassettes" compounds. These compounds combine the previous dosimeter with a BODIPY core. This strategy allows dopamine (donor) to react with formaldehyde and upon absorption generate a signal that will be transmitted through bond energy transfer to the BODIPY core (acceptor). This BODIPY core will be responsible of exhibiting a fluorogenic response.

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First homoleptic MIC and heteroleptic NHC–MIC coordination cages from 1,3,5-triphenylbenzenebridged tris-MIC and tris-NHC ligands

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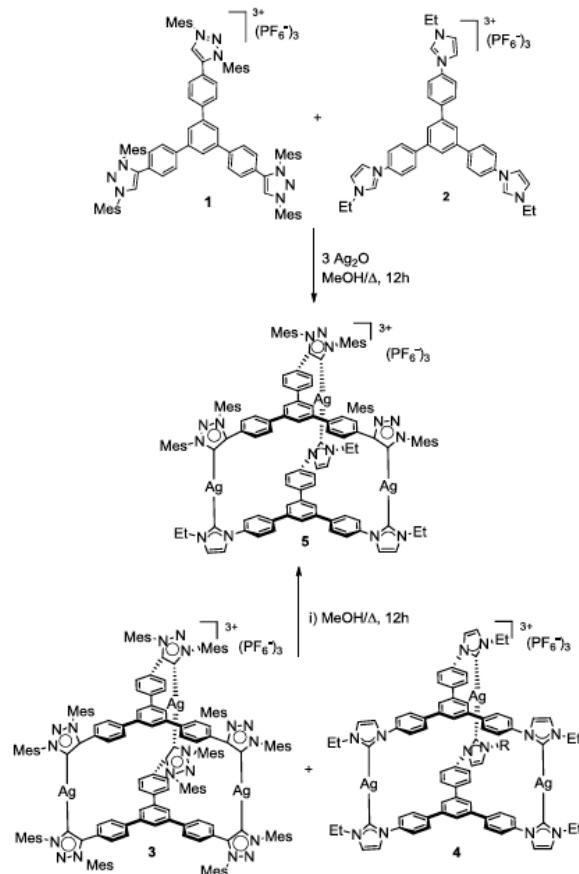
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The development of self-assembly architectures with very small cavities has become a very intense field of research, due to their ability for hosting molecules.¹

Based on our previous experience,² herein we present the preparation of a triphenylene-bridged tris-(1,2,3-triazolium) salt (**1**). This salt allowed us to obtain the first homoleptic tris-MIC cylinder-like cages of Ag and Au, proving that this type NHC-relatives may be used for the metal-controlled self-assembly of nanometer-sized cylinder-shaped molecules.

The silver MIC-based cage (**3**), reacts with the tris-NHC-Ag analogue (**4**), to form the corresponding heteroleptic NHC-MIC silver cage (**5**), by an unusual reaction involving the rearrangement of the tris-NHC and tris-MIC ligands, illustrating the lability of the tris-NHC and tris-MIC ligands on silver in solution. The heteroleptic **4** can also be obtained from the reaction of the tris-imidazolium and tri-triazolium salts **1** and **2** with Ag₂O.³



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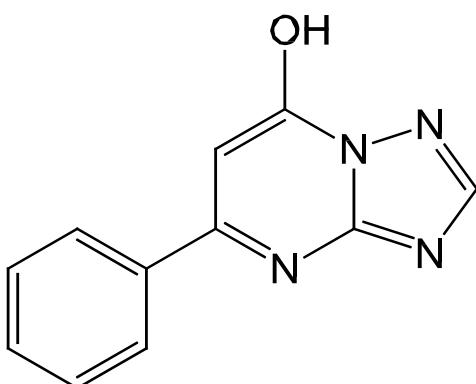
Síntesis y caracterización de nuevos complejos metálicos de derivados triazolopirimidínicos con potencial actividad leishmanicida

PO-46

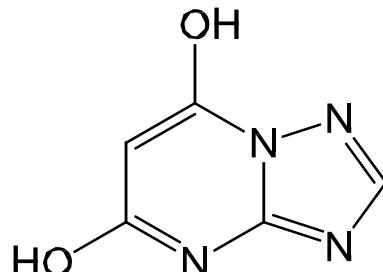
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En los últimos años, nuestro grupo de investigación ha sintetizado y caracterizado estructuralmente un importante número de complejos metálicos con derivados de la triazolopirimidina [1]. Para el caso concreto de la 5-fenil-7-hidroxi-1,2,4-triazolo[1,5-a]pirimidina (HftpO) se han obtenido dos series de acuocomplejos de este ligando con elementos de transición y lantánidos que responden a fórmulas del tipo $[M(\text{ftpO})_2(\text{H}_2\text{O})_4]$ siendo $M=\text{Cu, Co, Ni y Zn}$; y $[\text{Ln}(\text{ftpO})_3(\text{H}_2\text{O})_6]$ siendo $\text{Ln}=\text{La, Gd, Eu, Nd, Er, Tb, Dy y Yb}$. Como paso previo al estudio de la actividad leishmanicida de estos complejos se ha estudiado la actividad antiparasitaria del HftpO encontrándose unos valores de IC₅₀ superiores a 20 frente a *L. braziliensis* (28,40), *L. donovani* (22,68) y *T. cruzi* (53,41). En la actualidad los estudios antiparasitarios se han extendido a otros ligandos, como es el caso de la 5,7-dihidroxi-1,2,4-triazolo[1,5-a]pirimidina (H2tpO₂) y a los complejos metálicos de ambos que se han aislado.



Estructura del HftpO



Estructura del H2tpO₂

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H₂O₂ formation induced by Cu²⁺-Aβ(1-16) complexes.

PO-47

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During the on-set of Alzheimer's disease copper ions and pathologically accumulated amyloid-β (Aβ) peptides are all present in the synaptic region of neurons. Cu²⁺ can form stable complexes with Ab and several studies indicate that Cu²⁺-Ab interaction mediate the toxicity of the peptide through the catalytic production of H₂O₂.^{1,2} Specifically, these complexes could contribute to the production of H₂O₂ that in turn derives in the formation of ROS through Fenton and Haber-Weiss like reactions^{3,4} increasing the oxidative stress.

