YOUNG CHEMISTS SYMPOSIUM

An event by

Società Chimica Italiana
Gruppo Giovani

Hotel Embassy & Boston
Milano Marittima (Italy)
November 13th-15th, 2017

Proceedings of the

Merck Young Chemists Symposium

XVII edition

Edited by: F. Bella, L. Botta, A. Buchicchio, R. Cucciniello, A. D'Urso, A. Erba, P. Franco, E. Lenci, G. Mazzone, A. Soldà, S. Staderini, L. Triggiani, and D. Spinelli

ISBN: 978-88-86208-89-5

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SCI Giovani is extremely grateful to all the co-sponsors that contributed to this conference

Welcome message

Dear participants,
welcome to the 17th edition of the **Merck Young Chemists Symposium**, formerly SAYCS.

This conference is an international scientific event organized by the Young Group of the Italian Chemical Society (SCI Giovani) with the financial support of Merck.

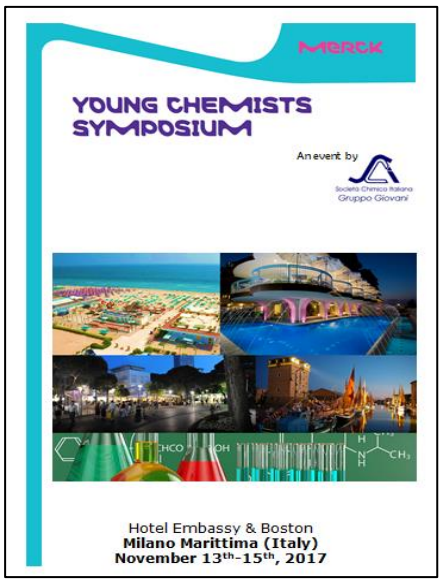
This symposium is fully devoted **to young researchers**, such as MSc and PhD students, post-doc fellows and young researchers in companies. All the disciplines of **Chemistry** are covered: analytical, physical, industrial, organic, inorganic, theoretical, pharmaceutical, biological, environmental, macromolecular and electrochemistry. This year, a special emphasis will be given to **chemistry without borders**: *how chemistry is increasingly present in all the fields that are fundamental for human life, i.e. energy, health, and environment?*

This year we have the exceptional number of 172 participants; we thank you for the great trust shown towards SCI Giovani and Merck.

Enjoy the conference!

Federico Bella
Coordinator of SCI-Giovani

HOW TO CITE YOUR WORK



The scientific contributions of this conference are collected in an international volume with ISBN code.

You can cite your work in this way:

N. Surname, *N. Surname*, … and *N. Surname*, *Abstract title*, in "Proceedings of the Merck Young Chemists Symposium", Ed. F. Bella, L. Botta, A. Buchicchio, R. Cucciniello, A. D'Urso, A. Erba, P. Franco, E. Lenci, G. Mazzone, A. Soldà, S. Staderini, L. Triggiani, and D. Spinelli, ISBN: 978-88-86208-89-5, *page number*, 2017, Rome".

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Program – Monday, 13th November

11.30	**Registration** desk opens @ Hotel Embassy & Boston	
15.00	**Opening Ceremony** @ Sala Plenaria	
	Chair: **P. Franco** (UniBO) and **D. Spinelli** (UniBO)	
15.20	OR-1 **Giovanni Valenti**, UniBO	
15.35	OR-2 **Francesca Arcudi**, UniTS	
15.50	OR-3 **Marianna Rossetti**, UniROMA-2	
16.00	OR-4 **Giulia Piana**, PoliTO	
16.10	OR-5 **Azzurra Stefanucci**, UniCH	
16.20	OR-6 **Vittoria Marzaroli**, UniPR	
16.30	OR-7 **Daniele Ragno**, UniFE	
16.40	OR-8 **Claudia Bonfio**, UniTN	
16.50	OR-9 **Valentina Cauda**, PoliTO	
17.00	**Coffee Break**	
	SALA ROSSINI Inorganic materials and reactions	**SALA PUCCINI** Electrochemistry in modern technologies
	Chair: **G. Mazzone** (UniCAL)	*Chair:* **A. Soldà** (UniBO)
17.30	OR-10 **Fabrizio Sordello**	OR-18 **Chiara Gaetani**
17.40	OR-11 **Luca Bellucci**	OR-19 **Luca Bartolini**
17.50	OR-12 **Valeria Caponetti**	OR-20 **Gregorio Bonazza**
18.00	OR-13 **Marco Chino**	OR-21 **Riccardo Brandiele**
18.10	OR-14 **F. Della Monica**	OR-22 **Francesca Colò**
18.20	OR-15 **Mattia Gatto**	OR-23 **Arnaud Gigot**
18.30	OR-16 **Chiara Parise**	OR-24 **Francesca Lorandi**
18.40	OR-17 **Silvia Ruggieri**	OR-25 **Amalia Velardo**
18.50		OR-26 **Alessandra Zanut**

SALA ROSSINI **18:50-19:40** Flash communications: medicinal & biological chemistry	**SALA PUCCINI** **19:00-19:40** Flash communications: organic & theoretical chemistry
Chair: **A. D'Urso** (UniCT)	*Chair:* **E. Lenci** (UniFI)
FL-1 **Michele Anselmi**	FL-11 **Nurgali Akylbekov**
FL-2 **Mariateresa Badolato**	FL-12 **Fortuna Ponte**
FL-3 **Fabio Bologna**	FL-13 **Emanuela Carrieri**
FL-4 **Francesca Carella**	FL-14 **Elisa Brambilla**
FL-5 **Luca Conti**	FL-15 **Edoardo J. Mattioli**
FL-6 **Matteo Mori**	FL-16 **Riccardo Innocenti**
FL-7 **Erica Rebba**	FL-17 **Elisa Bonandi**
FL-8 **Federica Sodano**	FL-18 **Arianna Massaro**
FL-9 **Giusy Tassone**	FL-19 **Marta Da Pian**
FL-10 **Martina Ciaravolo**	FL-20 **Giacomo Berton**
19.40	**Free time** *Those who will present a poster in the evening must hang the poster*
20.30	**SCI Social Dinner** @ Ristorante Basilico *Dress code:* Elegant
22.00	**Poster Session** *From POS-1 to POS-20 & from FL-1 to FL-20*
23.30	**SCI Cocktail** @ Foyer Bar Embassy & Boston *First cocktail offered by SCI Giovani Board*

Program – Tuesday, 14th November

7.30 **Breakfast**

SALA PLENARIA

Chair: **E. Lenci** (UniFI)

9.00 INV-1 **Kevin Sivula**, EPFL
9.35 OR-27 **Jan Willem Wijnen**, Elsevier
9.55 OR-28 **Alice Soldà**, EYCN
10.15 INV-2 **Andrea Cavalli**, UniBO

10.50 **Coffee Break**

SALA ROSSINI 11:20-13:30

Physical & theoretical chemistry

Chair: **L. Triggiani** (UniBA)

OR-29 **Andrea Ancona**
OR-30 **Margherita Bolognesi**
OR-31 **Massimo C. D'Alterio**
OR-32 **Ivan Grigioni**
OR-33 **Alessandro Landi**
OR-34 **Mattia Melosso**
OR-35 **Ylenia Miele**
OR-36 **Filippo Monti**
OR-37 **Marco Fabbiani**
OR-38 **Laura Falivene**
OR-39 **Giulio Latini**
OR-40 **Tainah D. Marforio**
OR-41 **Eduardo Schiavo**

SALA PUCCINI 11:20-13:30

Medicinal and clinical chemistry

Chair: **L. Botta** (UniTUS)

OR-42 **Stefano Cinti**
OR-43 **Giorgio Amendola**
OR-44 **Francesco Bavo**
OR-45 **Irene M. Carnovale**
OR-46 **Tommaso Felicetti**
OR-47 **Valeria Francesconi**
OR-48 **Mirko Scortichini**
OR-49 **Chiara Setti**
OR-50 **Valentina Straniero**

Flash communications - General

Chair: **A. Soldà** (UniBO)

FL-21 **Simone D'Agostino**
FL-22 **Jacopo De Maron**
FL-23 **Michele Iannone**
FL-24 **Martina Marinelli**
FL-25 **Alberto Martis**
FL-26 **Cristina Pizzolitto**
FL-27 **Andrea Vassoi**
FL-28 **Onur Yildrim**
FL-29 **Maria Sole Zalaffi**

13.30	**Lunch** @ Ristorante Basilico *Posters of the previous day must be removed and replaced with new ones.*	
	SALA ROSSINI **14:45-16:45** Chemistry for industrial and technological applications *Chair:* **R. Cucciniello** (UniSA)	**SALA PUCCINI** **14:45-16:45** Current trends in organic chemistry *Chair:* **S. Staderini** (CNR)
	OR-51 **Aurelio Bifulco**	OR-63 **Carlos Rodriguez D. Rio**
	OR-52 **Laura Campagnolo**	OR-64 **Chiara Biagini**
	OR-53 **Giuseppe Ferraro**	OR-65 **Michele Cacioppo**
	OR-54 **Simone Galliano**	OR-66 **Nunzio Cardullo**
	OR-55 **Angelo Garofalo**	OR-67 **Jacopo Ceccarelli**
	OR-56 **Claudio Imparato**	OR-68 **Graziano Di Carmine**
	OR-57 **Lorenza Maddalena**	OR-69 **Luca Leoni**
	OR-58 **Davide Magrì**	OR-70 **Alessandro Manfrin**
	OR-59 **Daniele Massella**	OR-71 **Luca Meschisi**
	OR-60 **Gaby B. Taptue**	OR-72 **Angela Pagano**
	OR-61 **Razieh Sadraei**	OR-73 **Francesca Piazzolla**
	OR-62 **Alessandro Sangion**	OR-74 **Luca Prati**
16.45	**Coffee-Break + Poster Session** – until 18:00 *From POS-21 to POS-42 & from FL-21 to FL-29*	
17.30	**Incontro col Presidente della Divisione di Chimica Organica: un brain-storming sulle attività future** *In sala plenaria – Rivolto ai soci della Divisione*	
17.30	**Incontro col Comitato Esecutivo** *Riservato al Direttivo del Gruppo Giovani*	

	SALA PLENARIA *Chair:* **D. Spinelli** (UniBO) and **F. Bella** (PoliTO)
18.00	INV-3 **Gianluca M. Farinola**, UniBA
18.35	OR-75 **Sara Tortorella**, Molecular Horizon
18.50	**Assemblea Ordinaria dei Soci del Gruppo Giovani**
19.30	List of **Awards** to be assigned @ MYCS-2017
19.40	**Free time** *Posters must be removed.*
20.30	**Merck Social Dinner** @ Ristorante Basilico *Dress code:* Semi-formal
22.00	**Party** @ Milano Marittima city center *First cocktail offered by SCI Giovani Board @ Caino Fashion Club*

Program – Wednesday, 15th November

7.30	**Breakfast**
9.00	**Check-out** from Hotel rooms (not later than 9:15)
	SALA PLENARIA
	Chair: **A. D'Urso** (UniCT) and **G. Mazzone** (UniCAL)
9.30	INV-4 **Gaetano Guerra**, UniSA
10.05	OR-76 **Luka Dordevic**, UniTS
10.15	OR-77 **Alice Tamburrini**, UniMI
10.25	OR-78 **Simona Ranallo**, UniROMA-2
10.35	OR-79 **Giorgio Grillo**, UniTO
10.45	OR-80 **Ritamaria Carpegna**, IIT
10.55	OR-81 **Adriano Intiso**, UniSA
11.05	OR-82 **Martina Catani**, UniFE
11.15	**Group Picture**
11.30	**Coffee Break**
	Chair: **P. Franco** (UniBO)
12.00	OR-83 **Patrizia Firmani**, UniROMA-1
12.10	OR-84 **Maria M. Salvatore**, UniNA
12.20	OR-85 **Maria Ricciardi**, UniSA
12.30	OR-86 **Cecilia Pozzi**, UniSI
12.40	**Closing Ceremony**
13.00	**Lunch** @ Ristorante Basilico
14.00	**Check your scheduled bus to Cervia train station**

Invited Talks

INV-1 Kevin SIVULA

INV-2 Andrea CAVALLI

INV-3 Gianluca M. FARINOLA

INV-4 Gaetano GUERRA

INV-1

Photoelectrochemical solar fuel production

Kevin Sivula

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To transition our energy economy into one that is fully sustainable and not dependent on fossil fuels, developing an economically viable "artificial photosynthetic" device for the overall storage of solar energy as chemical energy is an urgent goal. Using solar energy to drive the electrochemical production of fuels (e.g. the splitting of water into molecular hydrogen and oxygen) is a promising technology in this regard. High-efficiency solar-to-fuel energy conversion can be directly achieved using a photoelectrochemical (PEC) device consisting of an n-type photoanode in tandem with a p-type photocathode. However, the development of stable and inexpensive photoelectrodes are needed to make PEC devices economically viable.

In this presentation, our laboratory's progress in the development of economically-prepared, high performance photoelectrodes will be discussed along with the application toward overall PEC water splitting tandem cells. Specifically, how the use of scalable solution-processing techniques (e.g. colloidal processing of nanoparticles or sol-gels) leads to limitations in charge transport and charge transfer in the resulting thin-film photoelectrodes will be examined. Strategies to overcome these limitations using chemical innovations such as using charge extraction buffer layers, catalysts, annealing/doping and nanoparticle self-assembly will be additionally presented. Materials of interest are delafossite $CuFeO_2$ [1] CIGS [2], 2D-layered WSe_2 [3], and semiconducting carbon-based materials [4].

[1] M. S. Prévot, N. Guijarro, and K. Sivula, *ChemSusChem* **8** (2015) 1359-1367.
[2] N. Guijarro, M. S. Prévot, X. Yu, X. A. Jeanbourquin, P. Bornoz, W. Bourée, M. Johnson, F. Le Formal, and K. Sivula, *Adv. Energy Mater.* **6** (2016) 1501949.
[3] X. Yu, M. S. Prevot, N. Guijarro, and K. Sivula, *Nat. Commun.* **6** (2015) 7596.
[4] P. Bornoz, M. S. Prévot, X. Yu, N. Guijarro, and K. Sivula, *J. Am. Chem. Soc.* **137** (2015) 15338-15341.

INV-2

Thermodynamics and kinetics of drug-target binding through molecular simulations

Andrea Cavalli[a,b]

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Drug-target binding represents the first event at the basis of the therapeutic action of drugs. This complex phenomenon needs to be properly described at an atomistic level to identify the major determinants of drug potency and in vivo drug efficacy. Molecular dynamics (MD) is emerging as a powerful tool for investigating protein-ligand binding, and is getting increasing consensus from the drug discovery community. While extensive MD simulations in the microsecond to the millisecond timescale are nowadays able to simulate protein-ligand binding "spontaneously", enhanced sampling methods, including metadynamics, steered-MD, umbrella sampling, etc., can improve the sampling of that part of free energy landscape that can be relevant for the biological process under investigation.

In this talk, I will be presenting the use of extensive MD simulations to investigate spontaneous protein-ligand binding. Then, I will show how free energy calculations allow the identification of the minimum free energy path from the bulk of the solvent into the protein-binding pocket, as well as the determination of thermodynamic and kinetic parameters associated to drug-target recognition and binding. The presentation will finally be focused on applications of enhanced sampling methods to accelerate ligand binding and unbinding and to estimate kinetics (kon and koff) and thermodynamics, in simulation timescale more compatible with the requirements of speed and accuracy of the pharmaceutical research. All these simulations will be discussed in the framework of drug design and discovery, highlighting the role of these approaches in real-life drug discovery endeavors.

[1] M. De Vivo, M. Masetti, G. Bottegoni, and A. Cavalli, *J. Med. Chem.* **59** (2016) 4035-4061.
[2] L. Mollica, I. Theret, M. Antoine, F. Perron-Sierra, Y. Charton, J. M. Fourquez, M. Wierzbicki, J. A. Boutin, G. Ferry, S. Decherchi, G. Bottegoni, P. Ducrot, and A. Cavalli, *J. Med. Chem.* **59** (2016) 7167-7176.
[3] S. Decherchi, A. Berteotti, G. Bottegoni, W. Rocchia, and A. Cavalli, *Nat. Comm.* **6** (2015) 6155.
[4] A. Cavalli, A. Spitaleri, G. Saladino, and F. L. Gervasio, *Acc. Chem. Res.* **48** (2015) 277-285.
[5] J. S. Patel, A. Berteotti, S. Ronsisvalle, W. Rocchia, and A. Cavalli, *J. Chem. Inf. Model.* **54** (2014) 470-480.
[6] G. Grazioso, V. Limongelli, D. Branduardi, E. Novellino, C. De Micheli, A. Cavalli, and M. Parrinello, *J. Am. Chem. Soc.* **134** (2012) 453-463.
[7] F. Colizzi, R. Perozzo, L. Scapozza, M. Recanatini, and A. Cavalli, *J. Am. Chem. Soc.* **132** (2010) 7361-7371.

INV-3

Making smart materials with organic molecules and photosynthetic microorganisms

Gianluca M. Farinola

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Current synthetic methods offer powerful tools to develop advanced materials for photonics, electronics and biomedicine. However, this may be not the only route to achieve significant progress.

In this lecture I will discuss a possible different approach based on combination of organic synthesis and biotechnology, leading to new functional materials with fascinating properties.

Looking at the way photosynthetic microorganisms (algae, bacteria) collect energy and produce materials, the possibility to exploit their sophisticated nanostructures and molecular machineries for light management, photoconversion and many other functions is attractive. Two examples explored in our laboratories will be discussed.

1. Diatoms microalgae produce beautiful ornate biosilica shells. We have shown easy functionalization of the biosilica either chemically, or *in vivo* by feeding the algae with tailored molecules. The resulting biohybrid structures can be used as materials for photonics and for biomedicine [1].

2. Photosynthetic Reaction Centers (RCs) are photoenzymes capable to convert solar energy into charge separated states with almost unitary efficiency. Together with the group of Angela Agostiano (University of Bari) and Massimo Trotta (CNR IPCF), we have built-up hybrid materials for bioelectronics [2] by covalent functionalization of the RC from the photosynthetic bacterium *Rhodobacter sphaeroides* R26 with photo- and electroactive organic molecules [3,4].

Overall, the lecture will emphasize how the creativity and the molecular insight of chemists can lead to groundbreaking concepts in materials design and synthesis.

[1] S. R. Cicco, D. Vona, E. De Giglio, S. Cometa, M. Mattioli Belmonte, F. Palumbo, R. Ragni, and G. M. Farinola, *ChemPlusChem* **80** (2015) 1104-1112.

[2] A. Operamolla, R. Ragni, F. Milano, R. R. Tangorra, A. Antonucci, A. Agostiano, M. Trotta, and G. M. Farinola, *J. Mater. Chem. C* **3** (2015) 6471-6478.

[3] F. Milano, R. Tangorra, O. Hassan Omar, R. Ragni, A. Operamolla, A. Agostiano, G. M. Farinola, and M. Trotta, *Angew. Chem. Int. Ed*. **51** (2012) 11019-11023.

[4] O. Hassan Omar, S. La Gatta, R. Tangorra, F. Milano, R. Ragni, A. Operamolla, R. Argazzi, C. Chiorboli, A. Agostiano, M. Trotta, and G. M. Farinola, *Bioconjugate Chem.* **27** (2016) 1614-1623.

INV-4

Nanoporous crystalline polymers and industrial innovations

Gaetano Guerra

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For two commercial thermoplastic polymers, syndiotactic polystyrene (s-PS) [1-3] and poly(2,6-dimethyl-1,4-phenylene)oxide (PPO) [4,5], crystalline phases including empty cavities of molecular size in their unit cell have been obtained and named *nanoporous-crystalline* phases. These nanoporous-crystalline phases unprecedently exhibit density lower than the corresponding amorphous phases and are obtained by guest removal from co-crystalline host-guest phases, between a polymer host and low-molecular-mass guest.

These nanoporous-crystalline phases are able to absorb guest molecules also from very dilute solutions. Most studies have been devoted to s-PS, which exhibits two different nanoporous-crystalline phases, δ^1 and ε^2, whose nanoporosity is organized as isolated cavities and channels, respectively.

Physically crosslinked monolithic aerogels, whose physical knots are crystallites exhibiting a nanoporous crystalline form, will be also discussed [6,7]. These *aerogels* present beside disordered amorphous micropores (typical of all aerogels) also all identical nanopores of the crystalline phases. Their outstanding guest transport properties combined with low material cost, robustness, durability and easy of handling and recycle make these aerogels suitable for applications in chemical separations, purification and storage [6,7].

The final part of the presentation will be devoted to possible industrial innovations of materials based on co-crystalline and nanoporous crystalline s-PS phases. In particular, applications of nanoporous films for active packaging of fruit and vegetable (by removal of ethylene and carbon dioxide), of nanoporous staple for removal of pollutants from water and air [8] and of nanoporous aerogels as support for nanostructured catalysts [9] will be presented.