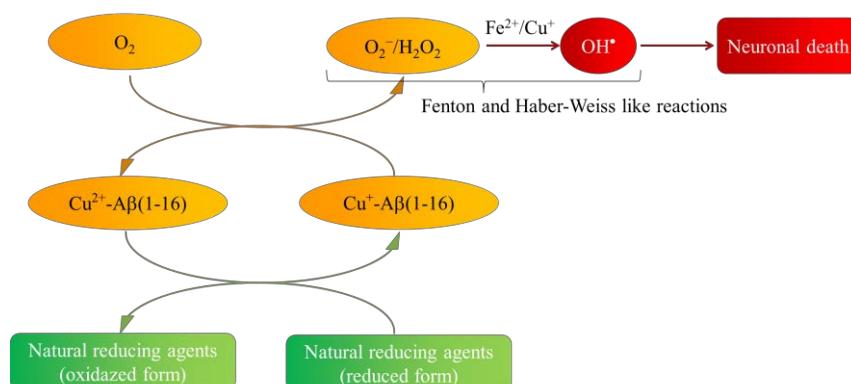


Figure 1. Schematic representation of the catalytic cycle of the Cu-induced ROS generation with the specific reactions studied in this work to the H₂O₂ formation.

In this work, we report computational simulations of H₂O₂ formation for a range of Cu(I)-Aβ(1-16) models previously obtained in Ref. 5 after reduction of Cu(II)-Aβ(1-16). Results show that in all cases the key step of the mechanism seems to be the superoxide formation. Moreover, the energy barriers for this step are small, thus corresponding to a fast process. The role of the coordination environment and second sphere interactions on superoxide formation is analyzed.

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Novel Cationic Alkynes as Scaffolds for Thermal and Cu(I) Catalyzed Azide- Alkyne Cycloaddition Reactions

PO-48

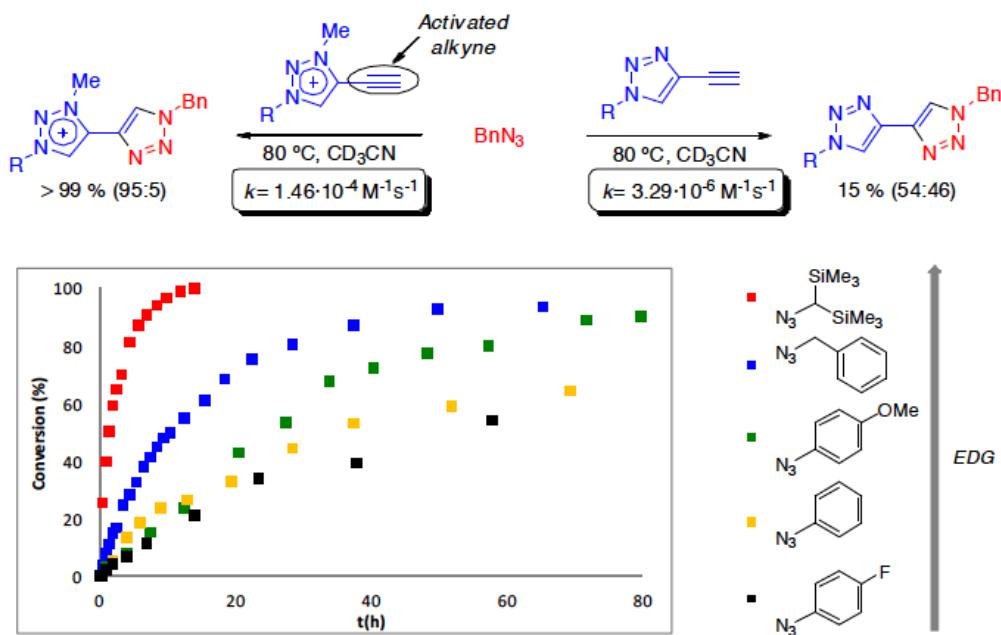
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Copper(I)-accelerated azide-alkyne [3+2] cycloaddition reaction has become one of the most reliable methods to connect molecules covalently; however the copper-free version of this reaction usually requires prolonged reaction times and lacks regioselectivity.¹ Therefore, different approaches have been developed to increase the reactivity of the alkyne groups to promote metal-free azide-alkyne cycloadditions under milder conditions and improved regioselectivity.²

Herein, we report the synthesis of novel cationic alkynes³ and their reactivity with azides under thermal and Cu(I)-activated conditions. Metal-free 1,3-dipolar cycloadditions showed a quasi-total regioselectivity (> 95 %) and an increase of the reaction rate of about two orders of magnitude, according to kinetic and computational studies. In addition, under Cu(I)-activated conditions, “ultrafast” click reactions (less than 1 minute) were carried out with several azides to yield nonsymmetrically substituted 4,4'-bis(1,2,3-triazolium) derivatives.



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Isoreticular series of Zirconium Metal-Organic Framework. Catalytic Applications

PO-49

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Nowadays, many research groups are trying to synthesize new Metal-Organic Frameworks (MOFs) with very large surface areas and pore volumes, in order to obtain highly porous materials suitable for the catalysis of middle/large size molecules. On top of this, renewed interest is addressed towards achieving novel porous structures exhibiting high stability in catalytic conditions that would result in their effective use under practical applications.

In this communication, we report the synthesis and structural characterization of an isoreticular MOF series based on zirconium clusters and novel dicarboxylate ligands with customized functionalizations. For this purpose, multiple Sonogashira coupling reactions have been used as the key step for linker synthesis, allowing thereby the introduction of different functionalization. The resulting materials are highly stable. We have studied the catalytic applications in comparison with other Metal-Organic Frameworks.

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Relevance of silicate surface morphology in interstellar H₂ formation

PO-50

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Among the molecules in space, H₂ is one of the most relevant of the universe. It is the most abundant one in the interstellar medium and is a key intermediate for the formation of more complex molecules. Its formation is complex, but due to its inherent relevance understanding its interaction and its formation can be considered as a paradigm of the astrophysical process. The association of two H atoms on the surfaces of cosmic dust, which consists partly of Mg,Fe-silicates, is thought to be the main reaction channel for H₂ formation in these regions. It involves first the adsorption of two H atoms on the surface, the subsequent diffusion of the ad-atoms and the final recombination to form H₂. In this presentation^{1,2} H₂ formation has been studied by means of B3LYP-D2* periodic calculations performed with the CRYSTAL09 code. The reaction has been studied on the (010), (001) and (110) surfaces of forsterite (Mg₂SiO₄), which represent surfaces of different stability and surface morphology. The most stable H adsorption states sport the H atom on surface O atoms, forming a SiOH group and transferring the H spin density to the neighbouring Mg ion. Because of that, the second H adsorption occurs on the neighbouring Mg ion, forming an Mg–H surface group, which enables the formation of a di-hydride OH···H–Mg hydrogen bond. The formation of a H₂ molecule adopting a Langmuir–Hinshelwood mechanism does not occur equally at the different forsterite surfaces. On the (010) surface, the formation takes place either starting from two physisorbed H atoms through a radical–radical coupling driven reaction or from a hydride-proton coupling with barriers surmountable at very low temperatures. On the (110) surface, the unique route is through a hydride- proton coupling, whereas on the (001) surface the reaction is disfavoured because the doubly-H-adsorbed initial states are more stable than the final product.

J. Navarro-Ruiz, M. Sodupe, P. Ugliengo, A. Rimola, *Phys. Chem. Chem. Phys.*, **2014**, 16 (33), 17447
J. Navarro-Ruiz, J. Á. Martínez-González, M. Sodupe, P. Ugliengo, A. Rimola, *Mon. Not. R. Astron. Soc.*, **2015**, 453 (1), 914

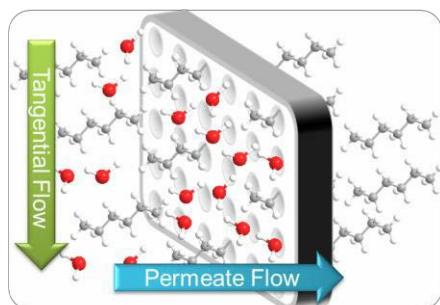
Modulación funcional de membranas monolíticas tubulares y aplicación en procesos de separación

PO-51

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La Química Verde y dentro de ésta la integración de procesos químicos adquiere hoy en día un rol muy importante y necesario. Así, el desarrollo de membranas monolíticas tubulares que sean capaces de separar mezclas bifásicas, emulsionantes o enriquecer mezclas homogéneas y, simultáneamente de servir como soporte para diferentes catalizadores puede facilitar la integración, en un único sistema, de procesos de reacción/separación.



En este trabajo se describe el método de preparación y la caracterización de diversas membranas poliméricas tubulares modificadas con utilidad en el campo de la ultrafiltración. Estas membranas, preparadas previamente a partir de una mezcla de monómeros estructurales y de entrecruzamiento en presencia de una sustancia porogénica, son modificadas posteriormente con la introducción de grupos funcionales específicos con el objetivo de modular sus propiedades, tanto la polaridad superficial como la porosidad, de modo que sean más selectivas en las separaciones de interés.

Agradecimientos: GV (PROMETEO/2012/020), UJI-P1-1B2013-37, MECD (CAS14/00001)

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Interacciones ADN-oligoescuaramidas cílicas

PO-52

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El desarrollo de compuestos capaces de interaccionar con moléculas biológicas como son el ADN u otros compuestos bioactivos, y facilitar su transporte a través de membranas biológicas, es de gran importancia para garantizar el transporte hacia el interior celular de forma eficiente¹. En este trabajo, se presenta la síntesis y evaluación de la interacción de una serie de oligoescuaramidas macrocíclicas frente a ADN. Los macrociclos sintetizados están formados por dos unidades escuaramida unidas entre sí mediante cadenas alifáticas decoradas con diferentes grupos funcionales. Las escuaramidas son unas excelentes unidades de reconocimiento con la capacidad de establecer enlaces de hidrógeno con oxoaniones. La combinación de grupos escuaramida con grupos tetraalquilamonio en una misma estructura, resulta muy adecuada a la hora de reconocer de forma selectiva oxoaniones como por ejemplo, fosfatos, sulfatos, carbonatos. Los estudios de interacción² oligoescuaramida cílica- ADN se han realizado mediante AFM e ITC utilizando como modelo de ADN el plásmido pmax-GFP, ADN de Salmón, ADN de esperma de Arenque y un pentanucleótido (CCTTT). Estos estudios junto con la determinación de las propiedades físico-químicas de los complejos ADN-cicloescuaramida como son el potencial zeta y el tamaño de los complejos han permitido establecer la relación estructura-interacción de cada uno de los macrociclos estudiados.

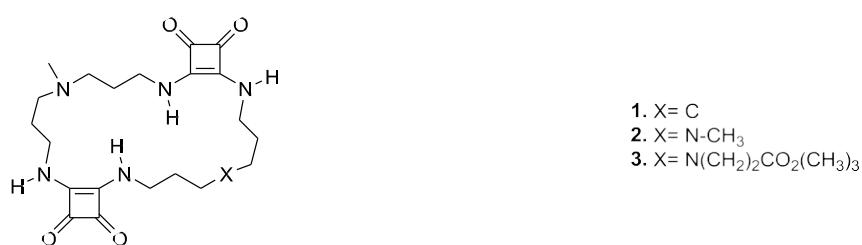


Figura 1. Estructura molecular de algunos compuestos cicloescuaramídicos.

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Pt(III) vs. Pt(IV) en la oxidación de complejos de Pt(II)

PO-53

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La tendencia que muestra un ligando didentado a actuar como quelato o como puente depende de la disposición de los átomos dadores en el esqueleto del ligando, de su rigidez y del volumen que ocupa el resto de ligandos que completan la esfera de coordinación del metal.¹

Se conoce una amplia variedad de complejos dinucleares de Pt(II) con propiedades de interés tanto ópticas como redox,² lo que permite además el acceso a complejos en estados de oxidación superiores con importantes aplicaciones en quimioterapia³ o para la acumulación de energía solar.⁴

En este trabajo se presenta y compara el comportamiento de complejos dinucleares de Pt₂(II,II) con distintos ligandos puente, [Pt(C₆F₅)Cl(m-napy)₂Pt(C₆F₅)Cl] y [Pt₂(C₆F₅)₄(m-ampy)₂], frente a procesos de oxidación con halógenos. Dependiendo de la flexibilidad del ligando puente, napy vs. ampy, se alcanzan estados de oxidación distintos en cada caso. Así, con el ligando ampy más flexible, se obtiene un complejo dinuclear de tipo Pt₂(IV,IV) que contiene además un ligando cloro monopuente (Fig. 1a). Por el contrario, con el ligando napy más rígido, la oxidación se detiene en el complejo de tipo Pt₂(III,III) que contiene un enlace Pt–Pt notablemente corto (Fig. 1b).