[1] C. De Rosa, G. Guerra, V. Petraccone, and B. Pirozzi, *Macromolecules* **30** (1997) 4147-4152.
[2] V. Petraccone, O. Ruiz de Ballesteros, O. Tarallo, P. Rizzo, and G. Guerra, *Chem. Mater.* **20** (2008) 3663-3668.
[3] M. R. Acocella, P. Rizzo, C. Daniel, O. Tarallo, and G. Guerra, *Polymer* **63** (2015) 230-239.
[4] C. Daniel, S. Longo, G. Fasano, J. G. Vitillo, and G. Guerra, *Chem. Mater.* **23** (2011) 3195-3200.
[5] P. Lova, C. Bastianini, P. Giusto, M. Patrini, P. Rizzo, G. Guerra, M. Iodice, C. Soci, and D. Comoretto, *ACS Appl. Mater. Interf.* **8** (2016) 31941-31948.
[6] C. D'Aniello, C. Daniel, and G. Guerra, *Macromolecules* **48** (2015) 1187-1193.
[7] C. Daniel, M. Pellegrino, V. Vincenzo, S. Aurucci, and G. Guerra, *Polymer* **105** (2016) 96-103.
[8] C. Daniel, P. Antico, H. Yamaguchi, M. Kogure, and G. Guerra, *Micropor. Mesopor. Mat.* **232** (2016) 205-210.
[9] V**.** Vaiano, O. Sacco, D. Sannino, P. Ciambelli, S. Longo, V. Venditto, and G. Guerra, *J. Chem. Technol. Biotechnol.* **89** (2014) 1175-1192.

Oral Presentations

OR-1	Giovanni VALENTI
OR-2	Francesca ARCUDI
OR-3	Marianna ROSSETTI
OR-4	Giulia PIANA
OR-5	Azzurra STEFANUCCI
OR-6	Vittoria MARZAROLI
OR-7	Daniele RAGNO
OR-8	Claudia BONFIO
OR-9	Valentina CAUDA
OR-10	Fabrizio SORDELLO
OR-11	Luca BELLUCCI
OR-12	Valeria CAPONETTI
OR-13	Marco CHINO
OR-14	Francesco DELLA MONICA
OR-15	Mattia GATTO
OR-16	Chiara PARISE
OR-17	Silvia RUGGIERI
OR-18	Chiara GAETANI
OR-19	Luca BARTOLINI
OR-20	Gregorio BONAZZA
OR-21	Riccardo BRANDIELE
OR-22	Francesca COLÒ
OR-23	Arnaud GIGOT
OR-24	Francesca LORANDI
OR-25	Amalia VERLATO
OR-26	Alessandra ZANUT
OR-27	Jan Willem WIJNEN
OR-28	Alice SOLDÀ
OR-44	Francesco BAVO
OR-45	Irene M. CARNOVALE
OR-46	Tommaso FELICETTI
OR-47	Valeria FRANCESCONI
OR-48	Mirko SCORTICHINI
OR-49	Chiara SETTI
OR-50	Valentina STRANIERO
OR-51	Aurelio BIFULCO
OR-52	Laura CAMPAGNOLO
OR-53	Giuseppe FERRARO
OR-54	Simone GALLIANO
OR-55	Angelo GAROFALO
OR-56	Claudio IMPARATO
OR-57	Lorenza MADDALENA
OR-58	Davide MAGRÌ
OR-59	Daniele MASSELLA
OR-60	Gaby B. TAPTUE
OR-61	Razieh SADRAEI
OR-62	Alessandro SANGION
OR-63	C. RODRIGUEZ DEL RIO
OR-64	Chiara BIAGINI
OR-65	Michele CACIOPPO
OR-66	Nunzio CARDULLO
OR-67	Jacopo CECCARELLI
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OR-32	Ivan GRIGIONI	**OR-75**	Sara TORTORELLA
OR-33	Alessandro LANDI	**OR-76**	Luka DORDEVIC
OR-34	Mattia MELOSSO	**OR-77**	Alice TAMBURRINI
OR-35	Ylenia MIELE	**OR-78**	Simona RANALLO
OR-36	Filippo MONTI	**OR-79**	Giorgio GRILLO
OR-37	Marco FABBIANI	**OR-80**	Ritamaria CARPEGNA
OR-38	Laura FALIVENE	**OR-81**	Adriano INTISO
OR-39	Giulio LATINI	**OR-82**	Martina CATANI
OR-40	Tainah D. MARFORIO	**OR-83**	Patrizia FIRMANI
OR-41	Eduardo SCHIAVO	**OR-84**	Maria M. SALVATORE
OR-42	Stefano CINTI	**OR-85**	Maria RICCIARDI
OR-43	Giorgio AMENDOLA	**OR-86**	Cecilia POZZI

OR-1

Co-axial nanostructures for energy conversion: synergic effects between carbon nanotubes and metal oxide

Giovanni Valenti,[a] Alessandro Boni,[a] Michele Melchionna,[b] Massimo Marcaccio,[a] Stefania Rapino,[a] Marcella Bonchio,[c] Maurizio Prato,[b] Paolo Fornasiero,[b] and Francesco Paolucci[a]

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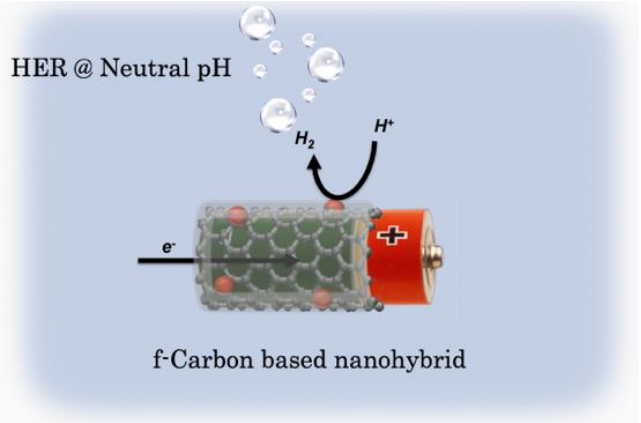
The growing need for energy on global scale and the realization that the so-called oil-based economy cannot sustain our world anymore, prompted researchers to find new ways to "power" the planet. In particular, a lot of efforts have been done in the field of chemical energy conversion, that remains very challenging because of the requirement for higher efficiencies. The splitting of water to high energy chemical fuels is one of the most attractive and pursued alternatives; among the major issues there is the need to find catalytic systems that are able to boost the overall reaction efficiently and durably.

In this context our group recently focused the attention on the study of catalytic systems for the oxygen reactions (such as oxygen reduction [1] and oxygen evolution [2]). Our last efforts have been done in the development of new C-based nanocomposites that combine the unique properties of multiwall carbon nanotubes (MWCNTs), metal oxides (TiO_2) and Pd nanoparticles (Pd NPs). The nanocomposite MWNT@Pd/TiO_2 has been designed and evaluated as electrocatalyst for the reaction of hydrogen evolution (HER) with resulting performance exceeding the state of-the-art electrocatalysts. [3]



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[2] F. Toma, A. Sartorel, M. Iurlo, M. Carraro, P. Parisse, C. Maccato, S. Rapino, B. Gonzalez, H. Amenitsch, T. Da Ros, L. Casalis, A. Goldoni, M. Marcaccio, G. Scorrano, G. Scoles, F. Paolucci, M. Prato, and M. Bonchio, *Nat. Chem.* **2** (2010) 826-831.
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OR-2

Rationally designed carbon nanodots

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Carbon nanodots (CNDs) are the latest members to join the carbon nanomaterials family, generating many expectations based on their interesting properties. These nanoparticles are characterized by their discrete and quasi-spherical shape, size below 10 nm, and fascinating luminescence properties. Furthermore, owing to their inexpensive and safe nature, CNDs could substitute conventional semiconductor quantum dots, generally considered to be supreme luminescent materials.

We present a facile bottom-up approach to nitrogen-doped CNDs, using a microwave-assisted protocol under controlled conditions. Our dots are highly soluble in water, display among the smallest size and the highest fluorescence quantum yield reported so far [1]. They have been successfully employed for the preparation of interesting hybrid materials, such as self-enhancing electrochemiluminescence platform, covalent donor-acceptor systems [2], or fluorescent thin films.

Moreover, our work provides a new avenue to size, surface controllable, structurally defined CNDs towards tailored fluorescent properties for specific applications. A simple and straightforward approach for CNDs able to emit light across the entire visible spectrum and resulting in white-light emission is presented [3].

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OR-3

Co-localization of DNA-based conformational switches for single-step fluorescence detection of small molecules

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The detection of small molecules, such as toxins, pharmaceutical drugs, metabolites, drugs, hormones, play an important role in drug discovery, food and environmental analysis, and clinical diagnosis. Traditional small molecule detection involves spectroscopic or chromatographic methods such as high-performance liquid chromatography (HPLC) and gas chromatography coupled with mass spectrometry (GC/MS), which require complex sample preparations, long testing cycles, slow result turnover, expensive equipment, and trained operators.

Hence, alternative methods that are rapid, simple, inexpensive and quantitative are needed.

Here, we report a sensitive fluorimetric competitive assay for the detection of small molecules that couples the advantageous features of DNA-based conformational switching probes with those of co-localization based approaches. The assay is based on our assay, recently proposed, for the rapid, sensitive and single-step detection of antibodies [1] in which we take advantage of the characteristic Y-shaped of antibody to co-localize on the same antibody DNA-based elements that are rationally designed to give a measurable fluorescence signal only in the presence of a specific target antibody. We have adapted this assay into a competitive format, that enables the rapid, inexpensive, one-step and quantitative detection of small molecules in homogeneous solution. We have demonstrated the adaptation of this assay for the rapid detection (<20 min) of Domoic acid, a neurotoxin produced by marine diatoms of the genus *Pseudo-nitzschia* [2], directly in seawater within nanomolar concentrations. The competitive assay could, in principle, be adapted for the detection of any small molecule for which a specific recognition element (e.g., antibody or protein) is available. Furthermore, the developed platform is also capable of enabling multiplexed detection of numerous small target molecules in the same solution, by using specific sets of DNA-based elements.

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[2] A. F. Saeeda, S. A. Awanb, S. Linga, R. Wanga, S. Wanga, *Algal Research* **24** (2017) 97-110.

OR-4

Photocured eletrolytes for lithium batteries

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To fulfill our needs, we all desire a long-lasting, non-explosive and small lithium-ion battery (LIB) for our portable electronic devices and (future) electric vehicles.

The use of a solid polymer as electrolyte, instead of a flammable solvent, is currently the most promising solution for thinner and safer LIBs. Poly(ethylene oxyde)-based polymers (PEO) are widely used because of their good ability to transport lithium ions at temperatures over 60 °C.

Our work is focused on the structuring of classic −EO− based backbones by photo-polymerization, which is a fast, cost-effective and solvent-free technique. Solid polymer electrolytes (SPEs) based on different monomers/oligomers (methacrylic and/or −EO− based) will be presented. By incorporating high amounts of plasticizers [1,2] and lithium salts, outstanding ionic conductivities are obtained ($\sigma > 10^{-4}$ S cm^{-1} at 20 °C) along with a wide electrochemical stability window (>5 V vs. Li^+/Li) as well as good interfacial stability. Besides, SPEs have remarkable morphological characteristics in terms of homogeneity, flexibility and robustness.

All-solid lithium-based polymer cells show very good cycling behavior in terms of rate capability and stability over a wide range of operating temperatures, which make them suitable candidates for future Li-ion polymer batteries working at ambient and/or sub-ambient temperatures.

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[2] J. R. Nair, L. Porcarelli, F. Bella, and C. Gerbaldi, *ACS Appl. Mater. Interfaces* **7** (2015) 12961-12971.

OR-5

Novel cyclic analogues of DPDPE and BIPHALIN with potent mixed μ/d opioid activity

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Biphalin and DPDPE have been modified by means of CLIPS approach, in order to obtain novel cyclic compounds with improved metabolic stability, potency and *in vivo* efficacy [1,2]. We evaluated the affinity at the μ and δ opioid receptors *in vitro* and analgesic *in vivo* potency of the novel cyclic compounds. DPDPE analogue with *m*-xylene regioisomer (**7b**) exerted a potent analgesic effect after i.c.v. and s.c. administrations, whereas the most active biphalin analogue contains the *o*-xylene bridge (**6a**). Finally we obtained two biphalin and DPDPE derivatives able to elicit a robust antinociceptive effect in rats both after central and local peripheral administrations.

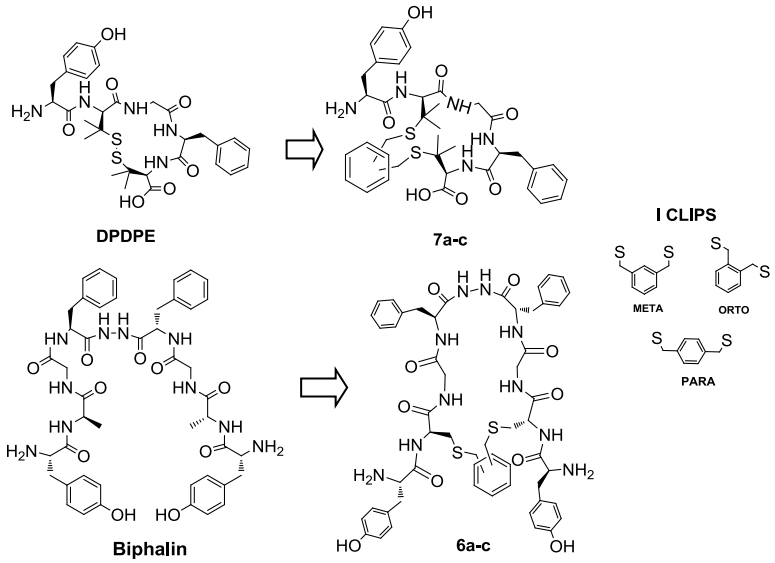

Figure 1: Design of Biphalin and DPDPE cyclic analogues performing CLIPS technology.

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[2] A. Stefanucci, A. Carotenuto, G. Macedonio, E. Novellino, S. Pieretti, F. Marzoli, E. Szűcs, A. I. Erdei, F. Zádor, S. Benyhe, and A. Mollica, *ACS Med. Chem. Lett.* **8** (2017) 858-863.

OR-6

Development of luminescent and magnetic materials combining MOF-like arrays and metallacrowns features

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Metal organic frameworks (MOFs) are porous coordination networks that usually exhibit high surface area [1]. Metallacrowns (MCs) are metallamacrocycles which might show luminescent and magnetic properties, that are tuned by the chemical neighborhood (solvent, counterions etc.) [2]. It's discussed here the combination of MOF-like arrays and MCs, that may lead to new functional materials, which can act as molecular recognition agents and find application as single-molecule magnets (SMMs) or luminescent probes in fields like quantum information processing and biological imaging. Two approaches are here described: the first consists into encapsulating MCs units inside the pores of the Zr-MOF PCN-777 (Fig. 1-left). The second one relates with the isolation of MOF-like metallacrown frameworks (*MMF*), where the MC units occupy the nodes and bear donor groups to connect at least two different MC units (Fig. 1-right).

The research leading to these results have received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° 611488. The MAECI (Italian Ministry of Foreign Affairs and Int. Cooperation) is acknowledged for financial support (Direz. Gen. per la Promozione del Sistema Paese).

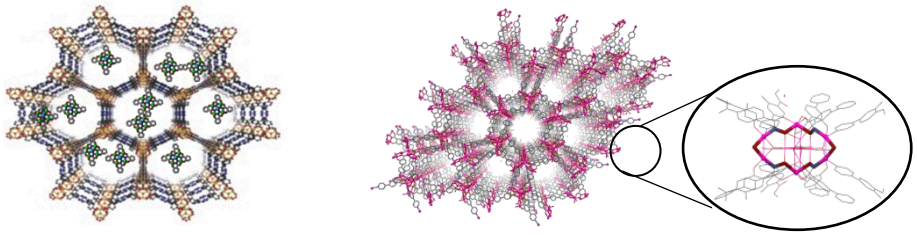

Figure 1: Left: Model of 12MC4 encapsulated in the MOF PCN-777 [1]. Right: X-Ray structure of the $Mn_{11}pPyHA_6AcO_3$ metallacryptate (the MC-motif is highlighted).

[1] D. Feng, K. Wang, J. Su, T. Liu, J. Park, Z. Wei, M. Bosch, A. Yakovenko, X. Zou, and H. Zhou, *Angew. Chem. Int. Ed.* **54** (2014) 149-154.
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OR-7

Immobilization of privileged triazolium carbene catalyst for batch and flow stereoselective umpolung processes

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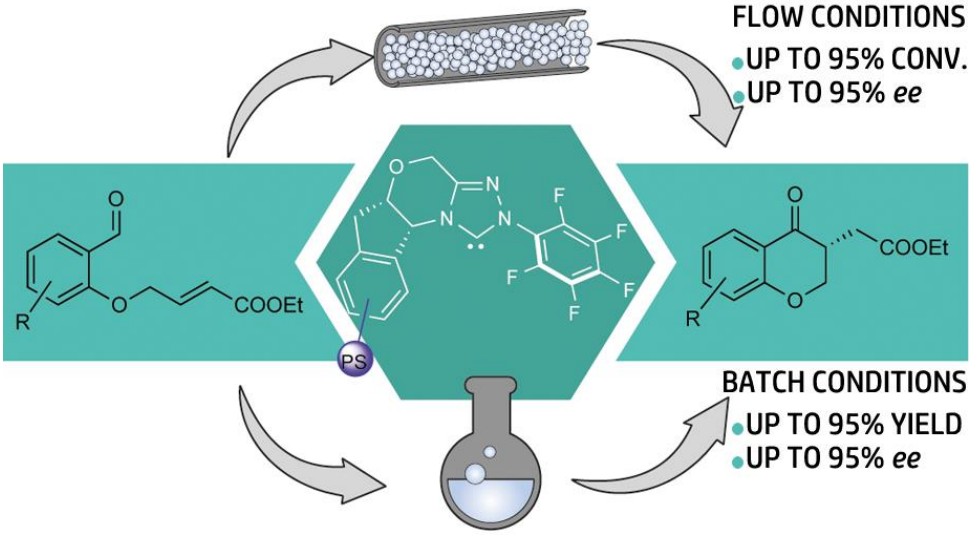
A strategy for the immobilization of the valuable triazolium carbene Rovis catalyst onto polystyrene and silica supports is presented [1].

Initially, the catalyst activity and recyclability were tested under batch conditions in the model stereoselective intramolecular Stetter reaction leading to optically active chromanones. Good results in terms of yield (95%) and enantioselectivity (ee: 81-95%) were detected for the polystyrene-supported catalyst (10 mol%), while poorer results were collected for the silica-supported analogue.

Also, continuous-flow experiments were performed by fabricating the corresponding polystyrene monolithic microreactors (pressure-resistant stainless-steel columns) to prove the benefits of the heterogeneous catalysis and the flow regime observing a high stability of the catalytic bed (48 h) with unaltered conversion efficiency and stereoselectivity [2].

To the best of our knowledge, our study represents the first example of heterogeneous NHC-catalyzed stereoselective process under continuous-flow conditions [3].



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OR-8

UV light-driven prebiotic synthesis of iron-sulfur clusters

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Iron-sulfur clusters are indispensable to extant metabolism and are thought to reflect an ancient role in mediating the chemical reactions that led to life. However, there has been no clear proposal for how these inorganic clusters came to occupy such an important position in biology. Therefore, it would be of great importance for prebiotic chemistry to delineate a plausible path from short, prebiotically plausible peptides to longer sequences with similar features to modern day iron-sulfur proteins.

Small organic thiolates and short cysteine-containing peptides can give rise to [2Fe-2S] and [4Fe-4S] clusters in aqueous solution when irradiated with UV light in the presence of iron ions [1]. Additionally, duplications of tripeptides coordinated iron-sulfur clusters give sequences which are better able to stabilize iron-sulfur clusters, resembling motifs with cysteinyl ligand spacing highly similar to contemporary ferredoxins [2]. Moreover, the studied iron-sulfur clusters are redox active and are able to mimic extant metabolic pathways, such as the first step of the electron transport chain, within protocells favouring the formation of a proton gradient which could be exploited for fundamental biosynthetic processes.

[1] C. Bonfio, L. Valer, S. Scintilla, S. Shah, D. J. Evans, L. Jin, J. W. Szostak, D. D. Sasselov, J. D. Sutherland, and S. S. Mansy, *Nat. Chem.* (2017) DOI: 10.1038/nchem.2817.
[2] S. Scintilla, C. Bonfio, L. Belmonte, M. Forlin, D. Rossetto, J. Li, J. A. Cowan, A. Galliani, F. Arnesano, M. Assfalg, and S. S. Mansy, *Chem. Commun.* **52** (2016) 13456–13459.

OR-9

The shielding effect of phospholipidic bilayers on zinc oxide nanocrystals for biomedical applications

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Zinc oxide nanocrystals (ZnO NCs), thanks to their unique properties, are receiving much attention for their use in nanomedicine, in particular for therapy against cancer [1]. To be efficiently employed as diagnostic and therapeutic (yet theranostic) tools [2], highly dispersed, stable and non-toxic nanoparticles are required. In the case of ZnO NCs, there is still a lack of knowledge about cytotoxicity mechanisms and stability in the biological context, as well as immunological response and haemocompatible features.

Most of these above-mentioned behaviours strongly depends on physico-chemical and surface properties of the nanoparticles. We thus propose a novel approach to stabilize the ZnO NCs in various biological media, focusing on NC aggregation and biodegradation as a function of the surface functionalization.We synthesized bare ZnO NCs, amino-propyl functionalized ones, and lipid bilayer-shielded NCs, and we characterized their morphological, chemical and physical properties. The stability behavior of the three different samples was evaluated, comparing their biodegradation profiles in different media, i.e. organic solvents, water, and different simulated and biological fluids. The studies aim to investigate how the particle surface functionalizations, and thus chemistry and charge, could influence their hydrodynamic size, zeta potential and consequent aggregation and degradation in the different solvents. We demonstrated that bare and amino-functionalized ZnO NCs strongly and rapidly aggregate when suspended in both simulated and biological media. Long-term biodegradation analysis showed small dissolution into potentially cytotoxic Zn-cations, also slightly affecting their crystalline structure. In contrast, high colloidal stability and integrity was retained for lipid-shielded ZnO NCs in all media, rendering them the ideal candidates for further theranostic applications [3].

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[2] E. Lim, T. Kim, S. Paik, S. Haam, Y. Huh, and K. Lee, *Chem. Rev.* **115** (2015) 327-394.
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The support from ERC Starting Grant – Project N. 678151 "Trojananohorse" and Compagnia di Sanpaolo are gratefully acknowledged.

OR-10

Photoelectrochemical performance of the Ag(III)-based oxygen evolving catalyst

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We report the electrosynthesis of a water oxidation catalyst based on Ag oxides (AgCat). AgCat is composed of mixed valence crystalline Ag oxides in the form of particle aggregates whose size is around 1 μm. Under positive applied bias this catalyst sustains current densities similar to other water oxidation catalysts, such as Co or Ir oxides. Dark bulk electrolysis demonstrated that AgCat can sustain high turnover number and is therefore stable in operative conditions, with production of molecular oxygen with faradaic efficiency larger than 90%. Oxygen evolution from water occurs in mild conditions: pH = 2-13, at room temperature and pressure, and moderate overpotentials (600 mV), compatible with the coupling with semiconducting oxides as sensitizers. When AgCat is coupled with TiO_2 and hematite, and under photo-electrochemical conditions, it substantially increases photocurrents in a wide range of applied potentials compared with bare and Co-Pi-modified photocatalysts. AgCat deposited on hematite produces O_2 with high faradaic efficiency during sustained electrolysis, both in the dark and under irradiation. Steady state is reached after an initial induction time of 50-60 minutes, in which modification of surface species occurs.

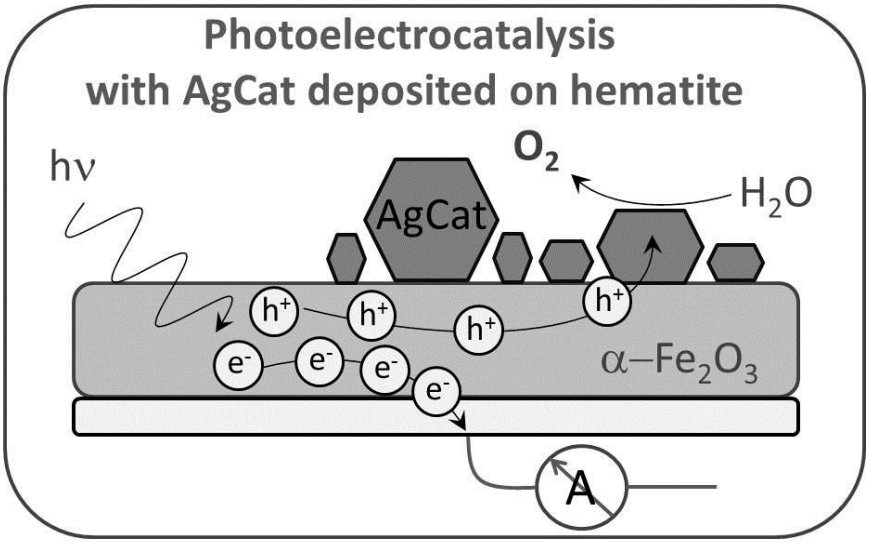

Figure 1: Schematic mode of operation of AgCat deposited on hematite (α-Fe_2O_3) in photoelectrochemical conditions.

OR-11

Smart grafting of lanthanides onto silica *via N,N*-dialkylcarbamato complexes

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Lanthanide ions play a relevant role in the advancement of new technologies, where their peculiar properties can be exploited (e.g. magnetic materials and luminescent sensors).

In this regard, the chemical grafting of metal ions onto the surface of inorganic, organic or hybrid (inorganic/organic) materials is an important route to add new functionalities [1].

N,*N*-dialkylcarbamato (cbm) lanthanide complexes are an attractive alternative to the other common organometallic precursors since they are easy to prepare and generally highly soluble in non-polar solvents. Furthermore, they show a prompt reactivity toward Brønsted's acid species releasing carbon dioxide and amine.

M-OH groups of various inorganic oxides (for example silanols on silica) are sufficiently acid to protonate the carbamate moieties allowing the grafting of the metal ion onto the inorganic material.

Since only a fraction of the carbamate ligands reacts with the surface, the residual cbm moieties may be easily substituted through reaction with a protic agent thus allowing a great flexibility.

In particular, in our work, we use β-diketonate or carboxylate ligands bearing suitable chromophores able to sensitize the emission of lanthanide ions exploiting the so-called "antenna effect" [2].

As an example, we report here the functionalization of silica surface with Eu^{3+} and Tb^{3+} ions using 1,4-benzendicarbocylic acid as a divergent ligand.

In this way, we can build step by step a molecular structure employing the lanthanide ions as nodes.

Upon varying the relative metal content it is possible to tune the luminescence output in a wide color range.

These systems are particularly appealing for the development of ratiometric, self-referencing, intensity-based luminescence thermometers.

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OR-12

Self-assembling supramolecular structures as stimuli-responsive systems for sensing pH and anions in water

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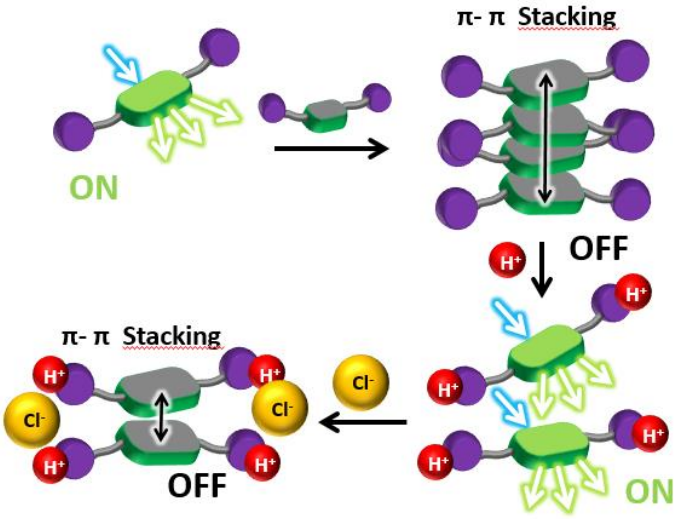
Multi-stimuli responsive materials are finding increasing importance in fields of high social and economic impact that include drug delivery, diagnostics, tissue engineering and 'smart' optical systems, as well as microelectronics, biosensors, microelectromechanical systems, coatings and textiles. Although different design approaches have been proposed, the self-assembly of molecular or nanostructured building blocks is, without any doubt, one of the most versatile, straightforward and powerful strategy to achieve stimuli-responsive materials. The response of these materials, either to environmental or external solicitation, can be, in fact, achieved by exploiting the same inter-components interactions that brings to their assembly.

Here we demonstrate that aggregation of properly designed perylene bisimide amino derivate can be controlled by pH in water solution. As shown in the figure the dye molecules (a) aggregate in water because of p-p stacking interaction (b), causing fluorescence quenching. The system can be disaggregated and the fluorescence switched on by protonation exploiting the electrostatic repulsion between the positive cations (c).



Even more interestingly we observed that the protonated system can be re-assembled by increasing the concentration of anion that partially shield the positive charge of the ammonium substituents.

Finally, our molecules show a unique response to protonation and anion concentration in water. These features make them very promising tools for ion sensing in view of biological and environmental applications.

OR-13

Bioinspired metal sites in four-helix bundle scaffolds

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Metal cofactors are involved in several key steps of life machinery. Metalloproteins regulate red-ox processes and efficiently catalyze difficult reactions under mild conditions. The protein matrix finely modulates the metal chemistry, despite the limited number of ligands, by a complex interplay of several interactions [1]. Thus, how the fine-tuning of the scaffolds hosting them imparts the wide spectrum of reactivity is of crucial interest both in the fields of structural biology and bioinorganic chemistry. Several scaffolds and metal binding motifs are object of intense work in the literature [2]. Here, we focused on the four-helix bundle as scaffold for metal binding sites in the context of protein *de novo* design.

To accomplish our objectives we expanded the designable space of a well-characterized *de novo* designed family of metalloproteins, the DFs (Due-Ferro). DF1, the progenitor of the family, bears a dicarboxylate bridged dinuclear metal center in its hydrophobic core constituted by the four-helix bundle unit [3]. We investigated the effect on the metal site exerted by loosening on the one side and tightening on the other the C_2 symmetric environment of the metal cofactor, giving raise to two new class of *de novo* designed proteins: DF-Click and 4[ED]H.

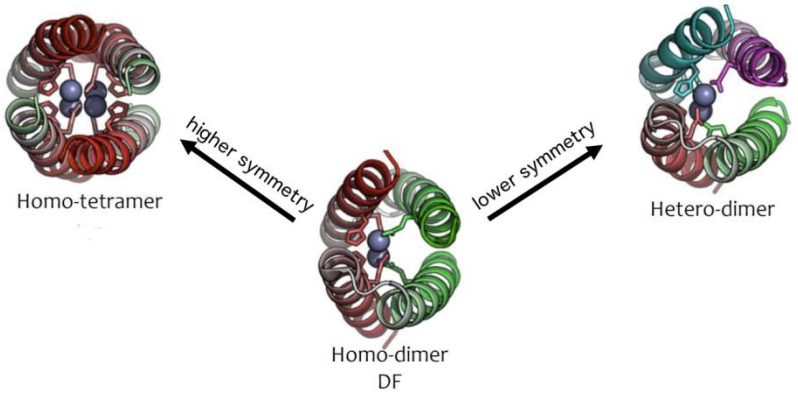

Figure 1: Top view of DF1 dimer and the two design strategy adopted.

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OR-14

[OSSO]-type Fe(III) complexes as catalysts for the reaction of CO_2 with epoxides

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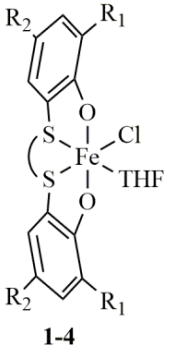
At present, the reduction of carbon dioxide deriving from anthropic activities is a challenging, but mandatory, objective to reach worldwide. Among the possible solutions, the reuse of CO_2 itself for the synthesis of chemicals, represent a valid strategy for the reduction of its concentration in the atmosphere [1]. One of the most interesting processes studied for this purpose is the reaction of CO_2 with epoxides for the synthesis of cyclic organic carbonates (COCs) and polycarbonates (PCs) [2].

Recently we reported on a series of dinuclear Fe(III) complexes, based on thioeter-tri-phenolate ligands, that resulted to be efficient catalysts for the selective synthesis of COCs [3]. To better understand the effect of nuclearity on the catalytic activity, saving the presence of sulfur neutral donor in the coordination sphere of the iron centre, we prepared a group of [OSSO]-type Fe(III) mononuclear complexes (Figure 1). In this contribution we describe the use of complexes **1**-**4**, in the presence of a co-catalyst, under mild reaction conditions. In detail the catalytic system is able to selectively produce COCs when the starting reactant is an acyclic epoxide while PC is obtained if the starting epoxide is cyclohexene oxide.



1-4

n	⌒	R_1	R_2
1	$(CH_2)_2$	CH_3	CPh_3
2	$(CH_2)_2$	$C(CH_3)_2Ph$	$C(CH_3)_2Ph$
3	$(CH_2)_2$	CH_3	CH_3
4	*c*-Hex	$C(CH_3)_3$	$C(CH_3)_3$

Figure 1: [OSSO]-type Fe(III) comlexes **1**-**4**.

[1] J. A. Martens, A. Bogaerts, N. De Kimpe, P. A. Jacobs, G. B. Marin, K. Rabaey, M. Saeys, and S. Verhelst, *ChemSusChem* **10** (2017) 1039-1055.
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OR-15

From neat to green solvents: steps towards sustainable homogeneous gold catalysis

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In literature, there are very few examples of gold homogeneous catalysis that works without silver additives, low catalyst loading, mild reaction conditions, simple work-up wth the possibility of recovery the catalytic system, and using green solvents or even in neat condition [1].

In this contribution, we obtained a greener pathways through the homogeneous gold catalysis, testing the activity of NHC-Au-X [NHC = (1,3-bis(2,6-di-isopropylphenyl)-imidazol-2-ylidene, X^- = BF_4^-, SbF_6^-, OTf^-,NTf_2^-, ClO_4^-, OTs^-, TFA^-)] as catalysts for the reactions of hydration, alkoxylation and cycloisomerization of alkynes and propargylamides. In our previous works, we notice that the anion plays an important role in the mechanism [2] and in order to obtain a reusable catalytic system, with a low catalyst loading (down to 0,01%), high values of TOF and TON, low Efactor and high EMY, the anion must be choose wisely in neat hydration of alkynes [3].

Once optimized the catalytic system, we extend the study to green solvents, instead of traditional volatile organic solvents (VOS) obtaining similar or, in some cases, better results.

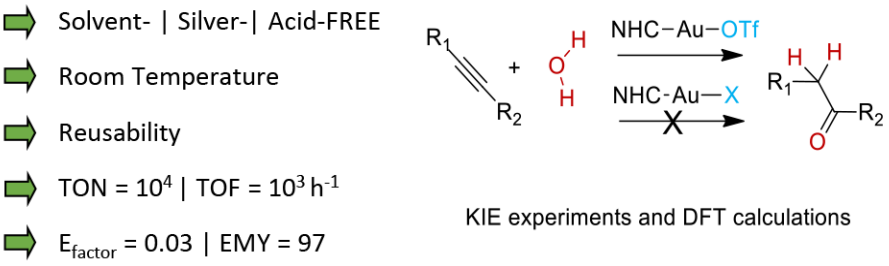

Figure 1: Hydration of alkynes.

[1] S. Dupuy, D. Gasperini, and S. P. Nolan, *ACS Catal.* **5** (2015) 6918-6921.
[2] L. Biasiolo, M. Trinchillo, P. Belanzoni, L. Belpassi, V. Busico, G. Ciancaleoni, A. D'Amora, A. Macchioni, F. Tarantelli, and D. Zuccaccia, *Chem. Eur. J.* **20** (2014) 14594-14598.
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OR-16

Synthesis, characterization and study of the catalytic activity of supported gold nanoparticles for alkynes hydroamination

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Our research group has previously reported the preparation of different silica supported gold nanoparticles (Au_{NPs}) catalytically active in the reduction of nitrophenol to aminophenol [1,2].

Recently, the focus of our research has shifted towards continuous flow nanocatalysis and for applications in packed bed reactors we have anchored Au_{NPs} on commercial micrometer oxide supports (SiO_2, Al_2O_3, TiO_2), previously modified by grafting of the organosilane [3-(2-propynylcarbamate)propyl]triethoxysilane (PPTEOS) (Figure 1).

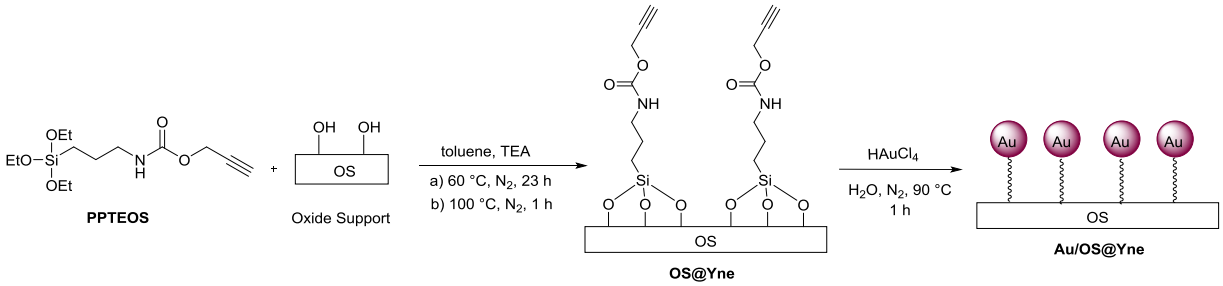

Figure 1: Synthesis of **Au/OS@Yne** (OS = SiO_2, Al_2O_3, TiO_2, Fe_3O_4).

After thorough characterization, the catalytic activity of these systems has been evaluated in the oxidation of a large variety of primary and secondary alcohols, both under batch and continuous flow conditions [3].

We now present the results in the field of the hydroamination of alkynes catalysed by **Au/SiO_2@Yne** and the new, magnetically recoverable **Au/Fe_3O_4@Yne** catalyst.

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OR-17

Synthesis, characterization and cytotoxicity of new Rh-Ge carbonyl clusters

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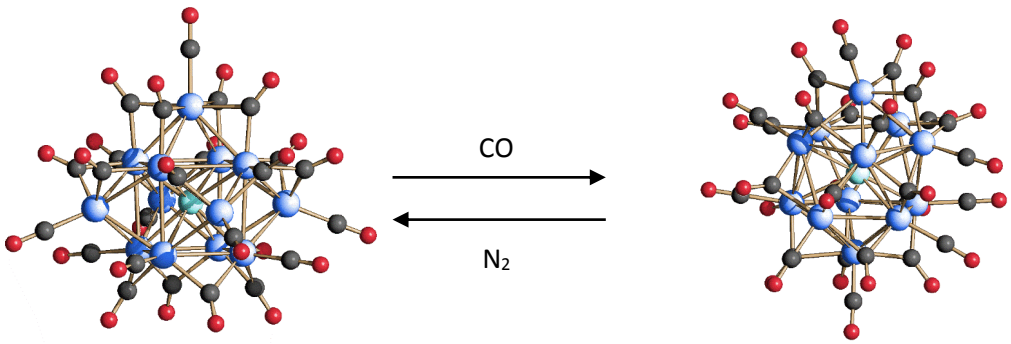
The chemistry of homo- [1] and hetero-metallic rhodium carbonyl clusters has been widely investigated in the last decades. Nevertheless, there are not so many examples of Rh clusters which interstitially host heavier elements than carbon [2] and nitrogen [3] and, among these, no one presents an inner germanium atom. Therefore, we have focalised our interest on the reactivity of the $[Rh_7(CO)_{16}][NEt_4]_3$ cluster precursor with Ge^{2+} and Ge^{4+} salts and we have obtained two new Rh-Ge carbonyl clusters, $[Rh_{13}Ge(CO)_{25}]^{3-}$ and $[Rh_{14}Ge_2(CO)_{30}]^{2-}$, both with Ge interstitially hosted.

Moreover, $[Rh_{13}Ge(CO)_{25}]^{3-}$ in solution under CO atmosphere undergoes a reduction process, forming the icosahedral species $[Rh_{12}Ge(CO)_{27}]^{4-}$.

These three new Rh carbonyl clusters have been characterised by IR spectroscopy and ESI-MS spectrometry and their molecular structures determined by X-ray diffraction studies.

Cytotoxicity tests of the two new compounds obtained under nitrogen atmosphere have been conducted against a human ovarian cancer cell line (A2780) and its cisplatin-resistant strain (A2780cisR).



$[Rh_{13}Ge(CO)_{25}]^{3-}$ $[Rh_{12}Ge(CO)_{27}]^{4-}$

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OR-18

IgY- and OVA- electrochemical immunosensor to detect egg temperas in works of art

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In the last few decades, due to their many advantages, immunosensors were deeply studied and applied in many research fields. By now only few papers regards the application of this effective devices to cultural heritage. One of the main goal of researches and analysis that involve works of art is to decrease the amount of sample required to have a detectable and reliable signal. Electrochemical immunosensors satisfies these (and more) requirements, due to their specificity and sensitivity. Moreover they ensure low costs, fast measurements and simple procedures [1].

To this aim, two immunosensors have been developed with the purpose to identify egg temperas. The target molecules are immunoglobulin Y (IgY – a specific marker for egg yolk), and ovalbumin (OVA – that properly represents egg white). Thanks to the simultaneous application of both the sensors, it is possible to fully determine the egg fraction that constitute a work of art, such as the binder in painting, when present. Both the immunosensors are electrochemical, the transduction element proposed is an ensemble of gold nanoelectrodes, an electrochemical devise suitable to be applied in the immunosensors field. Indeed the dual superficial composition on this electrode (polycarbonate and gold) is affine to biomolecules, as proteins and antibodies.

The immunosensors were applied to study mock-up samples simulating a complex multilayer painting, containing both the egg components at different concentration, to understand and study the reliability and sensitivity of the method.