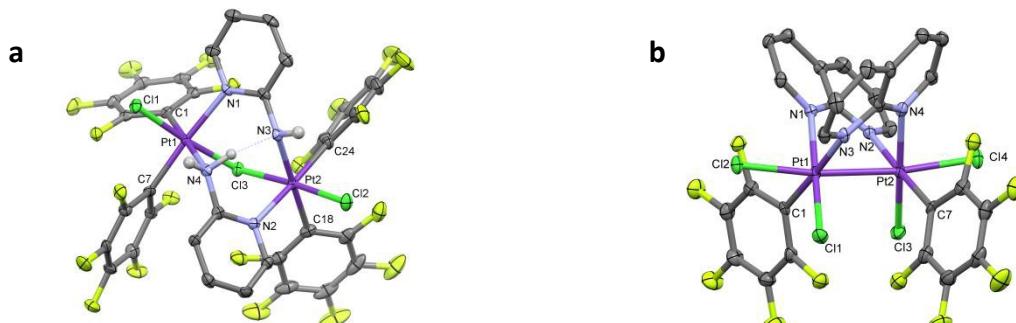


Figura 1. Estructura molecular de los complejos dinucleares de tipo: **a)** Pt₂(IV,IV) con el ligando 2-aminopiridina (ampy); y **b)** Pt₂(III,III) con el ligando 1,8-naftiridina (napy).

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SNF472 inhibe la calcificación cardiovascular en ratas inducida por vitamina D

PO-54

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Introducción: SNF472, una formulación intravenosa de myo-inositol hexafosfato, se está desarrollando para prevenir la calcificación cardiovascular en pacientes con enfermedad renal crónica (ERC) que están en tratamiento de hemodiálisis. En este estudio se evalúa la eficacia de SNF472 en la prevención de la calcificación cardiovascular inducida por vitamina D3 (colecalciferol) en ratas.

Métodos: El estudio se realizó con 50 ratas Sprague Dawley repartidas en 5 grupos. La calcificación cardiovascular se indujo por administración subcutánea de Vitamina D3 a una dosis de 75000 UI/kg durante los tres primeros días. El tratamiento consistió en administrar diariamente, y por vía subcutánea, 2 mL/kg de suero salino o dosis crecientes de SNF472. El grupo 1 (control) recibió suero salino y los grupos 2, 3, 4 y 5 dosis de 3, 10, 30 y 100 mg/kg de SNF472, respectivamente. El día 12 se sacrificó a los animales y se extrajeron aortas y corazones. Para evaluar la calcificación cardiovascular se determinó el contenido en calcio de estos tejidos por espectroscopia de emisión con plasma de acoplamiento inductivo (ICP-OES).

Resultados: La administración de vitamina D3 indujo un aumento en los niveles de calcio en aorta y corazón. Estos niveles se vieron reducidos al ir aumentando la dosis de SNF472. La administración subcutánea de SNF472 a dosis de 30 y 100 mg/kg inhibió significativamente la calcificación en aorta en un 63 y 75%, respectivamente. En el corazón, todas las dosis probadas produjeron inhibición significativa de la calcificación: dosis de 3, 10, 30 y 100 mg/kg de SNF472, inhibieron un 45, 54, 69 y 80%, respectivamente.

Conclusiones: El tratamiento subcutáneo con SNF472 a dosis de 30 y 100 mg/kg, inhibe significativamente la calcificación cardiovascular inducida por vitamina D3 en ratas. Por ello, se podría estudiar SNF472 como posible fármaco para prevenir la calcificación cardiovascular en pacientes con ERC.

Catalizadores fotomodulables de iridio(III) para la reacción de hidrosililación de iminas

PO-55

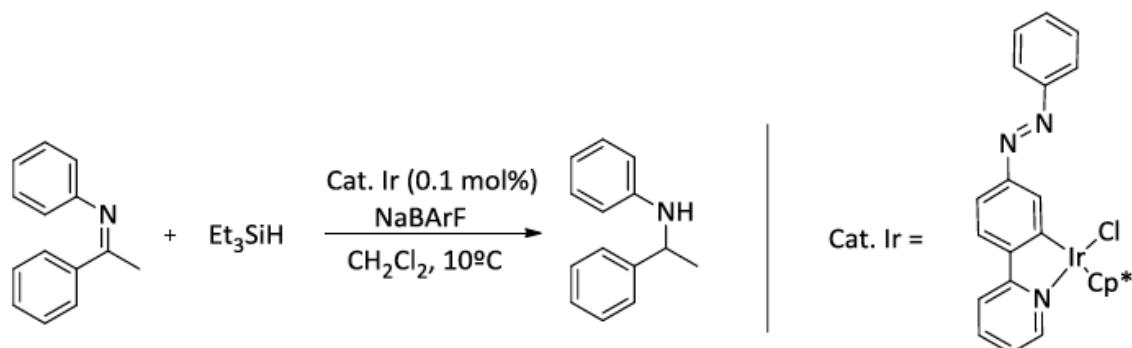
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El desarrollo de nuevas metodologías para la síntesis de aminas presenta interés industrial debido a que se trata de intermedios de reacción frecuentes en numerosos productos farmacéuticos y/o agroquímicos.¹ Uno de los posibles métodos de síntesis es la reducción de iminas catalizada por complejos metálicos, ya sea a través de procesos de hidrogenación, hidrogenación por transferencia o hidrosililación.² Muy recientemente se ha publicado la aplicación de complejos de tipo half-sandwich ciclometalados de iridio(III) como catalizadores muy efectivos para este último proceso en condiciones muy suaves y utilizando reactivos relativamente económicos (organosilanos).³

En nuestro grupo de investigación, trabajamos en la síntesis de complejos half-sandwich de iridio(III), con ligandos de tipo fenilpiridina que incorporan grupos azobenceno en su estructura. Este fragmento azobenceno, experimenta una fotoisomerización reversible de la forma *trans* a la forma *cis*, produciendo cambios estructurales y electrónicos en la molécula.⁴ En nuestro proyecto de investigación estudiamos si las propiedades y/o funcionalidad (actividad y/o selectividad catalítica) de dichos complejos fotosensibles se podrían modificar mediante estímulos externos (irradiación de luz y/o temperatura).

Los resultados preliminares de la aplicación de este tipo de compuestos en la reacción de hidrosililación de iminas en comparación con los sistemas ya publicados, así como su eventual fotocontrol, se discutirán en esta comunicación.



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Task specific Supported Ionic Liquid-Like Phases (SILLPs) for Strecker reactions under continuous flow conditions

PO-56

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Many research efforts are driven to the development of more efficient and sustainable synthetic processes for the preparation of Fine Chemicals and Pharmaceutical products. In last years, we have been exploring the combined use of continuous flow systems and heterogeneous reagents or catalysts immobilized onto Supported Ionic Liquid-like Phases (SILLPs) to achieve this goal. The immobilization of the catalyst onto a polymeric SILLP as support facilitates the separation and reuse of the catalyst, providing products not contaminated by elements of the catalytic system and, simultaneously, allowing for the implementation of continuous processes.¹ The structural design elements of SILLPs allows us to fine tune the catalyst activity in the case of supported Scandium Triflate allowing to obtain a catalyst for the Strecker reaction that is more active than any other supported $\text{Sc}(\text{OTf})_3$ previously reported.² This task specific Sc-SILLP provides, for the model Strecker reaction under continuous flow conditions, excellent yields, productivities and long-term catalyst stability.

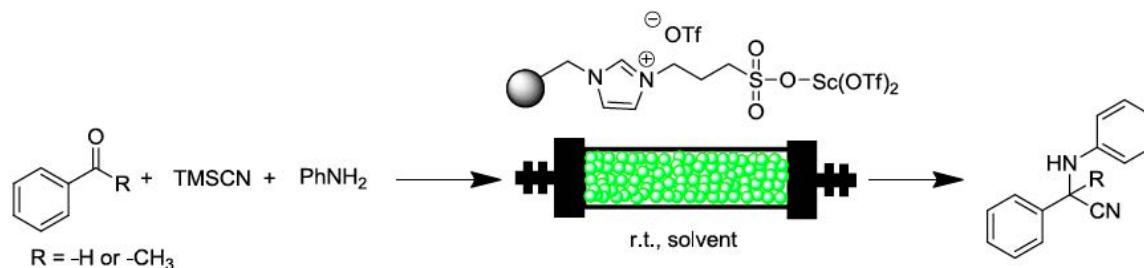


Figure 1. General scheme for Strecker reaction under continuous flow conditions

Despite of this success, other catalytic possibilities and conditions were studied in order to understand better this reaction that allows us to synthesize key compounds of importance as intermediates for the synthesis of some important drugs like Rivastigmine or (S)-Dapoxetine.

Acknowledgements: MICINN (FPU13/00685), GV (PROMETEO/2012/020) and UJI-P1·1B2013-37

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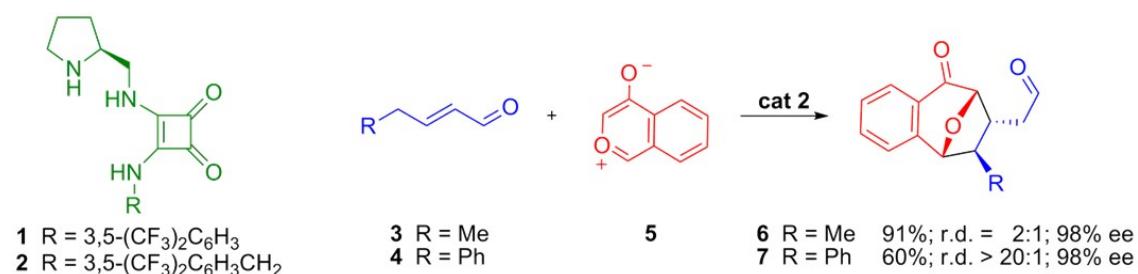
Estudio mecanístico de cicloadiciones catalizadas por un organocatalizador bifuncional derivado de pirrolidina y escuaramida

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Los catalizadores bifuncionales han jugado un papel fundamental en el desarrollo de la organocatálisis enantioselectiva: Como los enzimas, estos catalizadores son capaces de activar (al menos) dos reactivos simultáneamente, mediante interacciones covalentes y no covalentes, consiguiendo en el proceso altas estereoselectividades.¹

El patrón más utilizado en el diseño de nuevos catalizadores es, sin duda, la combinación de un grupo amino (capaz de reaccionar con carbonilos) junto uno o varios grupos capaces de formar puentes de H, típicamente una tiourea.² No obstante, recientemente las escuaramidas han emergido como una alternativa a las tioureas como organocatalizadores bifuncionales.³ En 2012, Jørgensen *et al.* publicaron los primeros catalizadores derivados de escuaramida y pirrolidina: **1** y **2**.⁴ En particular, el catalizador **2** demostró una gran eficiencia en la cicloadición enantioselectiva (5+2) entre los enales **3** y **4** y el oxidopirilico-4-olato **5** mediante activación vía dienamina.⁵



Los estudios computacionales llevados a cabo para esclarecer el mecanismo de la reacción, así como el modo de actuación de los catalizadores **1** y **2** serán analizados con el fin de racionalizar la enantio y diastereoselectividad observada.

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Simple HPLC determination of urinary theobromine: Cocoa products consumption and urinary theobromine levels in healthy children

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Uric acid nephrolithiasis accounts around 10 % of all kind of kidney stones in the adult population¹, and 2-3 % of the pediatric stone former patients². The main etiological factors associated with this type of stones are low urinary pH, hyperuricosuria and low diuresis. Until now, the intake of urinary basifying products (mainly citrate) is the gold standard for the treatment of these patients. Recently, theobromine, a dimethylxanthine present in cocoa products, has been described as a uric acid crystallization inhibitor, suggesting that its use may be useful in the treatment of uric acid stone formers³.

The objectives of this study are to validate an HPLC method for easy urinary theobromine determination, to assess urinary theobromine levels in 80 healthy children, and to relate these levels with the consumption of cocoa products.

Urine samples were diluted, directly injected into an HPLC system, separated by gradient elution on a C18 column, and detected by photodiode array (PDA). The method was validated for linearity, limits of detection and quantification, imprecision, accuracy, recovery and interferences. The proposed method was used to assess 12-h day and 12-h night urinary theobromine excretion by 80 healthy children, divided into four groups based on consumption of cocoa products. In addition, urinary excretion of magnesium and oxalate, also present in cocoa, were determined in these four groups.