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OR-19

Exploring cellular interactions with 2D organic monolayers by scanning electrochemical microscopy

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The morphology of cells changes consistently with the surface where they adhere [1]. As reported in literature, surfaces with micrometric and nanometric patterns affect the cell morphology, as well as surfaces with peculiar chemical functionalities [2]. In order to control both morphology and chemistry of the surface, mono-molecular layers of small organic molecules (specifically Pentacene, α-Sexithiophene and PDI8-CN_2) were deposited on SiO_x substrates by means of Organic Molecular Beam Epitaxy (OMBE). Through the partial annealing method, SiO_x substrates were fully covered with a mono-molecular layer, as confirmed by Atomic Force Microscopy measurements (surface coverage of about 98%). Such molecules enable SiO_x substrates to become biocompatible and to have flat morphologies with selective chemical functionalities. Epithelial cells were cultivated on such samples and their structure and shape has been investigated by optical and fluorescence microscope and Scanning Electrochemical Microscopy (SECM).

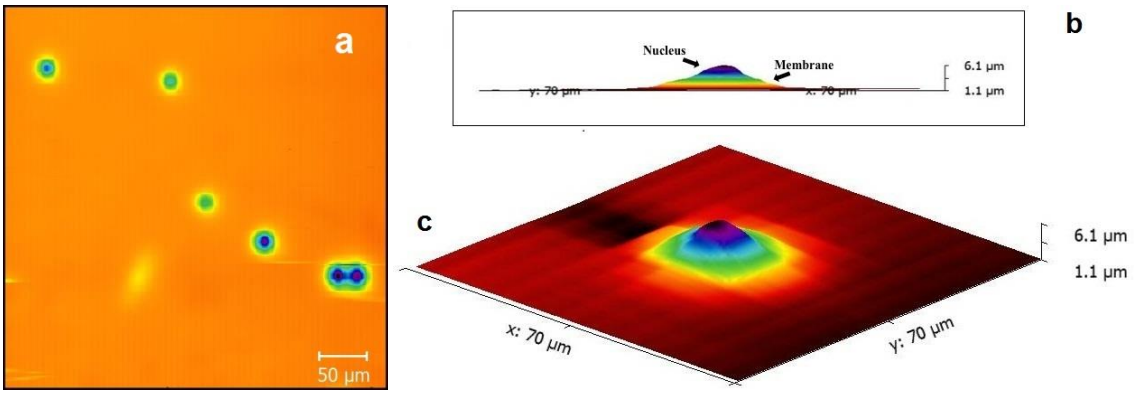

Figure 1: a) SECM image of cells on Pentacene; b) single cell profile and c) 3D image.

[1] D. Lehnert, B. Wehrle-Haller, C. David, U. Weiland, C. Ballestrem, B. A. Imhof, and M. Bastmeyer, *J. Cell Sci.* **117** (2003) 41-52.
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OR-20

Detection of irinotecan in plasma samples by coupling solid phase extraction and voltammetry

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Irinotecan (CPT-11) is an antineoplastic drug currently used in several cancer regimens. It is a pro-drug, activated by liver carboxylesterase to provide 7-ethyl-10-hydroxycamptothecin (SN-38), which is a potent topoisomerase I inhibitor [1]. CPT-11 has a narrow therapeutic window, because its pharmacokinetics and metabolism are extremely complex and depend from a number of factors such as patients' physical conditions and genetic background. Moreover, severe and unpredictable side effects are associated with CPT-11 overdosing. Thus, personalized drug treatments could avoid either over- or under-drug dosages, leading to a more selective chemotherapeutic use of CPT-11. In this respect, therapeutic drug monitoring (TDM) has become essential to assist in the determination of drug dosage for the individual patient [2]. TDM requires simple and fast analytical protocols for the detection and and control the drug concentration in patients' bloodstream. Among other approaches, electrochemical techniques appear very suitable for the purpose, as they are characterized by high sensitivity, minimum sample treatment, low cost and compact instrumentation [3].

In this paper, a simple method for the detection of CPT-11 in blood plasma samples is presented. It consists in a solid phase extraction (SPE) by means of commercially available SPE columns; this is followed by an electrochemical detection by differential pulse voltammetry (DPV). Current responses are evaluated against CPT-11 concentration and the method has a dynamic range between 3 and 15 μM, a LOD = 0.8 μM, a LOQ = 2.66 μM. It requires about 250 μL of blood sample. The method has been tested on a patient, affected by metastatic colorectal cancer, undergoing pharmacological treatment. Results obtained were compared with a validated HPLC-MS method and the absolute errors ranged between 11 and 24%.

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OR-21

New evidences of Pt_xY alloyed NPs formation on carbon support and catalytic activity for ORR

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Recently, the preparation of Pt bimetallic systems has attracted considerable attention because the amount of Pt could be reduced while the catalytic activity and stability may be maintained or even improved, due to the so called "*geometric effect*" and "*ligand effect*" [1,2].

In this work Pt_xY NPs, where Y atoms are in part alloyed with the Pt, were synthesized via a solid state method involving the chemical reduction of $Pt(acac)_2$ and $Y(NO_3)_3{\cdot}6H_2O$ salt precursors by H_2/N_2 flow at high temperature on different carbon supports [3]. The influence of the Pt_xY formation, NPs shape and dimension, and ORR activity was investigated with different commercial and homemade carbon support, which possess different surface area, porous distribution and surface functional groups. The best syntheses afforded small spherical Pt_xY NPs (2.71 nm) on a commercial CB (Pt_xY@MC7) and on MWCNT (Pt_xY@MC5), which showed a MA than the Tanaka catalyst but containing a lower amount of Pt. The mass activity determined were 606 mA/mg_{Pt} and 453 $mA/mg_{Pt,}$ respectively. The catalytic activity towards ORR was compared with Tanaka 50% Pt taken as standard reference confirming the increased activity of the Pt_xY alloy.

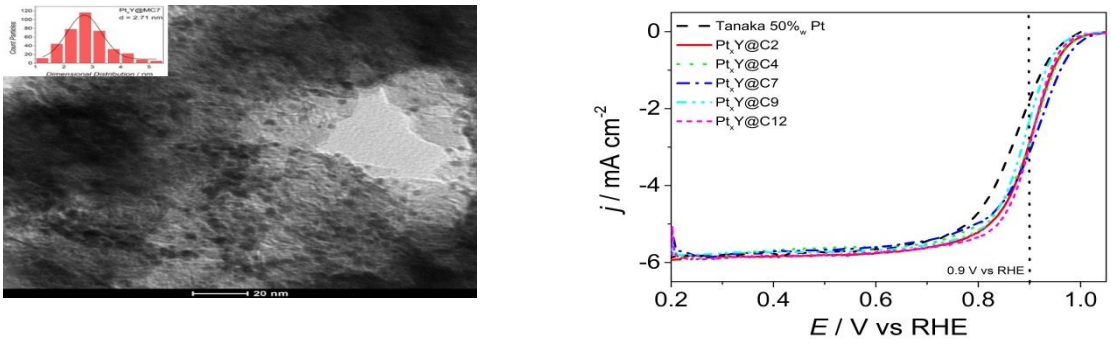

Figure 1: a) TEM image of Pt_xYMC7, b) LSV with RDE at 1600 rpm and 20 mV s^{-1} in $HClO_4$ O_2 saturated for Pt_xY catalysts.

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OR-22

An electrolyte study on Na_2BDA anode for Na-based organic batteries

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Thanks from the very high abundance on the Earth's crust and the low cost of sodium resources, Sodium-ion batteries (SIBs) are considered as attractive technology for application in the stationary state as energy storage and conversion systems.

The electrode materials chemistries actually used in batteries technologies are based on inorganic compounds (e. g. $LiCoO_2$, $LiMn_2O_4$, $Li_4Ti_5O_{12}$, etc…), that are expensive and synthesized from high temperature reactions, and also the end-of-life treatment is difficult and energy greedy.

One possible approach as alternative is switching to the organic based materials, in which a lot of synthesis routes can be chosen and a lots of compounds can be synthesized. Furthermore, the possibility to prepare materials from recyclable organic materials is really appealing [1].

However, organic compounds are often associated with drawbacks such as poor conductivity, low energy density and high solubility in liquid electrolytes. Especially for the last point an accurate study on the electrolytes involved in the batteries is mandatory, because is well known how the ion-transport media affect the performances of the batteries system.

In this work we present an overview on our recent results on using disodium benzenediacrylate (Na_2BDA) as electrode material for Na-based organic batteries [2], in different electrolyte media. In particular, the galvanostatic cycling behaviors in Na|electrolyte|Na_2BDA pouch-cell configuration are shown.

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OR-23

Mixed 1T–2H phase MoS_2/reduced graphene oxide as active electrode for enhanced supercapacitive performance

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Recently, the need of storage systems is crucial towards a clever energy management. Supercapacitors (SCs) are electrochemical power storage devices that can find many practical applications with the goal of replacing or going alongside with the already existing battery technology. Research is focused on the fabrication of nanostructured electrodes improves their energy density without affecting the high power density [1].

Aim of this work is the synthesis and assembly of hybrid SCs combining both EDLC and Pseudocapacitance properties. The hybrid material, based on graphene and a sulfur-based transition metal dicalchogenide, is synthesized by a green hydrothermal process [2]. The concomitant reaction between the metal precursor (e.g., Phosphomolybdic acid as Mo precursor) and L-cysteine, an amino acid acting as S source, allows to incorporate, in the RGO 3D matrix, the metal dichalcogenide layers. These materials enhance the supercapacitive performance [3].

The synthesized materials were fully characterized by FESEM, EDX, XRD, XPS, micro-Raman Spectroscopy and N_2 adsorption/desorption at 77 K. An in-depth electrochemical characterization of the SCs has been carried out using Cyclic Voltammetry, charge/discharge galvanostatic measurements and EIS.

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OR-24

Kinetic and thermodynamic parameters of atom transfer radical polymerization measured *via* rotating disk electrode

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Atom transfer radical polymerization (ATRP) is extensively used to build polymers with narrow molecular weight distribution, predetermined architectures and preserved chain end functionalities. Electrochemistry plays a crucial role in the complete definition of ATRP mechanism.

Particularly, k_{act}, rate constant of the activation step of ATRP initiators (alkyl halides) by the catalyst $[Cu^{I}L]^{+}$, is determined via rotating disk electrode (RDE). k_{act} values spanning over a 6 order of magnitudes range were measured under various conditions, setting up an easy, fast and highly reproducible procedure [1].

The equilibrium constant of ATRP, K_{ATRP}, is also precisely measured by RDE. Side reactions hampering ATRP process must be taken into account, mainly Cu(I) catalyzed radical termination (CRT) [2].

Thus, besides the direct determination of kinetic and thermodynamic parameters, electrochemistry allows to investigate harmful processes, and to define the best operating conditions for several ATRP setups.

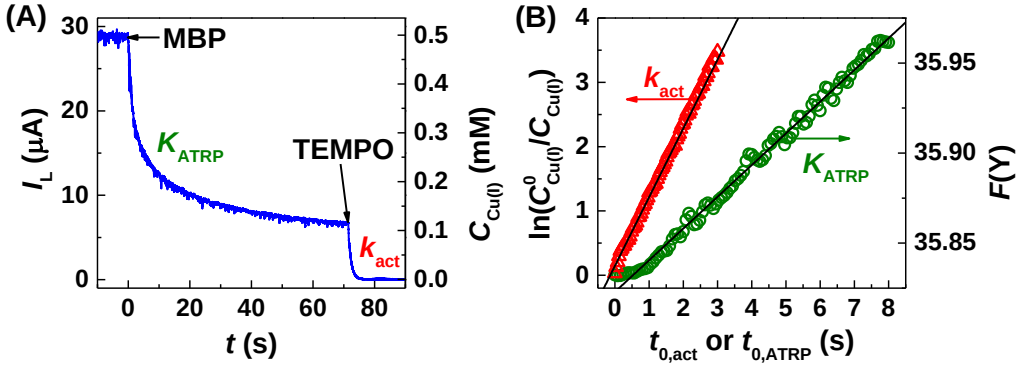

Figure 1: One-pot determination of k_{act} and K_{ATRP} via RDE for $[Cu^{I}TPMA]^{+}$ reacting with MBP, in MeCN/BA 1/1 v/v + 0.1 M Et_4NBF_4, T = 25 °C. Radical scavenger TEMPO was injected *ca.* 70 s after MBP injection.

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OR-25

First principle analysis of singlet-triplet transitions in organic molecules

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Organic molecules have revealed to be extremely useful building blocks for developing efficient optoelectronic materials. The theoretical design of new molecules has been mostly carried out by focusing attention on energetic aspects, but, as recently remarked, kinetic aspects can also play a predominant role. Herein, we present a full quantum approach for predicting the kinetics of some elementary processes frequently occurring in optoelectronic devices: i) photo-induced charge transfer; ii) charge diffusion within donor and acceptor domains; iii) charge recombination process at donor/acceptor interface, both via singlet and triplet states. Triplet state are indeed expected to play an important role both in organic light emitting diodes (OLED) and in solar energy conversion devices [1]. For better assessing the reliability of the adopted computational procedures for singlet-triplet transitions, we have also simulated from first principles the spectral band shapes of singlet-triplet transitions of some aromatic compounds used in solid-state optoelectronic devices [2]. Computed spectral shapes are indeed in excellent agreement with experimental results, opening the way for reliable calculations of the rates of nonradiative singlet-triplet transitions, an important step for the optimization of the molecular structure of dyes for solar energy conversion cells and for light-emitting diodes.

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OR-26

Single cell electrochemiluminescence imaging: from the proof-of-concept to disposable device-based analysis

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Electrochemiluminescence (ECL) is a powerful transduction technique gathering the advantages of the electrochemical sensitivity and the spatial resolution provided by fluorescence microscopy. Recently, the combination of ECL imaging and immunoassays resulted in an emerging approach for visualizing micrometer-size objects onto an electrode surface [1,2]. However ECL has never been reported for the resolved imaging of single cells showing up the distribution of proteins on their membrane. Here we report the development of coreactant-based electrogenerated chemiluminescence (ECL) as a surface-confined microscopy to image single cells and their membrane proteins. In order to present the potential diagnostic applications of our approach, we selected carbon nanotubes (CNT)-based inkjet-printed disposable electrodes for the direct ECL imaging of a labeled plasma receptor over-expressed on tumor cells. The presented surface-confined ECL microscopy should find promising applications in ultrasensitive single cell imaging assays.

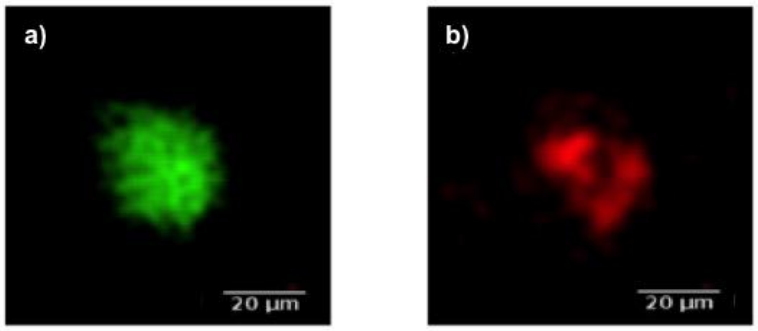

Figure 1: PL (a) and ECL (b) images of a MCF10A cell labeled with **Ab@Ru** adhered on an inkjet-printed CNT electrode.

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Elsevier: an overview from the Publishing Team

Jan Willem Wijnen

OR-28

EYCN – The European Young Chemists' Network

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The European Young Chemists' Network (EYCN), the young member's division of EuCheMS, is a motivated team of young scientists from 22 different European countries.

The EYCN spent the last years working towards promoting the exchange of knowledge, experience, new ideas and projects among young chemists coming from academia and companies. One of the aims is also to improve the visibility of chemistry, bring it closer to a wider audience and to people from outside the research field - such as industry, business&management. Moreover, the EYCN wants to support young chemists at the beginning of their career with awards and activities focused on developing soft-skills and expanding their possibilities. Every two years, the EYCN announce the Young Chemist Award (EYCA) in collaboration with SCI and the Italian Consiglio Nazionale dei Chimici. Moreover, the EYCN organizes career days and has promoted the Young Chemists Crossing Borders exchange program (YCCB) in collaboration with the Younger Chemists Committee of the American Chemical Society (ACS YCC) since 2011 [1]. In April 2016, the EYCN hosted its first European Young Chemists' Conference (EYCheM) in Guimarães (Portugal) and its 2nd edition is coming in 2019. Our network is working for supplying a mentoring program for Marie Curie fellowship and ERC starting grant applicants.

If you wish to get in touch with us, please visit our website **www.eycn.eu**, or contact us using our social media profiles on Facebook (@EYCN), Twitter (@YoungChemists) or LinkedIn. We look forward to collaborating with you!

Figure 1: EYCN Delegates attending the 12th Delegates Assembly in Heraklion (GR)

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OR-29

ROS-generating lipid-coated zinc oxide nanoparticles for photodynamic therapy

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Photodynamic Therapy (PDT) is a medical treatment that combines the administration of a nontoxic drug, called photosensitizer (PS), with light irradiation of the targeted region. It has been proposed as a new cancer therapy, promising better selectivity and fewer side-effects compared to traditional chemo- and radio-therapies. PSs indeed can accumulate specifically within the region of interest so that when the light is directly focused only in that region the therapeutic effect is highly localized.

Traditional PSs, like chlorins and porphyrins, suffer from several drawbacks such as aggregation in biological media and poor biocompatibility. Thus, the development of innovative photosensitizers able to overcome these issues is crucial to the therapeutic action of PDT. Among the others, nanostructured Zinc Oxide (ZnO) has been recently proposed as new therapeutic agent and PS thanks to its semiconducting properties, biocompatible features, and ease of functionalization [1]. Nevertheless, further efforts are needed in order to improve its colloidal stability in biological media and to unravel the effective therapeutic mechanism.

Here, we propose the synthesis and characterization of lipid-coated ZnO nanoparticles as new photosensitizer for cancer PDT [2]. First, by Dynamic Light Scattering (DLS) experiments, we show that the lipid-coating increases the colloidal stability of the ZnO NPs in Phosphate Buffered Saline (PBS). Then, using Electron Paramagnetic Resonance (EPR) coupled with the spin-trapping technique, we demonstrate and characterize the ability of bare and lipid-coated ZnO NPs to generate Reactive Oxygen Species (ROS) in water only when remotely actuated via light irradiation. Interestingly, our results aware that the surface chemistry of the NPs greatly influence the type of photo-generated ROS. Finally, we show that our NPs are effectively internalized inside human epithelial carcinoma cells (HeLa) via a lysosomal pathway and that they are able to generate ROS inside cancer cells.

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OR-30

A grandma's recipe: oil canned phosphorene

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In recent years, 2D phosphorene has attracted growing attention for potential applications in electronic devices because of its high carrier mobility and tunable bandgap [1]. However, its fast oxidation in air severely hinders its practical applications. The most widely used approach to overcome this issue involves the use of thick protecting layers, such as PMMA or Al_2O_3, which anyway have to be removed (with long and costly lithographic techniques) for the preparation of electronic devices. Some effort has also been made on the passivation of phosphorene through atomic layer deposition, covalent functionalization, and covering with monolayers of boron nitride, graphene, or organic materials. However, the stability in air and performance in device of phosphorene passivated with such materials/techniques is not optimized yet.

In sight of this, the chemical inertness and hydrophobicity of linear alkane chains, together with their well known self-ordering properties onto 2D materials [2], prompted us for the study of epitaxially gowth mono- and oligo-layers of linear alkanes onto exfoliated phosphorene, as efficient passivating agents. Evidence of the self ordering, through non-covalent bonding, of the alkane chains on the surface of phosphorene was given through SPM techniques, showing one preferential and one secondary orientation of the chains, corresponding to the in-plane crystalline axis of the underlying phosphorene. Then, the protecting properties of such layers towards oxidation were proven through the study of the oxidation time in air of pristine *versus* passivated phosphorene.

The authors thanks the European Research Council (ERC) under the European Union Horizon 2020 research and innovation program (grant agreement no. 670173) for funding the project PHOSFUN "Phosphorene functionalization: a new platform for advanced multifunctional materials" through an ERC Advanced Grant.

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OR-31

Models for stereocontrol in polylactide polymerization

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Polylactide (PLA), is one of the most important synthetic biodegradable polymers used for a wide range of biomedical and pharmaceutical applications [1]. Moreover, recent concerns with our environment call for the development of eco-friendly materials derived from renewable resources such as corn and sugar beets.

The most efficient method for the generation of PLA is the ring-opening polymerization (ROP) of the six-membered cyclic ester lactide (LA). The presence of two stereogenic centers in the LA monomer may give rise to different polymer stereoregularities which affect physical and mechanical properties of the material.

A large number of aluminum complexes, including tetradentate-dianionic sequential [ONNO]-type ligands (Al-Salan, Al-Salen and Al-Salalen) producing stereoregular PLAs, have been recently synthesized.

Even if this plethora of catalytic systems exists, little is known about the mechanism(s) of stereocontrol in the PLA synthesis obtained by ROP.