The method was linear to a theobromine concentration of 278 µmol/L (50 mg/L). LOD and LOQ for urine samples, diluted 1:5 (vol/vol) with water, were 1.1 and 3.6 µmol/L respectively. Within-run and between-run imprecisions (CV) were each <2%. Average recovery was 99%, and analysis of a certified reference sample showed an error <2.5%. Theobromine excretion levels were significantly higher in healthy children with higher consumption of cocoa products ($p<0.001$), but oxalate ($p=0.098$) and magnesium ($p=0.068$) excretion levels did not differ significantly.

This validated method resulted in urinary theobromine determination with 100% recovery, without sample pretreatment. Urinary theobromine levels in healthy children were directly related to the consumption of cocoa products.

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**Zn-NanoMOFs: estudio de su estabilidad coloidal y aplicación
como sistemas de transporte/liberación de fármacos**

PO-59

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Existe un creciente interés por el desarrollo de nanopartículas para el transporte y la administración de fármacos. El uso de “nanotransportadores” mejora la eficacia en la liberación, dirección y protección del fármaco encapsulado hasta la diana deseada. En los últimos quince años, se ha desarrollado un nuevo tipo de materiales inorgánicos porosos conocidos como redes metalorgánicas (MOFs), que tienen una potencial aplicación como agentes liberadores de fármacos.¹ En este sentido, hemos sintetizado una serie isoestructural de nanoMOFs (ZnBDP_X) basados en iones Zn²⁺ y espaciadores orgánicos funcionalizados del tipo 1,4-bis(1*H*-pirazol-4-il)-2-X-benceno (H2BDP_X), donde X = H, NO₂, NH₂ y OH. Asimismo, se ha estudiado la estabilidad coloidal de estos sistemas en distintos medios fisiológicos simulados (condiciones orales e intravenosas). Los resultados obtenidos demuestran que el derivado ZnBDP_OH presenta una mayor estabilidad química y coloidal en los medios ensayados atribuida a la formación de una corona proteica que evita la agregación de las partículas. Por otra parte, hemos investigado la incorporación/liberación de los fármacos antitumorales mitoxantrona y RAPTA-C ([Ru(*p*-cimeno)Cl₂(pta)] (pta = 1,3,5-triaza-7-fosfoadamantano) en esta serie de nanoMOFs con el fin de determinar el efecto de la funcionalización de la matriz en su capacidad para incorporar/liberar estas moléculas bioactivas. Hemos demostrado que la capacidad de adsorción de los fármacos depende del área superficial de la matriz. Además, la funcionalización de los ligandos afecta tanto a la cinética como a la cantidad total de droga liberada.

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Synthesis of 1-Benzyl-1,2,3,4-Tetrahydroisoquinoline Alkaloids via Organocatalyzed Pictet-Spengler Reaction

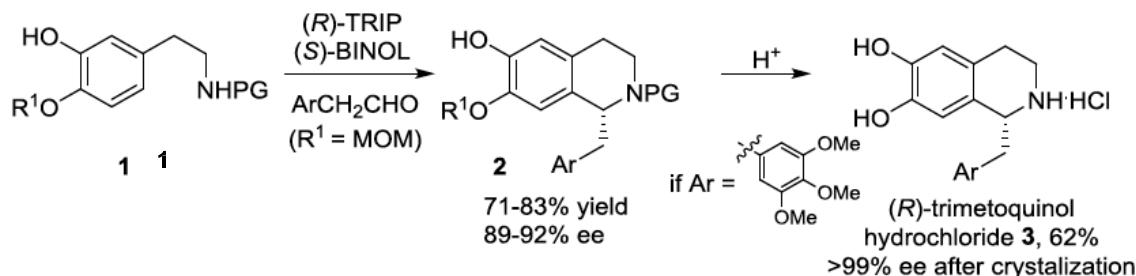
PO-60

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There is a wide array of methods to synthesize 1-substituted tetrahydroisoquinolines (THIQ's) but they are not metal-free¹ and a more desirable synthesis would be required in view of pharmaceutical applications. The original Pictet-Spengler reaction carries out the cyclization between β -arylethylamines (as tryptamine) and aldehydes or ketones. Nevertheless, due to the fact that norcoclaurine synthase, identified as Pictet-Spenglerase, produces the condensation between dopamine and 4-hydroxyphenylacetaldehyde, it was envisioned that a synthetic method with phenylethylamines, which are less nucleophilic, could be achieved. Previous work of the group showed the successful organocatalyzed enantioselective Pictet-Spengler reaction of protected phenylethylamines and aromatic and aliphatic aldehydes. It was catalyzed by the combination of (*R*)-TRIP as organocatalysts with (*S*)-BINOL as co-catalyst.² This work presents a new phenylethylamine derived substrate **1**, which was prepared for the organocatalyzed Pictet-Spengler reaction with substituted phenylacetaldehydes achieving the cyclization products **2** in high ee's. Afterwards, the synthetic route towards enantiopure (*R*)-trimetoquinol hydrochloride **3** was completed and other 9 pharmaceutically relevant THIQ alkaloids were uneventfully synthesized.³

"Ayudas para la movilidad para la realización de estancias breves, 2013" of the Ministerio de Economía y Competitividad of Spain is acknowledged.



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FTIR studies to characterize the kinetics of nanocomposite polyurethane foams

PO-61

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Polyurethanes (PUs) foams are cellular materials (Fig. 1) formed by the simultaneous poly-addition reaction of isocyanates and polyols (gelling reaction, Fig 1.a), and a second reaction where a gas is generated (blowing reaction, Fig 1.b) due to the addition of a blowing agent.¹ Water is a common blowing agent, and gives rise to the foam expansion by final formation of CO₂ and urea groups. These two simultaneous reactions should be adequately controlled in order to obtain polymer foam (Fig 1.c) with the desired cellular structure and physical properties.

The kinetics of these reactions is usually strongly modified by the presence of additives in general and nanoadditives in particular. The aim of this work is to study systematically the effect of different nanoparticles on the reaction kinetics of polyurethane formation. In this work, we present the FTIR monitoring of the phase evolution and the kinetics of the reactions involved in polyurethane foam formation. Deconvolution of the Amide I region (Fig 1.d) absorptions belonging to the stretching vibrations of the carbonyl of the urea and urethane groups allow us to study in a separate way the blowing and gelling reactions involved and their progress.