Aim of this work is to use DFT calculations to unveil the reasons which lead to a stereocontrolled ROP for the PLA synthesis promoted by two Al-Salen systems: the achiral (**1**) and the chiral (**2**) Al-Salen precursors (see Figure 1). It has been reported in literature that system **1** may forms stereoregular PLAs by Chain-End control whereas a Site control mechanism may operate with system **2** [2,3]. The main whish of this work is to get insights to lead a rational tuning of the catalysts.

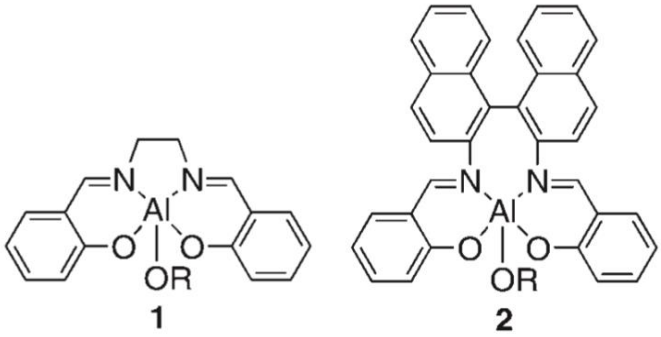

Figure 1: Structure of achiral (**1**) and chiral (**2**) Al-Salen complexes.

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OR-32

The wavelength dependent ultrafast charge carrier dynamics in the $WO_3/BiVO_4$ heterojunction

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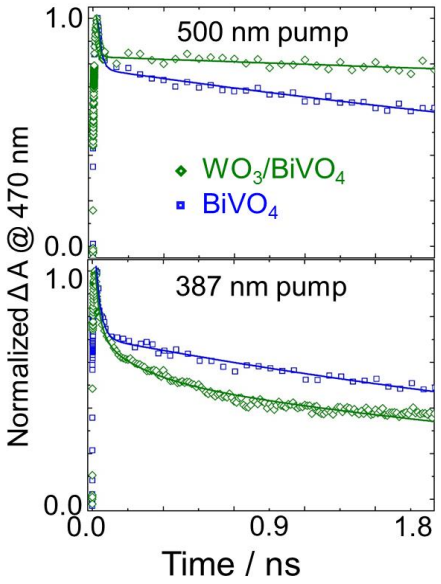

Figure 1. Effect of the pump wavelength (500 and 387 nm) on the normalized TA signal recorded at 470 nm in $BiVO_4$ (blue squares) and $WO_3/BiVO_4$ films (green diamonds).

Photoelectrocatalytic water splitting into H_2 and O_2 is a promising way to store solar light in the form of chemical energy. $WO_3/BiVO_4$ photoanodes show remarkable efficiency due to the favorable band alignment between the two oxides, which is commonly considered the key factor of their high activity [1,2].

The charge carrier dynamics and the interactions between WO_3 and $BiVO_4$ in the $WO_3/BiVO_4$ system have been investigated through femtosecond transient absorption (TA) spectroscopy. By tuning the pump wavelength, we observed wavelength dependent interactions, *i.e.* under selective $BiVO_4$ excitation the lifetime of trapped holes in $BiVO_4$ increases, while by exciting both oxides a recombination channel leads to shorter lived holes [3]. These interactions allow to explain the overall photoelectrochemical performance of this heterojunction and should be taken into account in the design of other efficient heterojunction systems for better charge separation.

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OR-33

Modeling hole transfer in DNA oligonucleotides

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Since its discovery, the ability of singly ionized DNA to provide long-range hole transport (HT) has attracted considerable interest. Apart from the biochemical implications connected with the oxidative damage of nucleic acids, long range HT makes DNA a potentially well-suited material for nanoelectronics, either by exploiting its self-assembling properties or by using it as the active component in nanocircuits.

Herein, we analyse the rates of hole transfer between guanines separated by up to five adenines or thymines, exploring both the coherent single step superexchange mechanism by the numerical solution of the time dependent Schrödinger equation [1] and the incoherent multi step hopping. Hole site energies and intra-strand electronic coupling elements have been estimated by differential pulse voltammetry of isolated nucleobases in solutions of A rich and G rich oligonucleotides, both in single and double strands, or by reliable ab initio computation, which are in optimum agreement with photoelectron spectroscopy and voltammetric measurements [2].

Theoretical simulations show that in short oligomers, consisting of two guanines separated by a bridge of up to three thymine bases, intrastrand hole tunnelling between guanines can occur on picosecond timescales, about three orders of magnitude faster than hole hopping, whereas interstrand charge transfer becomes faster in oligomers with longer bridges of four or five thymines. Tunnelling becomes extremely slow in longer oligomers, containing more guanine sites in the strand, because charge can bounce among them. Our results are able to reconcile conflicting experimental results [3], showing the great complexity of charge transport in molecular systems.

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OR-34

High-resolution rotational spectroscopy of doubly-deuterated Amidogen radical ND_2

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The formation mechanism of deuterated molecules in the interstellar medium (ISM) is still being debated. Detection of deuterium-bearing species in various astronomical sources represents a powerful constraining tool to improve our comprehension of the interstellar chemistry. The doubly-deuterated form of the Amidogen radical, ND_2, could be a target for observation in space.

In the present work, the rotational spectrum of the ND_2 radical in its ground vibrational and electronic states has been investigated in selected frequency regions between 588 and 1131 GHz using a frequency modulation millimeter/submillimeter-wave spectrometer. This radical has been produced in a free-space glass absorption cell by discharging a mixture of ND_3 and Ar. More than sixty new transition frequencies involving J values ranging from 2 to 5 and K_a values from 0 to 4 have been recorded.

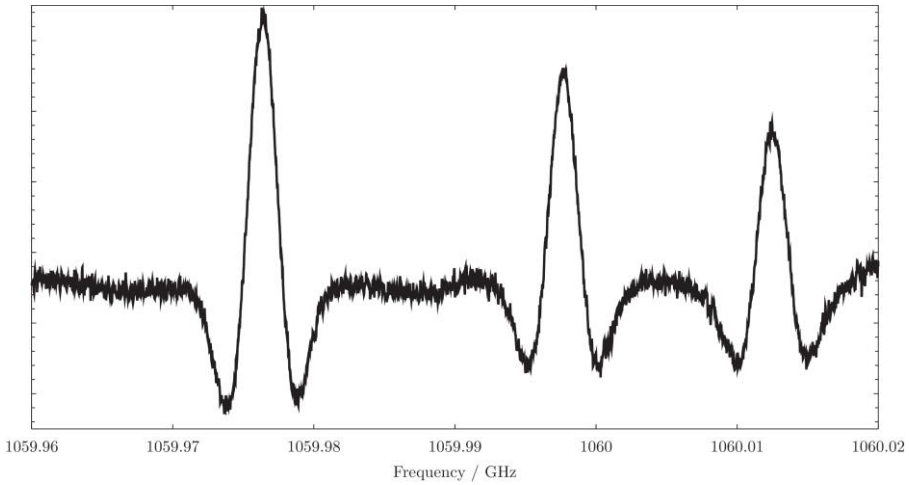

Figure 1: Portion of the THz spectrum.

A global analysis including all the previous field-free pure rotational data [1-3] has been carried out, allowing for a more precise determination of a large set of spectroscopic parameters. Accurate predictions of rotational transition frequencies of ND_2 are now available up to 8 THz, providing a facility set of data for radio-observations of doubly-deuterated Amidogen.

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OR-35

pH-sensitive vesicles for the confinement of nonlinear chemical reactions

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It is now well established that chemical reactions, far enough from their equilibrium state, can give rise to complex phenomena such as oscillations of concentrations in time and space. Such oscillations have been observed in many instances including redox reactions and heterogeneous catalytic systems [1].

One of the most innovative projects in the field of nonlinear dynamics is the design of chemical systems that can show pH oscillations in batch and biocompatible conditions. Due to the ubiquity of the H^+ ion in biological and chemical processes, these oscillators may have potential applications in medicine as drug delivery systems [2].

In an attempt to design a biocompatible batch pH oscillator, some years ago, our research group recovered the well-known urea-urease reaction. Numerical simulations showed that this enzymatic reaction can give rise to pH oscillations if the transport rate of the substrate (urea) is lower than that of a negative feedback species (H^+). We first coupled the urea-urease reaction with POPC lipid vesicles as this kind of membrane guarantees a differential transport of the reactants [3]. However, in this system, oscillations have not been observed yet.

Currently, our strategy to obtain pH oscillations includes the coupling of the urea-urease reaction with pH-sensitive membranes that can be made of either pH sensitive polymers (polymersomes) or lipids and pH-sensitive polymers (hybrid vesicles). The polymers we are synthetizing are block copolymers with the general structure ABC where A is the hydrophilic block of monomethoxypoly(ethylene glycol) (mPEG), while BC is a copolymeric random chain of methyl methacrylate (MMA) and the pH sensitive monomer 2-(Dimethylamino)ethyl methacrylate (DMAEMA). The pure polymersomes will be produced with the thin-film hydration method, while the hybrid ones with the electroformation technique.

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OR-36

Anilino-substituted multicyanobuta-1,3-dienes: strong electron acceptors for photoinduced charge-separation systems with thermally accessible conical intersections

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The electrochemical and photophysical properties of three multicomponent systems featuring a Zn(II) porphyrin linked to aniline-substituted pentacyano- (**PCBD**) or tetra-cyanobuta-1,3-dienes (**TCBD**), with and without a spacer, are presented [1]. By means of steady-state and time-resolved spectroscopy, photoinduced intramolecular energy and electron transfer processes are evidenced, upon excitation of the porphyrin unit. These results suggest that the strongly electron-accepting cyanobuta-1,3-dienes might become promising alternatives to quinone-, perylene-diimide-, and fullerene-derived acceptors in multicomponent systems featuring photoinduced electron transfer.

Unfortunately, these electron acceptors are not luminescent and their lowest singlet excited state (S_1) decays to S_0 within few picoseconds, preventing a simple and straightforward photophysical characterization of any system featuring cyanobuta-1,3-dienes as electron acceptors. This is also a significant drawback if cyanobuta-1,3-dienes are to be considered as active materials in photovoltaic devices where generation of charge-separated states must compete with internal deactivation processes.

By means of CASSCF calculations we were able to locate accessible sloped S_1/S_0 conical intersections for these acceptor molecules, which are responsible for their observed fast non-radiative deactivations [2]. At present, we are also investigating the role of triplet excited states (and of intersystem crossing) in the deactivation pathways of these molecules [3].

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OR-37

Siliceous zeolites with mono-dimensional linear channels as host for adsorption and reaction of technologically relevant organic molecules

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Beyond their traditional applications as shape-selective catalysts, selective absorbers and cation exchangers, zeolites can be considered as small chemical laboratories [1]. ZAPPING project (www.zapping-prin.it) aims to merge the potentialities of high-pressure technologies with microporous materials properties, to induce and control chemical reactions proved effective in driving the formation of arrays with desired dimensionality [1]. The project will exploit the porous template effectiveness of zeolites in inducing the aggregation and polymerization along preferential directions, not easily achievable under bulk nor confined conditions. This will allow the development of materials with enhanced functionalities, such as confined polymers with low dimensionality, to be integrated in devices (i.e. gas sensing devices).

The use of all silica zeolite is fundamental to obtain organization of molecules in the channels. Specific framework types were selected according to specific needs: i) the dimensions of the pores must allow the penetration of the molecules of interest. ii) to promote the synthesis of isolated 1D polymer chains the framework must have a mono-dimensional channel system; iii) a residual porosity should be maintained after polymerization to allow the gas transit. For these reasons MOR and MOZ framework type were selected.

Within the first months of the project, we report the tuning of the synthesis conditions for a nanocrystalline ZSM-10 material using dm-DABCO as templating agent and the de-alumination of a MOR type zeolite.

Acknowledgment: this research work was carried out in the frame of the PRIN 2015 Project ZAPPING (code 2015HK93L7).

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OR-38

A DFT rationalization of a two metals strategy to tune selectivity in catalysis

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Selectivity is among the most important properties of an effective catalyst. In homogeneous catalysis this can be achieved by appropriate design of the ligand around the metal. In heterogeneous catalysis this is a more complex issue, since selectivity is often associated with different reactivity at different surfaces of the catalyst, as well as at steps, edges, and any type of defects. A promising strategy to improve the selectivity of a metallic catalyst is alloying a second metal [1]. In this communication we will present DFT insights in the dry reforming of methane promoted by Ni/Co catalysts [2]. In details, we performed DFT simulations aimed to elucidate the availability of the different active sites on the surface of the reduced CoNi particles to supplement the experimental techniques.

Moreover, calculations allowed to rationalize the catalytic behavior of the alloy showing that the CoNi metal surface has an intermediate energy of oxygen chemisorption, between those of monometallic Co and Ni (see Figure 1).

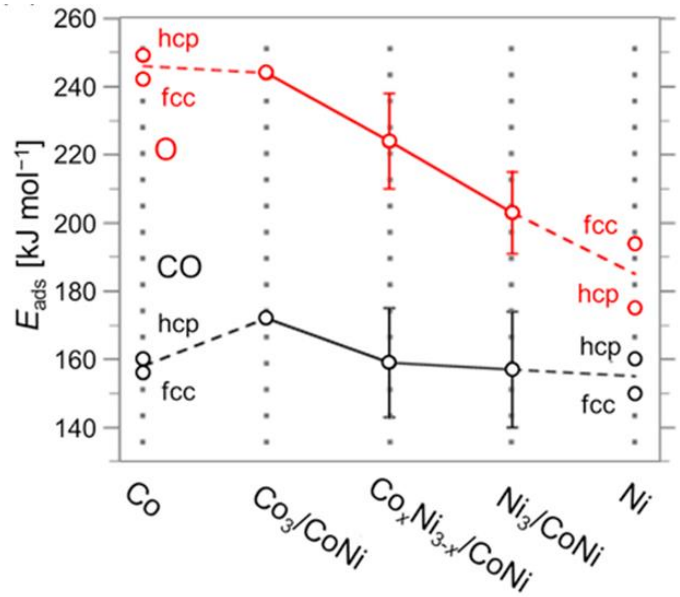

Figure 1: Adsorption energies of CO and O on Co(111), Ni(111) and CoNi(111) sites with various composition.

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OR-39

Amino-acid-based task specific ionic liquids for CO_2 capture

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The problem of the high concentration of CO_2 in the atmosphere is encouraging the development of novel and efficient system for the reversible capture of the CO_2. The amine scrubbing of flue gases is a well-known technology but it still has several drawbacks (*e.g.* corrosion and toxicity). Recently Task Specific Ionic Liquids (TS-ILs) have been considered as alternative for the highly efficient capture of CO_2 via chemical fixation [1] and overcome the performance of the usual aqueous amine solution. Nonetheless, the most common cations employed in ILs, imidazolium, pyridinium and phosphonium, revealed to be not environmental friendly and to be toxic for the microorganisms and cells. Instead, the cholinium-based ILs demonstrate to be an interesting alternative to usual ILs [2]. The Choline is a water-soluble essential nutrient, it has relatively low toxicity and it consists of a tetraalkyl-ammoniun head linked to a polar hydroxyl tail. On the anion side, the amino acids (AA) are a fully sustainable and non-toxic source of counter-ion with amine functionalities. The first synthesis of Choline AA-ILs was carried out through Choline Hydroxide intermediate [1]. Only recently, a newer and simpler method was developed to synthetize the Choline AA-ILs [3].

In this work, the CO_2 absorption of two Choline-based AA-ILs were studied, aiming to enlight the mechanism of absorption. Choline Glycinate and Choline Alaninate were synthetized using the newer method. The absorption of the pure AA-ILs and their solutions with DMSO were measured, as well as other chemo-physical properties. The overall mechanism of absorption was deeply investigated by means of infrared spectroscopy using a peculiar Attenuated Total Reflectance setup in order to determine the interaction between the IL, the solvent and the CO_2.

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OR-40

Carbocatalysis: a computational insight into the metal-free oxidation of ethylbenzene by carbonanotubes

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During the last two decades it has been demonstrated that nanostructured carbon materials (*i.e.* graphene sheets, carbon nanotubes and fullerenes) can play an active role as catalysts in heterogeneous catalysis [1].

Experiments on oxidized carbonanotubes (o-CNTs) have shown that ketonic carbonyl groups on the o-CNT surface are responsible for the oxidative dehydrogenation of ethylbenzene (ODE) to styrene with the loss of a water molecule [2].

Up to date, the ODE reaction mechanism is still unclear. A very general hypothesis suggests a mechanism that proceeds through a first hydrogen radical abstraction. Our purpose was to investigate, at a quantum-mechanical level (DFT), the potential energy surface of the reaction and elucidate the mechanism in detail. For the sake of simplicity, we studied a (6,6) armchair CNT (12-Å long) on which we modelled the chemisorption of one $^3O_2$ molecule. On the two most stable geometries, we physisorbed ethylbenzene obtaining two model systems. On each model, we computed the dehydrogenation of ethylbenzene to styrene finding that the rate determining step corresponds to the first hydrogen abstraction. The results also suggest that the nature of the first intermediate strongly depends on the catalytic oxygen-group that participates in the catalysis.

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OR-41

Doped graphene-metal interfaces as ORR and OER electrocatalysts for fuel cells applications

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Hybrid organic-inorganic systems are widely applied in different technological devices thanks to the peculiar combination of molecular functions (*e.g.*, molecular recognition) and solid-state inorganic features (*e.g.*, fast charge and heat transport) [1]. 2D materials such as graphene nanostructures (GNS) can be easily combined with inorganic substrates for designing new materials for clean energy conversion devices. In particular, the optimization of effective and cheap alternatives to traditional expensive platinum-based electrocatalysts for oxygen reduction reaction (ORR) in fuel cells is attracting a lot of attention. Recent experiments support the idea that dopants or interfacing with a metallic support can enhance GNS catalytic activity [2].

In this context, we have studied the energy conversion capabilities of a hybrid material based on GNS and doped-GNS on a metallic substrate with first-principles calculations. We investigated the properties of the interface with an *in-house* modified DFT-D approach (DFT-DM) for treatment of dispersion forces. We characterized how the structural, electronic and catalytic properties of GNS are tuned by dopants and by direct interaction with the supporting metal surface. In this contribution, we will first discuss minimum-energy geometries, binding energies and electronic structure features of pristine and doped graphene on the hexagonal Ag(111) surface slab. Both p- and n- doping effects have been investigated using boron and nitrogen as dopant atoms, respectively. Then, we address the ORR/OER catalysis at the surface of the hybrid electrode in the framework of the theoretical hydrogen electrode (TSHE) [3]. We focus on the reaction intermediates and the minimum energy pathways for the ORR in order to understand the effects of the metal substrate on the physical and chemical properties of GNS. Our final objective is to design a new and effective GNS-silver hybrid cathode for low temperature fuel cells by identifying the dopants and/or defects that can boost ORR catalysis without weakening the excellent electronic features of graphene.

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OR-42

Sustainable electronalysis: paper-based (bio)sensors in clinical field

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In the era of sustainability, the reduction of both the environmental and the economic impact related to mass-scale processes represents the leitmotiv. Regarding the analytical methodologies, the development of real-time, in-process monitoring, and environmental friendly analysis have been placed in top of the list of required features. A sustainable analytical method should minimize the production of hazardous waste during the analysis to reduce environmental impact and it should provide a more sustainable use of recyclable materials. Furthermore, the measurement should be cost-effective allowing for cost-effective analysis. The electroanalytical techniques, compared with the other analytical methods, require non-sophisticated equipment, small amount of sample, and are suitable for measurements on field. In addition, screen-printed electrodes own high adaptability: customizing shape, dimension, conductive-ink material, and substrate, allow for selective and finely calibrated electrodes to be fabricated for specific target analytes. However, even if glucometers represent a keystone as self-monitoring device, drawbacks related to their production cost and waste removal need to be carefully evaluated. In this keynote, paper-based substrates are proposed as novel materials for the sustainable production of printed electroanalytical platforms. An overview regarding the various manufacturing processes will be provided, and the properties of both chromatographic and office papers will be showed, highlighting the diverse experimental setup that are adopted depending on the type of involved paper. Herein, paper patterning will be focused on the well-known wax printing technology which allows to create hydrophobic/hydrophilic areas, making paper an all-in-one platform. The analytical relevance of the proposed approach will be proposed in terms of healthcare applications. More specifically, paper-based (bio)sensors to detect chloride, zinc, and DNA in biological fluids will be taken into account. By merging type of printing substrate, conductive inks, (nano)modifiers, and biological components, paper is a candidate towards the development of a low-cost and reagentless substrates, being capable to load, react, and filter the samples.

OR-43

Structure-based virtual screening of novel SMO antagonists: a ligand repurposing approach

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Dysregulation of the Hedgehog Signaling Pathway is involved in the development of wealth of solid tumors, as it has been well established [1]. Notably, the aberrant activation of this pathway is linked to metastasis growth and acquisition of resistance to traditional chemotherapeutic agents. The GPCR-like receptor Smoothened (SMO) is part of this pathway and represents an attractive target to antagonize in cancer treatment. Thus, we devised an in silico protocol which is fine-tuned to identify new potential ligands for this receptor in databases of known active compounds against other targets (Figure 1) [2]. The ligand repurposing approach paves the way for new and synergistic therapeutic strategies which could help overcome cancer resistance to treatment. Such a protocol employs the renown docking software AutoDock Vina, which allows for fast and comprehensive virtual screening (VS) campaigns. To probe the predictive power of our method, we screened a database of inhibitors active against the tyrosine kinase MET, whose overexpression is also heavily implied in cancer progression. The most promising hits resulting from this campaign proved to be active in the nanomolar range in biological assays against SMO [3], representing the first dually-active ligands against these two structurally different targets.