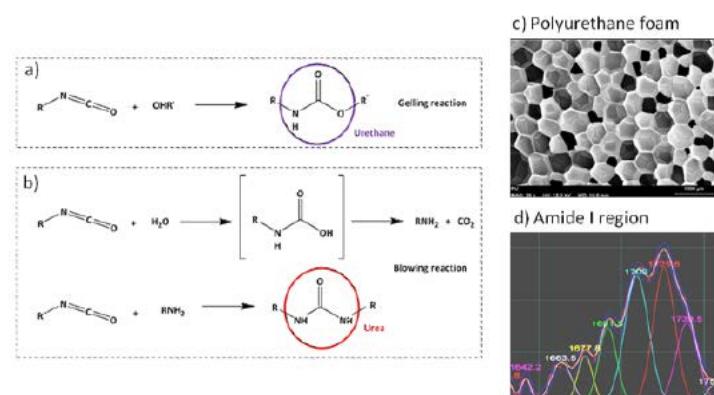


Figure 1

Figure 1. a,b) Main reactions involved in the production of PU foams, c) cellular structure of a rigid PU foam, d) deconvolution of the FTIR spectrum in the amide I region.

The presented methodology indicates that the presence of nanoparticles in this process produces important modifications on the PU foaming kinetics. The phase development and hydrogen bonding equilibrium of a series of nanocomposite polyurethane foams are herein studied.

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Direct reductive alkylation of amine hydrochlorides with aldehyde bisulfite adducts

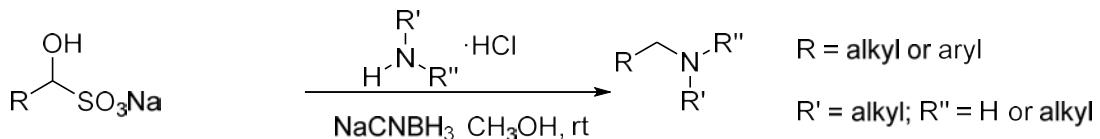
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The reaction of aldehydes with ammonia, primary amines or secondary amines under reductive conditions (*reductive alkylation* of the amines or *reductive amination* of the aldehydes) is a very useful and versatile method for the synthesis of amines.¹ A widespread problem while working with aldehydes is their instability (e.g. tendency to epimerize, undergo air oxidation to the carboxylic acid). Moreover, several liquid aldehydes are difficult to purify.

Bisulfite adducts are usually crystalline solids with desirable physical properties which allow a facile isolation and purification and their storage for prolonged periods of time, easing the experimental working conditions. This adducts are readily accessible compounds via one step, consisting in mixing the aldehyde with aqueous sodium bisulfite.

In this work we present a new, mild, one-pot procedure for the direct reaction of equimolecular amounts of aromatic and aliphatic aldehyde bisulfite adducts and primary and secondary amine hydrochlorides in the presence of NaCNBH₃ in methanol.



Specifically, two aliphatic aldehydes and five aromatic benzaldehydes, were used. Regarding the amines, three secondary and three primary amine hydrochlorides were tested. Typically, the raw yields ranged from 60 to 90%. Notably, this novel methodology has permitted the synthesis of the calcimimetic drug cinacalcet hydrochloride in 90% yield.²

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3. "Sulfolefinas": Ligandos Sulfinamido-olefinas para adiciones conjugadas enantioselectivas catalizadas por Rodio

PO-63

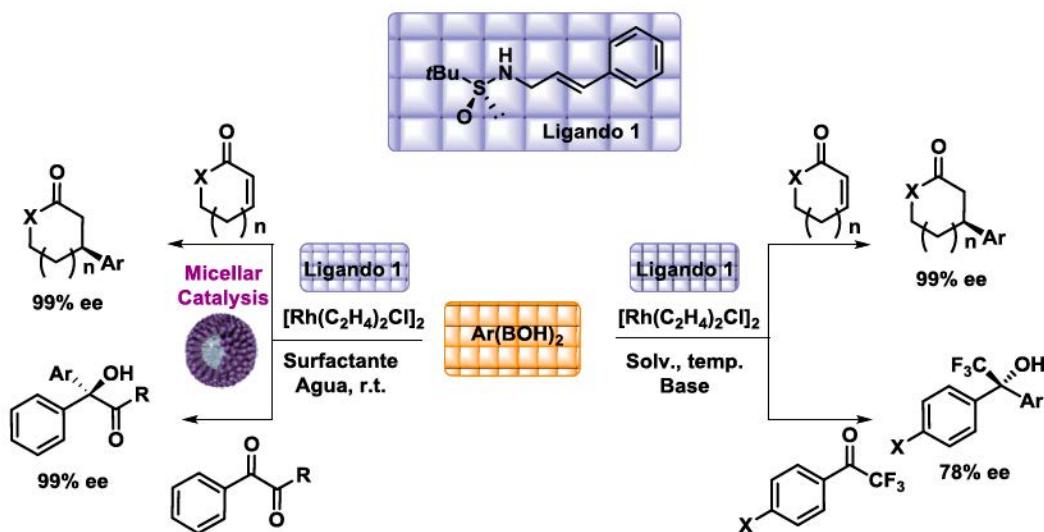
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La realización de reacciones catalíticas enantioselectivas, especialmente la formación de enlaces carbono-carbono, es uno de los objetivos más importantes en la síntesis asimétrica moderna. Dentro de nuestros intereses hacia la síntesis de derivados quirales de azufre y sus aplicaciones en catálisis asimétrica orgánica y organometálica, en el presente trabajo se presenta una aproximación altamente enantioselectiva de adiciones 1,4- y 1,2 de ácidos arilborónicos a cetonas α , β -insaturadas, a-cetoésteres y a-dicetonas catalizada por Rh, utilizando la sencilla sulfinamido-olefina 1 como precursor del catalizador quiral (Esquema 1). Este sistema catalítico ha demostrado ser altamente eficiente no sólo en disolventes orgánicos¹, sino también en agua en combinación con un agente tensioactivo,² lo que permite la síntesis de cetonas ariladas y alcoholes terciarios con altos rendimientos y altas enantioselectividades.