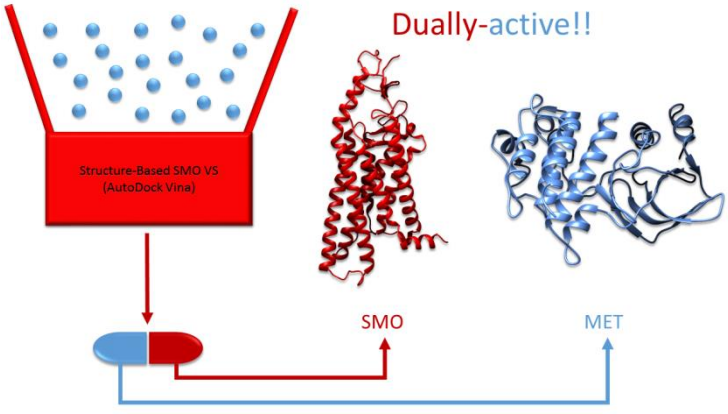

Figure 1: Project workflow.

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OR-44

Novel α7 antagonists as potential anticancer agents

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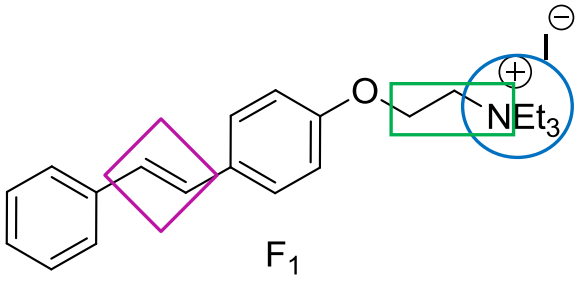
Homomeric α7 nicotinic acetylcholine receptors (α7 nAChR) are overexpressed in several extra-neuronal tumours, like non-small-cell lung carcinomas, small cell lung carcinomas, gliomas and glioblastomas [1].

Nicotine, a non-selective α7 agonist, promotes tumour growth and metastases through different mechanisms, among which the activation and induction of the α7 subtype [2]. The nicotine-induced cell proliferation effect can be also obtained with a subtype selective α7 agonist, while specific α7 antagonists such as methyllycaconitine (MLA), α-Bungarotoxin (αBgtx) or the widely used pharmacological tool F1 can revert it, acting as anti-proliferative agents [1,3].

The aim of our work is the synthesis and the biological evaluation of more potent and more selective analogues of F1 as novel α7 antagonists and potential anti-proliferative agents.



F1

First, the triethyl ammonium group of F1 was replaced with other differently hindered quaternary ammonium heads. Then, the role of the terminal styryl moiety and the flexibility of the alkyl linker were investigated.

All the F1 analogues were assessed in terms of binding affinity and selectivity at the α7, α4β2 and α3β4 subtypes. The results, which will be discussed during the presentation, highlighted some interesting α7 ligands that will be assessed in electrophysiological functional activity. Particularly, we obtained a novel compound with improved affinity at the α7 subtype and a markedly enhanced α7/α4β2 and α7/α3β4 selectivity.

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OR-45

Synthesis of new gadolinium complexes for magnetic resonance imaging with improved relaxivity

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Magnetic resonance imaging (MRI) is a widespread noninvasive diagnostic technique that provides images dependent on proton density and on the relaxation times of water proton nuclei.

Paramagnetic ions (e.g. Gd^{3+}, gadolinium) can decrease via dipolar interactions the nuclear relaxation times and gadolinium-based contrast agents (GBCAs) are currently used to enhance MRI image contrast.

The optimization of relaxivity properties of GBCAs is still a need. In this respect, prototropic exchange of mobile protons can play a significant role and it may be modulated by pendants arms of ligands [1,2].

A series of new Gd-complexes (compounds **1-4**, **Fig. 1**) was designed to rationalize the prototropic exchange effect. The coordination cage is the same of the commercial Gd-HP-DO3A, but with an additional phenol moiety. Ligands of the new Gd-complexes differ in the position of the hydroxyl phenolic group (**1-3**) or in substituent of the phenol moiety (**4**), respectively to modify the distance between mobile protons and Gd ion and to tune the pH value at which the prototropic effect is exploited.

The relaxivity of **1** and **4** was proved to be twice the value of the commercial Gd-HP-DO3A and, interestingly, the effect of the prototropic exchange reaction occurs at physiological pH [3]. Complexes **2** and **3** did not share these properties and the enhancement of r_1 was shifted toward more basic pH values (up to pH 9).

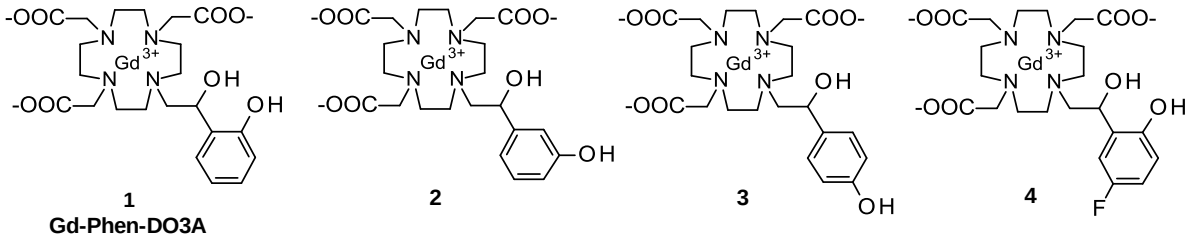

Figure 1: Chemical structures of novel Gd-complexes.

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OR-46

Inhibition improvement of the *Staphylococcus aureus* efflux pump NorA by methoxy group introduction on the 2-phenylquinoline core

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To date, antimicrobial resistance is a global health threat causing several difficult-to-treat infections. The large misuse of common antibacterials to control or prevent bacterial infections is increasing the development of new multi-drug resistant strains. Moreover, the discovery of new antibacterial agents for years now is being on the wane and the new drugs are doomed to a rapid resistance insurgence [1]. Therefore, the strategy aimed to identify a molecule devoid of antibacterial effect but specifically targeting the resistance mechanisms looks promising. In particular, our group has long been focused on the search for molecule inhibiting bacterial efflux pumps (EPIs) with the aim to restore antibacterial efficacy [2].

In this work, we report the optimization of the previously reported 2-phenylquinoline derivatives [2] as EPIs of NorA, the most expressed efflux pump in *S. aureus*. By the introduction on the 2-phenylquinoline core of a methoxy group, a substituent recurrent in both natural and synthetic NorA EPIs, we designed four series of methoxy-2-phenylquinoline derivatives (Figure 1). Compounds, bearing at C-4 different alkylamino chains selected on the basis of the previous SAR, were initially tested by ethidium bromide (EtBr) assay on SA-1199B, a *S. aureus* strain overexpressing NorA. Then, all the compounds having no antibacterial effect and an EtBr efflux inhibition higher than 80% were evaluated in synergism with ciprofloxacin against different resistant *S. aureus* strains. For the best compounds cytotoxicity was evaluated on HepG2 cells, showing as the new derivatives possess an EPI activity at not toxic concentrations. Results of this study will be presented.

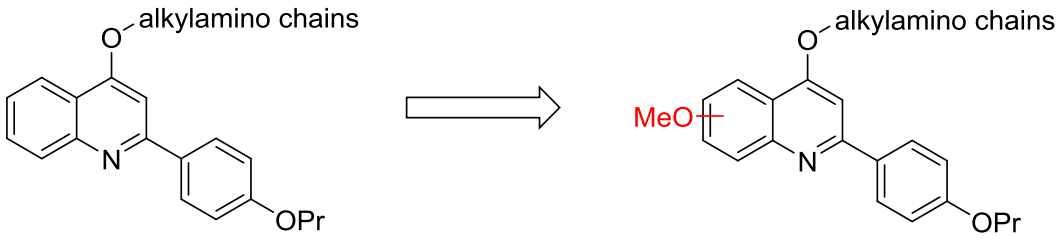

Figure 1: new series of methoxy-2-phenylquinoline derivatives

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OR-47

9-aminoacridine-based agents impair the bovine viral diarrhea virus (BVDV) replication targeting the RNA-dependent RNA polymerase (RdRp)

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Bovine Viral Diarrhea Virus (BVDV), the prototype of Pestivirus genus (Flaviviridae family) is a major pathogen of cattle, responsible for significant economic losses for food industries worldwide. Currently, there are no effective antiviral drugs to control Pestivirus infections, whereas vaccination is used in some countries with different success rates.

Recently, we identified a novel class of 9-amino-6-chloro-2-methoxyacridine derivatives [1], structurally related to quinacrine and acranil, capable of inhibiting BVDV replication in cell-based assays with potency profile comparable to reference compounds (ribavirin and NM 108). Thus, starting from these lead compounds we synthesized new 9-aminoacridine derivatives featuring additional chemical features with the two-fold ultimate goal of increasing antiviral potency while preserving low toxicity. The relevant viral protein target – the RNA-dependent RNA polymerase – the binding mode, and the mechanism of action of these new antivirals have been determined by a combination of in vitro (i.e., enzymatic inhibition and isothermal titration calorimetry assays) and computational experiments.

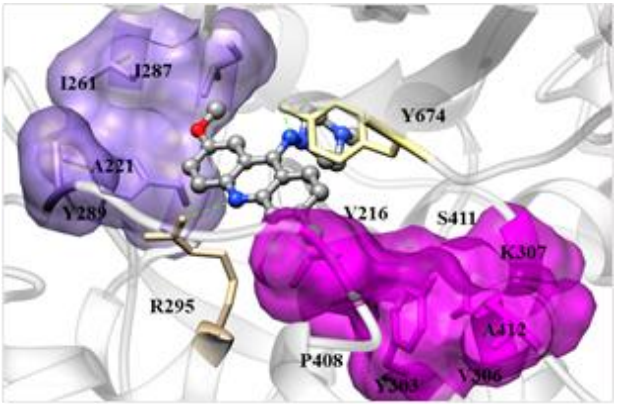

Figure 1: Docking pose for 6-chloro-2-methoxy-9-(4'-methylpiperazin-1'-yl)amino-acridine into the putative BVDV RdRp binding site

[1] M. Tonelli, G. Vettoretti, B. Tasso, F. Novelli, V. Boido, F. Sparatore, B. Busonera, A. Ouhtit, P. Farci, S. Blois, G. Giliberti, and P. La Colla, *Antivir. Res.* **91** (2011) 133-141.

OR-48

N^6-substituted-5′-*C*-ethyl-tetrazolyl-adenosine derivatives: potent dual acting A_1 and A_3 adenosine receptor ligands with analgesic properties

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Adenosine (Ado) is the endogenous ligand of a family of G-protein coupled receptors (GPCRs) represented by four subtypes: A_1, A_{2A}, A_{2B}, and A_3 adenosine receptors (ARs). They are widely distributed in all the human body including the central nervous system (CNS), peripheral neurons, cardiovascular system, respiratory tract and immune system [1].

Affinity and selectivity towards the four ARs can be modulated through substitutions at both purine and sugar moiety of adenosine. The replacement of the 5'-hydroxyl group with a chlorine atom in N^6-substituted adenosine derivatives led to discovery of 5'-chloro-5'-deoxy-N^6-(±)-(*endo*-norborn-2-yl)-adenosine (5'Cl5'd-(±)-ENBA), a potent and selective A_1AR agonist that showed analgesic effects in mice without affecting cardiovascular and motor functions [2].

Introduction of a 5'-*C*-ethyltetrazol-2-yl group, together with the appropriate N^6-substitution in adenosine derivatives, furnished compounds endowed with an increased affinity versus both hA_1AR and hA_3AR, reaching affinities in subnanomolar range [3].

In this work, a new series of 5'-*C*-ethyltetrazol-2-yl-N^6-substituted adenosine derivatives were designed, synthesized and tested *in vitro* in binding and functional assays and *in vivo* in a mouse model of pain. The molecular features necessary for the hA_1- and hA_3AR recognition and activation by this series of derivatives were explained through an *in silico* receptor-driven approach.

[1] K. A. Jacobson, and C. E. Müller, *Neuropharmacology* **104** (2016) 31-49.
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[3] R. Petrelli, I. Torquati, S. Kachler, L. Luongo, S. Maione, P. Franchetti, M. Grifantini, E. Novellino, A. Lavecchia, K.-N. Klotz, and L. Cappellacci, *J. Med. Chem.* **58** (2015) 2560-2566.

OR-49

Hydrophilic and lipophilic dual model drug release from bio-polymeric matrices produced by sodium alginate - MaterBi® emulsions

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Emulsion science and technology is proven to be an indispensable tool for pharmaceutical formulations, able to overcome issues such as stabilization of poorly soluble drugs in aqueous media, as well as combination or encapsulation of hydrophilic and lipophilic molecules in a single medium [1].

In this study, we used an emulsion solution casting process to fabricate sodium alginate - MaterBi® biopolymer matrices that can retain both hydrophilic (a cutaneous antiseptic) and lipophilic (curcumin) model drugs. The obtained matrices were characterized in terms of their ability to release the model molecules, either individually or simultaneously *in vitro*. Recently, different alginate-based biomedical systems, obtained by processing alginate in the form of fibers, microspheres, films and hydrogels [2], have been exploited for tissue engineering, drug delivery, and wound healing applications [2]. However, the novelty of this research resides in the combination of this widely used material with Mater-Bi®, a commercial, hydrophobic, biodegradable polymer composite consisting of polycaprolactone (PCL) and thermoplastic starch. This bio-polymer, obtained by a proprietary compound extrusion method, is actively marketed as sustainable food packaging material [3], but it has not been applied in the biomedical field so far. Moreover, the exploitation of the emulsion technology as facile, inexpensive, quick method for bio-composite fabrication, allows the combination of different materials in an easy-to-scale approach.

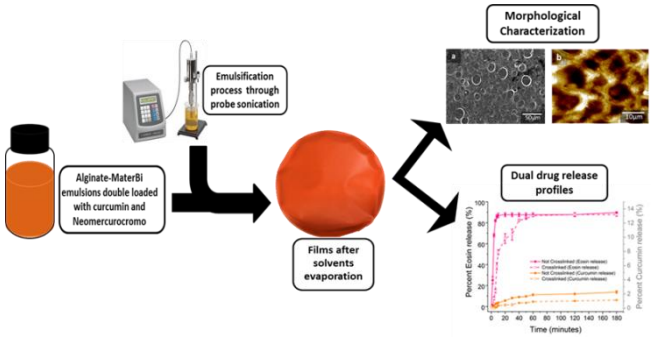

Figure 1: Alginate – MaterBi® bio-matrices. Fabrication process, morphological characterization and dual drug release kinetics.

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OR-50

Solvent- and substrate- dependent regioselective synthesis of 2- and 3- substituted 2,3-dihydro-1,4-benzoxathiine

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The 1,4-benzoxathiane scaffold is a common moiety present in several therapeutic agents, acting as adrenoceptor antagonists [1], or as anticancer agents [2].

Very recently, designing novel antibacterial agents, and aiming to afford 2- or 3- substituted benzoxathiine derivatives, we initially followed an established synthetic scheme previously used for the synthesis of 2-substituted 1,4-benzodioxane scaffold [3].

We then broaden the reaction conditions, finding an easy and reliable method for the obtainment of both 2,3-dihydro-1,4-benzoxathiine-2-yl derivatives and 2,3-dihydro-1,4-benzoxathiine-3-yl ones (Figure 1).

As a result, we observed that the right choice of an appropriate solvent and a correct substrate allow the exclusive formation of one of the two possible regioisomers. The relative solvation of O- and S- anions induced the regioselectivity; specifically, when the 1,2-mercaptophenol is treated with an organic base, in a lipophilic solvent, in the absence of water and in the presence of the lipophilic ethyl 2-bromo acrylate, the thiolate succeeds as nucleophile and thus the 2-substituted compound is fully accomplished.

On the other hand, the treatment in the presence of water and with a polar 2-bromo acrylamide let the phenoxide to manage the nucleophilic substitution and therefore to afford 3-substituted compounds.

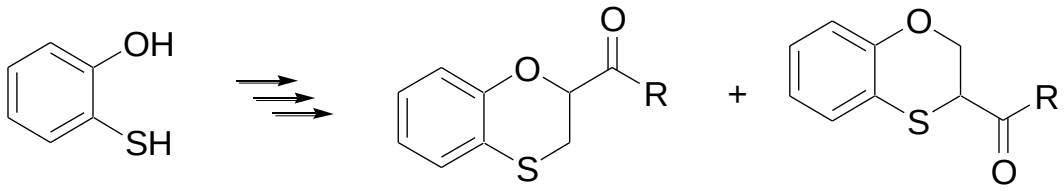

Figure 1: Simplified synthetic scheme for the obtainment of the desired 2,3-dihydro-1,4-benzoxathiine.

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OR-51

A fire retardant strategy for hemp fabric/epoxy composites

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A new and ecofriendly chemical approach uses inexpensive waterglass solutions in order to promote the formation of a silica-based coating on hemp fabrics; this green coating is able to act as a thermal shield and to protect the latter from heat sources [1, 2]. Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR_FTIR) and Nuclear Magnetic Resonance (NMR) confirm the formation of –C–O–Si– covalent bonds between the coating and the cellulosic substrate. The waterglass treatment improves the fire behavior of hemp fabric/epoxy composites, also in combination with ammonium polyphosphate, and favors a remarkable decrease of the heat release rate, total heat release, total smoke release and specific extinction area (respectively by 83%, 35%, 45% and 44%) as compared to untreated hemp/epoxy composites, favoring the formation of a very stable char, as also assessed by Thermogravimetric Analysis (TGA) [1].

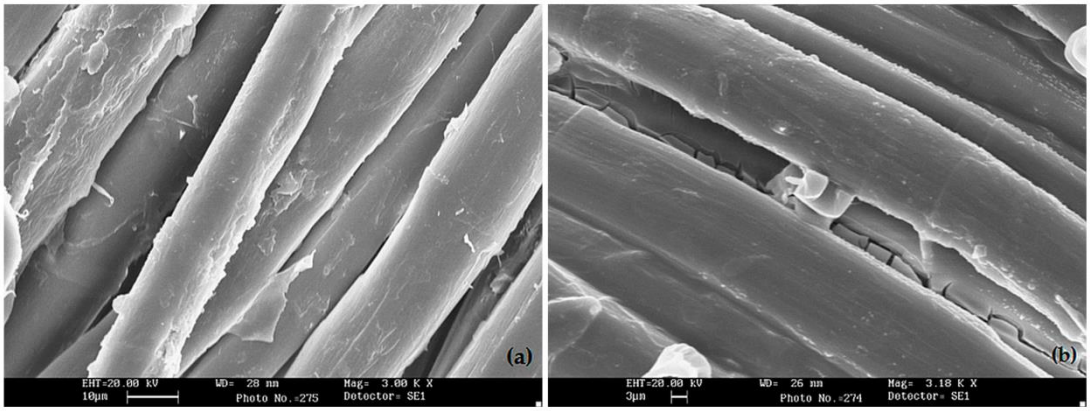

Figure 1: Scanning Electron Microscope images of: (a) untreated hemp fabric (scale bar: 10 µm); (b) hemp fabric after the waterglass treatment (scale bar: 3 µm).

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OR-52

Porous biopolymeric material for the removal of organic pollutants from water

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Among the water treatment methods, adsorption processes are considered a better choice due to cost effectiveness and ease of operation. The limitations of the currently available adsorbent materials, such as high cost and high level of required maintenance, dictate the research and the development of new materials with better performance. Here we present the formation of a novel highly porous adsorbent based on the combination of silk fibroin, a biopolymer derived from Bombyx mori cocoons, with orange peel powder. The embedding of an agricultural food waste peel into a mechanical and environmentally stable fibroin matrix allows to obtain a composite material which is capable to interact efficiently with organic pollutants like dyes, due to the presence of specific functional groups, such as hydroxyl and carboxylic group [1]. The highly porous biocomposite foam is prepared using carbon dioxide assisted critical point drying of the orange peel-fibroin alcogel. The composite alcogel is obtained by the addition of an appropriate amount of methanol in the fibroin-orange peel powder mixture, which induces the self-assembly of ordered β-sheet structures in the protein [2]. The morphological study of the foams reveals that the presence of 50%wt. of orange peel in relation to the fibroin induces the formation of pores with sizes ranging from few tens to hundreds of nanometers, increasing thus the porosity of the system and allowing the more efficient internal diffusion of the aqueous solution into the material. This, in combination with the functional groups of the orange peel increases the sorption capacity of the foam towards a model molecule, methylene blue (MB), in aqueous solution as evaluated by UV-vis spectroscopy.