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Síntesis de nuevos compuestos tripodales pseudopeptídicos como receptores de cloruros

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El diseño y síntesis de nuevos ligandos que actúen como receptores selectivos de aniones continúa teniendo un gran interés en la comunidad científica.¹ En este sentido, el anión cloruro es importante a nivel biológico y medioambiental. El transporte de cloruro a través de las membranas celulares es uno de los procesos biológicos más importantes en organismos vivos. Por ello, se están llevando a cabo estudios de transporte utilizando como agentes transportadores compuestos capaces de imitar a los receptores naturales. En este sentido, nuestro grupo de investigación ha sintetizado recientemente compuestos pseudopeptídicos, basados en unidades de imidazolio, como receptores de aniones.² A raíz de estos resultados, aquí se presenta la síntesis de nuevos compuestos tripodales basados en unidades de imidazolio, sintetizados a partir de L-Valina (ver Figura 1), como receptores de cloruros.

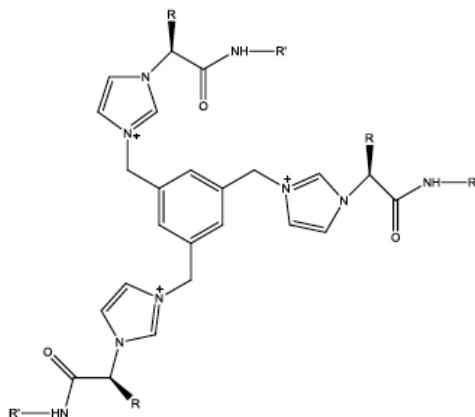


Fig.1. Estructura general de los compuestos tripodales sintetizados

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**BO radical-metal interaction: computational study of structure
and bonding**

PO-65

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Boron chemistry is well known and has been studied for many years. One of its main characteristics is that the boron atom finds stability with six valence electrons. Thus, many of its compounds are usually good electron acceptors (Lewis acids, oxidants, etc.). This is the main feature which addresses both its chemical behaviour and reactivity.

However, despite the enormous amount of information related to boron chemistry, BO radical chemistry still remains unknown to a large extent. BO radical shows resemblances to CN radical and carbon monoxide, CO, both of which are good π -acceptor ligands in coordination chemistry. It is isoelectronic to the CN radical and it has a similar molecular orbitals structure to carbon monoxide. Therefore, it is interesting to study the BO radical due mainly to its possible applications in synthetic chemistry. Up to now, just one BO-complex has been synthesised and characterised. In addition, experimental data for BO-carbon and BO-gold clusters has been given. However, very little information exists regarding the structure and bonding situation which this group displays in BO-bearing compounds. So within this framework a theoretical study of the BO radical would render relevant information.

To study BO radical characteristics, some BO-metal model systems were chosen. A structural study has been carried out at several levels of calculation for the different chemical species with the aim of predicting their main properties and making their possible experimental characterisation easier. The isomerization processes have also been studied. Eventually, topological analysis of electron density and the study in terms of natural bond orbitals have thrown light on the nature of the chemical interaction between BO radical and the metallic atoms.

**Theoretical study of tetratomic {C, H, N, Zn} compounds:
molecular structure and bond characteristics**

PO-66

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The structural and spectroscopic parameters of the most relevant tetratomic {C, H, N, Zn} isomers have been studied employing high-level quantum-chemical methods. For each isomer, predictions for its molecular geometry, thermodynamic stability and rotational and vibrational spectroscopic parameters, which could eventually help in the experimental detection, are provided. In addition, a detailed study of the bonding situations has been carried out by means of a topological analysis of electron density in the framework of the Bader's Quantum Theory of Atoms in Molecules.

The analysis of the relative stabilities suggests two linear isomers for neutral tetratomic {C, H, N, Zn} compounds, namely the cyanidehydridezinc, HZnCN ($^1\Sigma$), and the hydrideisocyanidezinc, HZnNC ($^1\Sigma$), as possible candidates for the experimental detection. For the monocationic tetratomic {C, H, N, Zn} compounds the most stable isomers are the ion-molecule complexes arising from the direct interaction between the Zn+ ion and the nitrogen or carbon atom from hydrogen cyanide, HCN, or hydrogen isocyanide, HNC, respectively: HCNZn⁺ ($^2\Sigma$) and HNCZn⁺ ($^2\Sigma$).

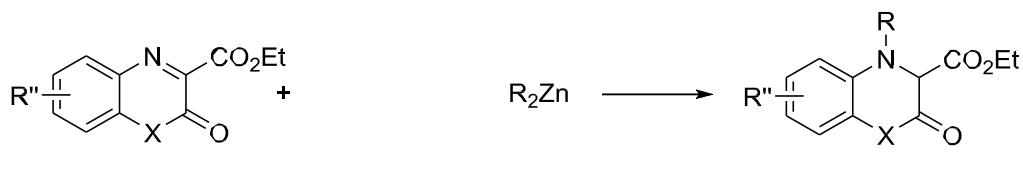
N-Alkylation of benzoxazinone and quinoxalinone derivatives with organozinc reagents via *umpolung*

PO-67

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Dihydrobenzoxazinone and dihydroquinoxalinone are ubiquitous structures in biologically active molecules such pharmaceutical or agrochemical compounds, so their synthesis is still in great demand.¹ On the other hand an *umpolung* reaction of an α -imino ester involving nucleophilic addition to the nitrogen atom is difficult due to the electron-withdrawing effect of the imino group.² Despite the progress over the past years of Kozlowski³ and Shimizu⁴ groups in the *N*-alkylation of acyclic α -imino ester, the *N*-alkylation of cyclic α -imino ester is less unstudied.⁵ In this communication, we present our efforts in the study of the *umpolung* *N*-alkylation of benzoxazinone and quinoxalinone derivatives with organozinc reagents.



X= O, NR'

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Rebecca Brodie

Deputy Editor of Analyst, Analytical Methods & JAAS



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Chemistry software solutions - A world of possibilities outside the lab

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Dr. Bernardo Herradón García
Investigador Científico en el Instituto de Química Orgánica General
(IQOG) del CSIC y Divulgador Científico



Divulgación Científica: como impactar en la Sociedad.

Bernardo Herradón compartirá con los asistentes al Simposio su experiencia como narrador científico en los medios de comunicación y las actividades de divulgación que ha realizado a estudiantes de ESO y Bachillerato.

Porqué es importante transmitir nuestra investigación al resto de la sociedad? Qué ganamos con ello? Como se puede conseguir? Preguntas que siempre nos hacemos y Bernardo nos intentará contestar.

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