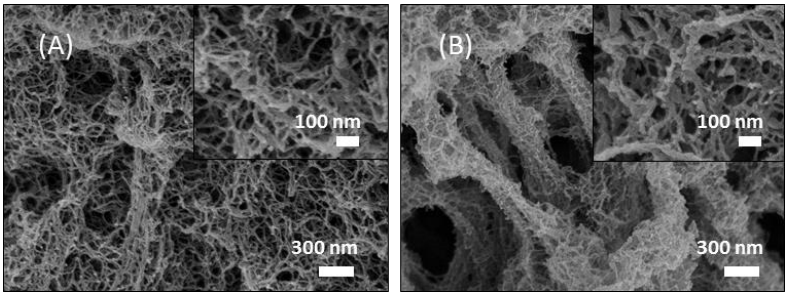

Figure 1: HRSEM imagine of silk fibroin (A) and composite (B) foams.

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OR-53

Supramolecular functionalization of graphene-related materials for the engineering of heat transfer materials

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The oustanding thermal conductivity measured for graphene (2000-5000 W/mK) attracted a lot of interest for possible exploitation into heat management application. However, the thermal conductivity of devices based on graphene and graphene-related materials, including reduced graphene oxide, multilayer graphene and graphite nanoplatelets, depends mainly on the contact thermal resistance between nanoplatelets.

The aim of this work is to build a molecular bridge between nanoflakes using non-covalent functionalization of graphite nanoplatelets (GnP) with bispyrene derivatives in order to decrease the thermal contact resistance preserving the high conductivity related to defect-free sp^2 structure [2].
Supramolecular functionalized GnP (s-GnP) were characterized by UV-Vis, X-ray diffraction and Raman spectroscopy, confirming the formation of a GnP linked network by bispyrene molecules.

s-GnP were used to fabricate films by flow-directed filtration-induce technique and they were characterized by field emission scanning electron microscopy (FESEM) and by Light Flash Analysis (LFA) showing higher value of cross-plane thermal conductivity compared to films from unfunctionalized GnP.

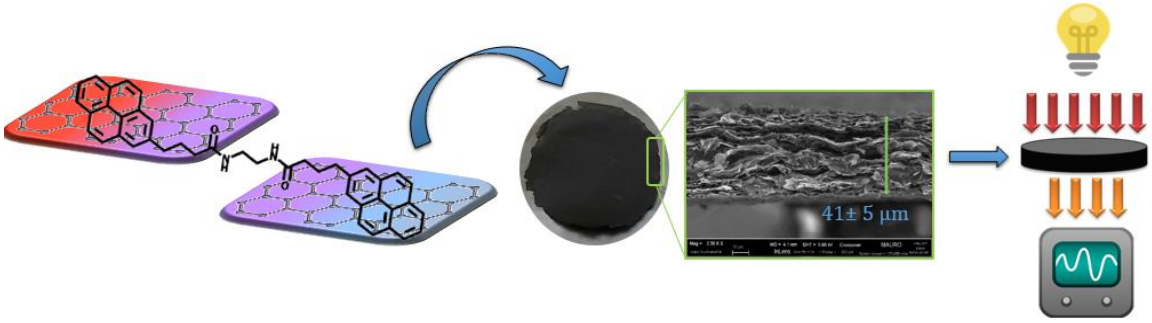

Figure 1: Representation of supramolecular functionalization of GnP to fabricate films for thermal conductivity investigation.

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OR-54

Hydrogel electrolytes based on bio-derived polymers for solar cells

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In recent years, with the idea of creating efficient, safe, stable and low-cost dye-sensitized solar cells (DSSCs), the research moved the attention towards alternative solvent-based electrolytes. In particular, DSSCs with water-based electrolytes have been proposed as one of the possible solution providing reduced costs, non-flammability and environmental compatibility. Recently we demonstrated that stability issues can be properly addressed by choosing the appropriate dye [1]. Moreover, the possibility of gelling the liquid solvent into a polymeric matrix can reduce the electrolyte leakage outside the device, thus increasing the long-term stability. Above all, bio-derived polymers appear promising being renewable and easy available with low cost.

In this work, the study on a series of iodine and cobalt-based 100% aqueous electrolytes is presented. Thanks to our previous experience [2] and to a multivariate approach (Design of Experiment), the effects of the photoanode preparation and the electrolyte compositions have been evaluated on DSSCs performances. Finally, the gelation of aqueous electrolytes with bio-derived polymers has been performed and evaluated [3]. Photovoltaic performances and stabilities will be discussed by comparing liquid and gel electrolytes. In lab-scale solar cells interesting photovoltaic performances superior to 4% were achieved.

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OR-55

Scale up of MFI membranes for water treatment

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Today, the absence of sufficient available water resources may be considered one of the most important and serious question that affected every continent. In fact, the water scarcity is in continuous growing and represents a significant global problem concerning our community.

Recently, membrane technology has emerged as one of the main contributor to solve the issue of the water demand. Intense research efforts are being made for the use of membranes combined with distillation process, in applications related to the water treatment, such as desalination of seawater or brackish water and drinking water purification [1]. In this context, zeolite membranes, due to their crystalline structure and to their pore diameters close to molecular size of different species, represent a potential device. In particular, wide attention was focused on the MFI (silicalite, ZSM-5) membranes, that have a pore size lower (about 5.5 Å) than the major kinetic diameters of hydrated ions.

In this work, supported silicalite membranes with a length of 30 cm were synthesized using the secondary growth method coupled with the cross flow seeding procedure. Besides, the prepared membranes were characterized and then used in vacuum membrane distillation (VMD) to investigate their performance and to compare them with those obtained for the membranes 10 cm long, previously used [2].

The distillation process was carried out using as feed both deionized water and salty solutions at different NaCl concentration (0.2, 0.6, 0.9 and 1.2 M).

The experimental results evidenced the possibility to reach good permeate fluxes constant in the time and salt rejection values higher than 99.5 % up to 0.9 M of NaCl [3].

Furthermore, it was possible to restore the original performance of the membrane after an identified cleaning procedure.

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OR-56

Sol-gel synthesis of hybrid TiO_2 photosensitized through charge transfer complexes

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Titanium dioxide is a wide band gap semiconductor with recognized photocatalytic properties, but its light absorption is limited to UV range. Visible light photosensitization can be obtained by chemical modifications anchoring to the oxide a dye or, alternatively, a smaller complexing molecule (e.g. a diol, diketone or carboxylic acid), which induces a direct ligand-to-metal charge transfer [1].

The role of complexing compounds is usually studied after their surface adsorption on crystalline TiO_2 nanoparticles. We propose a different approach for the synthesis of inorganic-organic hybrids containing chelating ligands such as catecholate and ascorbate through sol-gel method, a simple and versatile "bottom-up" procedure: adding the ligand to the titanium alkoxide precursor, heteroleptic alkoxide complexes are formed before the hydrolysis and condensation reactions occur. The final material is a chemical or physical gel with the ligand stably bound into the oxide amorphous structure.

We observed that the presence of ascorbic acid fosters the gelation of TiO_2 sols, while homogeneous gels with catechol can be obtained through the addition of an auxiliary ligand, like acetylacetone or citric acid, which also form interesting hybrids with TiO_2 by themselves [2].

The structural and physicochemical properties of different xerogels are studied by complementary analytical techniques (XRD, FT-IR, TG/DTA, UV-vis DRS, EPR), evaluating the effects of sol-gel synthesis variables, such as reagents concentration or solution pH. UV-vis DRS and EPR spectra confirm the charge transfer in all samples, showing wide absorption in the visible range, with significant band gap decrease, and the presence of radical species. These hybrid materials are potentially useful for photocatalytic or related applications.

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OR-57

Multilayers of graphene oxide to reduce the flammability of PU foams

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The Layer by Layer (LbL) technique has been adopted for the construction of nanoarchitectures capable of improving flame retardant properties of organic polymers [1]. In particular, it has been applied to an open cell poly(urethane) (PU) foam in order to increase its thermal and flame stability. PU foams represent one of the first item to be ignited in fires as they can ignite and burn very quickly, releasing toxic gases and optically dense smoke [2]. LbL deposition technique has proven to be an extremely versatile tool able to penetrate inside the foam and homogeneously coat each available surface with a nanostructured layer (Figure 1).

The aim of this work is to produce a coating capable to improve flame reaction of the foams introducing Graphene Oxide(GO) as flexible high aspect ratio nanoparticle. In this way, the LbL growth of the GO and different polymers, including natural and synthetic polyelectrolytes, was monitored with FT-IR spectroscopy. In order to improve the efficiency of the process, different deposition conditions were evaluated on the bases of ionic strength and pH. The homogeneity of coatings was characterized by FE-SEM. Flammability tests in horizontal configuration demonstrated the complete suppression of the melt dripping phenomenon and self-extinguishing behaviour for foams treated at high ionic strength. Surprisingly, by cone calorimetry some of the treated foams showed no ignition at all when exposed to heat flux typical of developing fires. The proposed GO multilayer coatings represent a valuable and efficient alternative for the reduction of the fire threat of PU foams.

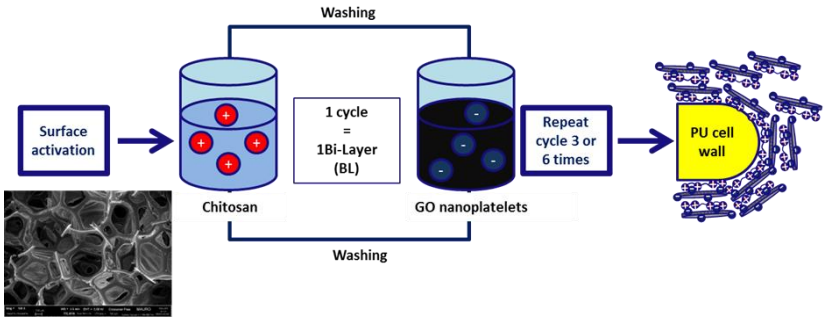

Figure 1: Layer by Layer deposition and SEM imagines of untreated PU foam.

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OR-58

Titanate-fibroin nanocomposites for the removal of heavy metal ions from water

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Metal oxide nanostructures exhibit good properties for the removal of heavy metal ions from water and can be structured in several shapes. Particularly titanates possess high cation exchange capacity due to their high surface-volume ratio, high concentration of hydroxyl groups and easily adaptable interlayer distances [1]. We produced and characterized a nanocomposite made of titanate nano-sheets immobilized in a solid matrix of regenerated silk-fibroin as a novel heavy metal ions removal system. The capacity of this nanocomposite to remove Pb^{2+}, Hg^{2+} and Cu^{2+} from water was investigated, revealing a removal capacity of ~73 mmol/g for all the ions tested. We demonstrate that this system can efficiently retain the adsorbed ions, and as already observed in literature, the presence of Na^{+} increases the sorption selectivity of the system towards the Pb^{2+} [2]. Due to the contribution of the silk fibroin, which entraps the titanate nano-sheets, in its solid structure, the risk of release of those nanostructures in the aqueous medium is prevented. The combination of good adsorption capacity, selectivity and structural integrity make this material an ideal candidate for heavy metal removal from water in real case scenarios.

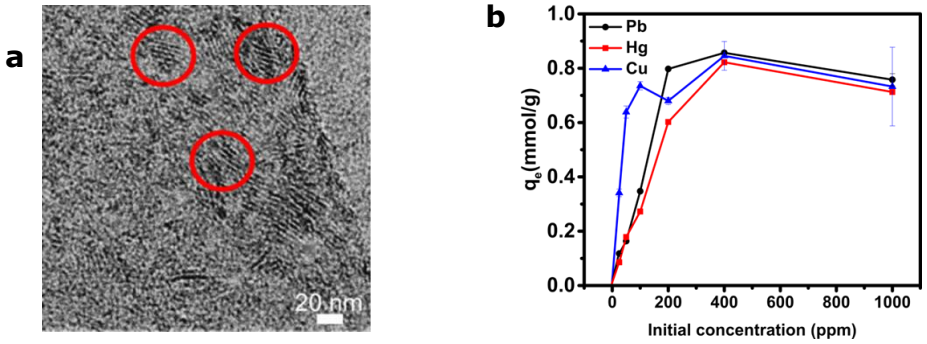

Figure 1 (a) TEM images of Titanates nano-sheets; **(b)** Removal capacity q_e in mmol/g after 24h of incubation at different of ions concentration (Pb^{2+}, Hg^{2+} and Cu^{2+}, respectively).

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OR-59

Production of PCL nanoparticles by flash nanoprecipitation for controlled release of caffeine

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Caffeine (CAF) is one of the most consumed drug worldwide due to its large application in food, pharmaceuticals, cosmetics and supplements; upon oral administration caffeine is cleared into the stomach in 20 minutes and absorbed into the blood within 1 hour [1].

Polycaprolactone (PCL) is biodegradable polymer extensively studied in drug delivery applications where long lasting releases are required [2].

Caffeine was encapsulated in PCL nanoparticles by exploiting the Flash nano-precitation technique which is well known method to encapsulate hydrophobic drug [3], but not yet studied on hydrophilic active principles. The nanoparticles were produced in a confined impinging jet mixer by dissolving caffeine alternatively in the solvent (acetone) or in the antisolvent (water).

The effect of the process parameters on the mean particle diameter and zeta potential of the nanoparticles was investigated by Dynamic Light Scattering. A novel procedure to accurately quantify drug Loading Capacity (LC) and Encapsulation Efficiency was developed and implemented.

The in vitro release kinetic was assessed by dynamic dialysis method.

Nanoparticles with average diameter ranging from 250 to 500 nm were successfully produced, the mean size was correlated to the flow rate. LC and EE were assessed in the range of 10-45% and 5-25% respectively. The release test showed a delay in the peak of caffeine in blood mimicking solution up to 6 hours.

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[2] V. R. Sinha, K. Bansal, R. Kaushik, R. Kumria, and A. Trehan, *Int. J. Pharm.* **278** (2004) 1-23.
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OR-60

Water-soluble polyester-based amino acids-modified dendrimers loaded with ursolic and oleanolic acids as promising prodrugs suitable for intravenous administration

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Dendrimers, are characterized by high controlled architecture, presence of inner cavities to accommodate small molecules and many peripheral functional groups and are of eminent interest for biomedical applications. The well-known pharmacological activities of Ursolic and Oleanolic acids are limited by low water solubility, non-specific cells distribution, poor bioavailability and pharmacokinetics and the research for new formulations of UA and OA is very extensive and concerns the use of carriers, such as liposomes or PAMAM. The present study describes the physical incorporation of the two triterpene acids inside amino acids-modified polyester-based dendrimers [1]. NMR, zeta potential, mean size of particles and buffer capacity of prepared materials were reported.

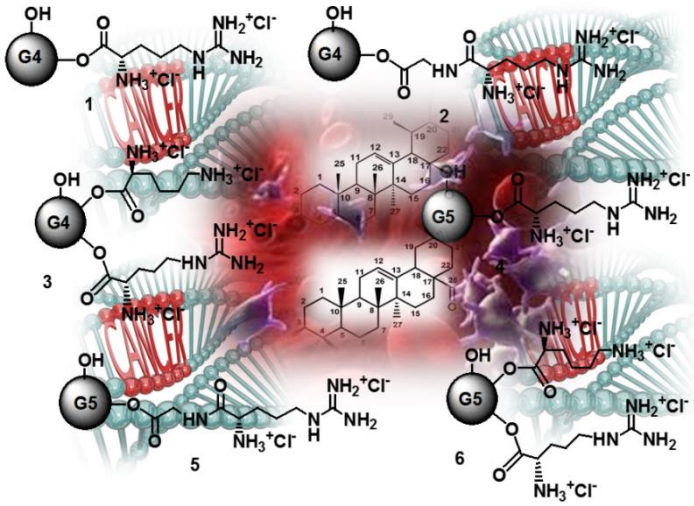

Figure 1: An eye-catching representation of the prepared complexes

The achieved water soluble complexes harmonize a polycationic character and a buffer capacity which presuppose efficient cells penetration and increased residence time with a biodegradable scaffold thus appearing as a promising team of new non-toxic prodrugs for safe intravenous administration of Ursolic and Oleanolic acids (Figure 1).

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OR-61

Soybean peroxidase adsorption from aqueous solution by alumina supports: a new process for enzyme recovery and reuse

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Enzymes are the biocatalysts of the living world, but their properties render them also exploitable in many applications that range from industrial catalysis to therapeutics, including synthetic and pharmaceutical chemistry, wastewater bioremediation, fabrication of high performance biosensors, among others [1-3].

The use of enzymes, however, is limited by their recovery since this aspect plays a significant role in the evaluation of the cost of the biocatalytic processes, therefore several methods have been proposed for their immobilization on stable supports. This study investigates the possibility of using different phases of nano-alumina for enzyme capture and reuse.

Alumina nanoparticles were synthesized in the γ and δ-θ phases with different shapes starting from boehmite and dawsonite thermally calcined at 500 and 1000 °C respectively and tested as adsorbent of commercial soybean peroxidase.

The alumina samples were characterized by thermogravimetric analysis, specific surface area, X-ray powder diffraction, scanning electron microscopy, zeta-potential and Fourier transform infrared spectroscopy.

The kinetic of recovery was evaluated in different experimental conditions (enzyme dosage, pH and temperature, presence of buffer) indicating that the supports can easily capture the enzyme which can be almost completely released for a subsequent cycle of reaction.

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OR-62

Human and fish biotransformation QSARs to refine PBT assessment of PPCPs

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The correct investigation and quantification of potential effects due to the accumulation of substances in human and animals is essential to improve and refine general screening of the properties Persistence, Bioaccumulation and Toxicity. However, the quantification of the various processes that characterize bioaccumulation, such as uptake, metabolism and excretion, is challenging due to the extensive costs and the time required to perform bioaccumulation testing.

In this work, we present different Quantitative Structure-Activity Relationship (QSAR) models for the prediction of biotransformation half life (HL; days) measured in humans, starting from five literature data sets and over 1000 compounds [1].

The models were developed focusing on statistical robustness and external predictivity, applicability domain and interpretability. Multiple Linear Regression and the Genetic Algorithm Variable Subset Selection procedure were performed in the software QSARINS by using as independent variables the theoretical molecular descriptors calculated from molecular structures.

The models were then applied to refine the assessment of the potential behavior as Persistent, Bioaccumulative, and Toxic compounds (i.e. PBTs) of over than 1300 Pharamceuticals and Personal Care Products (PPCPs). Principal Component Analysis was used to combine HLs predicted by different models, and to project the studied PPCPs in a new multidimensional space where the compounds are ranked according to their increasing biopersistence. This approach allowed for the identification of slowly biotransformed PPCPs among those predicted as potential PBTs. Results from this study show that QSAR models are useful tools not only to fill data gaps but also to refine previous assessment such as the potential for PBT behaviour.

[1] E. Papa, A. Sangion, J. Arnot, and P. Gramatica, *Food Chem. Tox.* (2017), DOI: 10.1016/j.fct.2017.04.016.

OR-63

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Carboxylic acids as chemical fuels for a catenane based molecular switch: tuning the motion rate

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In this work, activated carboxylic acids are presented as new chemical fuels for a catenane based, bistable chemical switch composed of two identical macrocycles incorporating a 1,10-phenanthroline unit. While the transition between two different states of a molecular switch has often been made possible by the sequential addition of a fuel and a proper antifuel [1], here one only chemical species, 2-cyano-2-phenylpropanoic acid **1**, is employed to drive the whole cyclic operation (**Figure 1**).

Decarboxylation of acid 1 is fast and quantitative when carried out in the presence of 1 molar equivalent of the chemical switch and, when decarboxylation is over, all of the catenane molecules have experienced large-amplitude motions from state **A** (neutral) to state **B** (protonated), then to state **A** again [2].

In this communication, the principle at the basis of the above system will be illustrated. Furthermore, it will be shown that is possible to control the rate of the cyclic motion of the switch (ranging from 100 s to 100 h timescale) by a fine tuning of the fuel chemical structure.

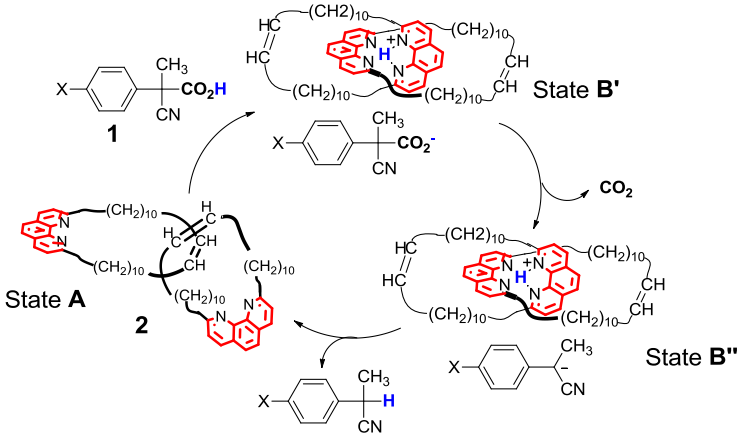

Figure 1: Cyclic operation of the catenane-based switch **2** coupled to decarboxylation of fuel **1**.

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Nitrogen-doped carbon nanodots based hybrids as functional materials

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Carbon Nanodots (CNDs) are quasi spherical carbon-based nanoparticles with sizes below 10 nm.[1,2] CNDs have interesting properties, such as fluorescence, chemical inertness, photobleaching resistance, low toxicity and good solubility in water, as well as a variety of organic solvents. All these features make CNDs promising candidates for a wide range of biological and optoelectronic applications.[1,2] Recently, our group reported a simple bottom-up approach to Nitrogen-Doped CNDs (NCNDs), through a bottom-up microwave assisted hydrothermal process.[3] These nanoparticles were designed to expose amine functional groups on their surface, which were exploited for post-synthetic functionalization with organic chromophores, in order to prepare novel donor-acceptor nano-hybrids (Figure 1, left). Lately, we focused on tuning the fluorescence emission of NCNDs from blue to green, in order to facilitate their application in the biomedical field. Similarly to the photofunctional hybrid, we further exploited the amine rich surface for preparing hybrids that carry biologically active molecules, such as antibiotics and antifungal agents (Figure 1, right).

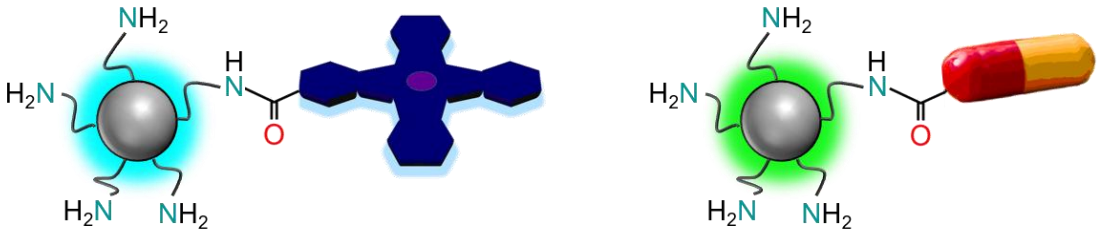

Figure 1: Representative structures of CNDs couplings: photofunctional hybrid (left) and drug delivery system (right).

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[2] X. Li, M. Rui, J. Song, Z. Shen, and H. Zeng, *Adv. Funct. Mater.* **25** (2015) 4929-4947.
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OR-66

Tannin fractions from *Castanea sativa* with antioxidant and antidiabetic properties: an HPLC/ESI-MS/MS and ^{1}H NMR study

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In recent years, the interest for products of natural origin and for natural extracts has been renewed. Natural extracts and naturally occurring products can be used as food additives/supplements, nutraceutical, cosmetic components or over-the-counter (OTC) drugs. Among healthy natural products, vegetable tannins, originally called 'plant polyphenols', represent the most structurally complex group of the polyphenol family, and often the chemical composition of tannin mixtures is not suitably defined. A growing number of research studies have been reported on these phenolic compounds, highlighting their promising biological properties [1], including prevention of degenerative diseases as well as antioxidant, antimicrobial, and antidiabetic activity. Moreover, tannins have many industrial applications: in the leather-making process, but also in wine-making and ageing processes, to improve the organoleptic properties of wine; as food additives; in dyestuff. More recently, tannin extracts have been introduced in animal feed as antimicrobial agents to overcome the problem of antibiotic resistance, and to reduce the greenhouse gas and ammonia emissions from ruminant manure.

On the basis of the above, we report here some results obtained by extraction and fractionation of a commercial tannin obtained from chestnut (*Castanea sativa*) wood, and produced by Silvateam Spa (http://en.silvateam.com/), a company operating in more than 60 countries. We privileged an assay-guided fractionation protocol [2] pointing to obtain polyphenol-enriched fractions displaying α-glucosidase inhibition and antioxidant activity, suitable for agro-food or nutraceutical applications. The main bioactive constituents of the most promising fractions were identified by means of HPLC/ESI-MS/MS and ^{1}H NMR spectroscopy.

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OR-67

A facile access to benzo[*e*]indolizidine derivatives from 1-(2-quinolyl)-2-propen-1-ol

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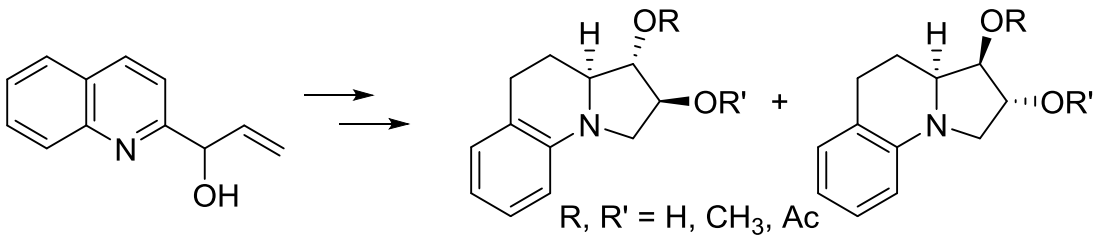
Nitrogen heterocycles are well established as privileged scaffolds commonly present in many biologically active molecules and, in particular, polyhydroxylated indolizidine alkaloids have received considerable attention because of their remarkable biological activities and applications as pharmaceutical tools. In this context, natural (+)-lentiginosine [(1S,2S,8aS)-octahydroindolizine-1,2-diol] is a potent and selective inhibitor of fungal amyloglucosidases as well as Heat shock protein 90 (Hsp90), while the non-natural enantiomer acts as an apoptosis inducer on tumor cells of different origin [1]. These results stimulated intense synthetic efforts to access different analogues and to text their biological activities.



Scheme 1: Synthesis of benzo[e]indolizidine derivatives from quinolyl-propenol.

On this ground, following a procedure previously developed for the synthesis of (±)–lentiginosine from 1-(2-pyridyl)-2-propen-1-ol [2], we studied the conversion of 1-(2-quinolyl)-2-propen-1-ol, obtained by vinylation of commercially available 2-quinoline-carboxaldehyde [3], into benzo[*e*]indolizidine derivatives through a four-step process involving bromination, reduction, and nucleophilic substitution (via elimination/addition).

Synthetic applications and mechanistic aspects of this new methodology will be presented.

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OR-68

Synthesis of functionalized 5-hydroxy-imidazolidine-2-thiones via *N*-heterocyclic carbene/base-promoted aza-benzoin/aza-acetalization domino reactions

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Imidazolidine-2-thione and imidazol-2-thione are acknowledged biologically relevant thiourea derivatives endowed with antithyroid, antitumor, antimicrobial, and dopamine inhibition activities [1].

Here we present a strategy for the synthesis of biologically relevant 5-hydroxy-imidazolidine-2-thione derivatives (which can be simply elaborate to imidazole-2-thione). A novel class of α-sulfonylamines have been suitably prepared (46-81% yield) as precursors of formal benzylidenethiourea acceptors; these are generated *in situ* and intercepted by N-heterocyclic carbene (NHC)-activated aldehydes affording open-chain aza-benzoin-type adducts, which in turn undergo an intramolecular aza-acetalization reaction in a one-pot fashion. A thiazolium salt/triethylamine couple proved to be the more effective system to trigger the domino sequence giving the target heterocycles in good yields (45-97%) and diastereoselectivities (up to 99:1 dr) [2]. The multigram scale synthesis and elaboration of a selected 5-hydroxy-imidazolidine-2-thione compound is also described.

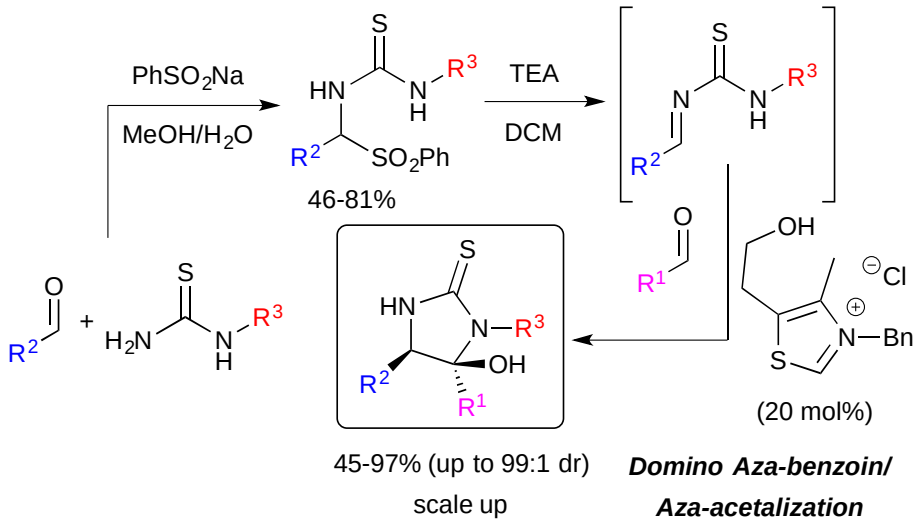

Figure 1: Synthetic strategy for the preparation of imidazolidin-2-thiones

[1] F. Isaia, M. C. Aragoni, M. Arca, F. Demartin, F. A. Devillanova, G. Floris, A. Garau, M. B. Hursthouse, V. Lippolis, R. Medda, F. Oppo, M. Pira, and G. Verani, *J. Med. Chem.* **51** (2008) 4050-4053.
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OR-69

Catching anion-π interactions through uranyl-salophen receptors

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Uranyl-salophen compounds are efficient receptors for anions and suitable supramolecular systems to be studied both in solution and in the solid state for many supramolecular applications spreading from recognition to catalysis [1].

In such systems, the driving force for anion complexation is provided by the interaction with the hard Lewis acidic uranyl center. The presence of electron-deficient aromatic pendants on the main skeleton, beside the metal center, increases the selectivity of the recognition of anions through an additional supramolecular interaction, i.e., anion- π interaction [2].

To elucidate the contribution of this quite elusive interaction, a series of uranyl-salophen complexes with one or two properly substituted aromatic pendant arms, Figure 1, have been synthesized.

Investigation has been undertaken in solution and in the solid state using a series of tetralkylammonium halide salts. The data here reported represent the first example of the occurrence of anion-π interactions in systems in which the main driving force for recognition is controlled by Lewis acid-base interactions.

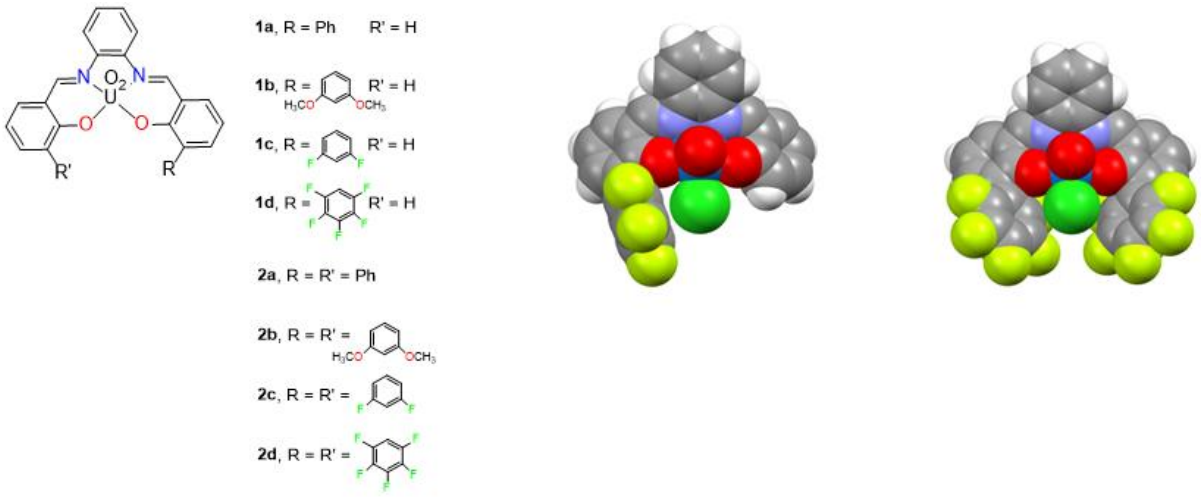

Figure 1: Left: Uranyl-salophen receptors used in this study; right: X-Ray crystal structures of **1d**@$Cl^-$and **2d**@Cl^- complexes respectively.

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OR-70

Environmental photostability of oxazoles and thiazoles found in NRPs and RiPPs

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Nonribosomal peptides (NRPs) and ribosomally synthesized post-translationally modified peptides (RIPPs) are important amino acid-based biomolecules with potent bioactivities, they often contain non-canonical amino acids and frequently incorporate oxazoles and thiazoles [1]. In aquatic systems, these compounds are susceptible to oxidation by photochemically generated reactive oxygen species [2]. Model oxazole and thiazole peptides were designed and synthesized, and found to be incredibly stable under environmentally-relevant conditions. $^1O_2$ bimolecular reaction rate constants were measured, and it was found that the electron-withdrawing or donating effects of ring substituent play a key role in their aquatic photostability. This effect was experimentally proved and results were supported by a theoretical study. Products of the reaction with $^1O_2$ were also detected and elucidated. $^1O_2$ bimolecular reaction rate constant was measured for the thiazole-containing natural product Aerucyclamide A.

This study provides insight into the aquatic environmental fate of oxazole- and thiazole-containing peptides, and highlights the potential of using model peptides to study the transformations of other environmentally relevant NRPs and RiPPs.

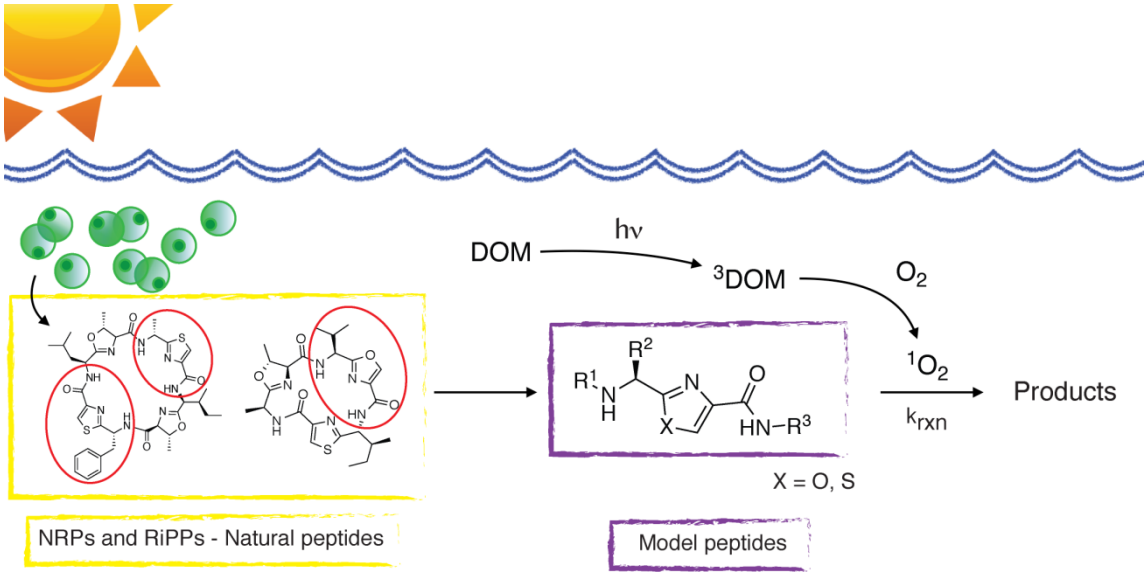

Figure 1: Aquatic photodegradation of oxazole- and thiazole-containing peptides as models for NRPs and RiPPs.

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OR-71

Biorefinery from *Nannochloropis oceanica* F&M-M24

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Biorefineries are facilities employing biomass to obtain chemicals useful for chemical industry as well as biofuels. The sustainability of a biorefinery is strongly dependent on the choice of raw materials to produce high value derivatives or commodities. In this research project, extraction processes from algal biomass were studied for the optimization of biofuel production as well as for the recovery of biomolecules or to develop high value products such as biopolymers and chemical industry intermediates for the pharmaceutical and nutraceutical sectors. Nitrogen starved and nitrogen replete *Nannochloropsis oceanica* F&M-M24 biomasses were provided by Fotosintetica & Microbiologica Srl (F&M), spin-off company of the University of Florence, within the activities of VALORE (Centro di Competenza *Gino Florenzano* of the University of Florence for the valorization of algal and residual biomasses). *N. oceanica* is a microalga widely used at research level to produce biodiesel from its triglycerides. The lipid content of biomasses can be increased by decreasing nitrogen availability during the cultivation of lipogenic microalgae (starvation process) [1]. In this work, a quantitative and qualitative comparison between the lipid fractions of the nitrogen starved and nutrient replete *N. oceanica* F&M-M24 has been performed. A new extraction protocol has been designed and tested with the aim to obtain triglycerides with high purity, low amounts of other fatty acid derivatives as well as protein-rich and sugar-rich fractions. The main components extracted were characterized by NMR, FT-IR, GC-MS and CHN elemental analysis, and synthetic processes to transform some of these products in high value-added derivatives were studied. The triglyceride fraction has been subjected to transesterification reaction with TMSCl [2,3] for biodiesel production.

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OR-72

From dinitrobutadiene building-blocks to nitroindoles: an appealing access to otherwise not easily attainable functionalized heterocycles

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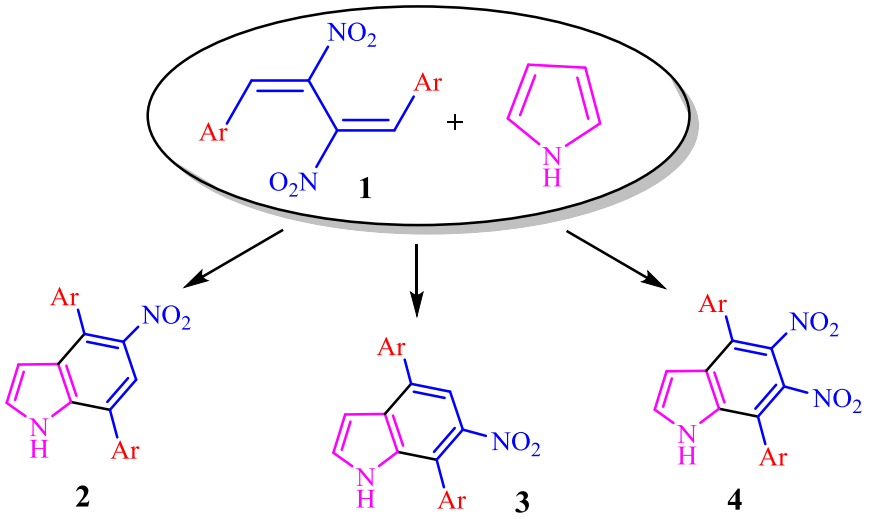
The long-standing synthetic efficacy of dinitrobutadienes **1** [1-3] has been more recently applied to the preparation of 5-nitro **2**, 6-nitro- **3**, and, even more interestingly, 5,6-dinitroindole **4** (a rare substitution pattern in literature), through an original strategy based on the construction of the benzene ring onto a pyrrole (Figure). The protocol represents an appealing access to new entries, otherwise not simply attainable, in the biologically and technologically exploited field of nitroheteroaromatics and derivatives therefrom. Latest achievements in such synthetic efforts will be presented and discussed also from a mechanistic point of view.



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OR-73

Metal-free approach to selenoesters

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The growing importance of selenoesters in several fields of science [1] encouraged us to broaden our ongoing research in organoselenium chemistry [2] in order to develop a simple, general and metal-free approach to these compounds, to overcome the drawbacks of the known synthetic approaches.

The present method [3] involves an unprecedented reduction of phenyl diselenide in ethyl acetate in the presence of sodium borohydride. The subsequent addition of symmetrical or unsymmetrical anhydrides, obtained from various carboxylic acids, resulted in the desired selenoesters with good to excellent yields.

These compounds were then used as highly chemoselective N-acylating reagents of various functional groups, such as amines, amino alcohols, amino acids and amino esters **(Figure 1)**.

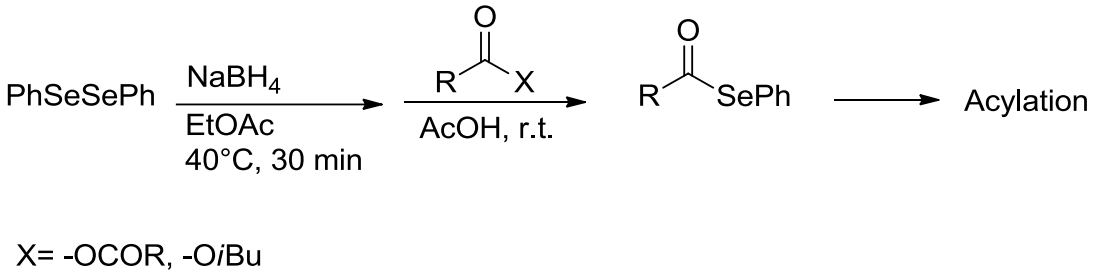

Figure 1: Metal-free synthesis and practical applications of phenyl-selenoesters.

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OR-74

Tetrasubstituted cyclopentadienones as suitable enantiopure ligands with axial chirality

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Tetraphenylcyclopentadienone is well-known to be a propeller-like molecular rotor, in which the aryl substituents do not lay in the plane of the cyclopentadienone. The rotation of one of them activates the rotation of the others with a domino mechanism [1]. The introduction of a 2',2" bond between the two phenyl moieties in 4,5 positions of cyclopentadienone yields a planar phenanthrene scaffold, resulting in the formation of a phencyclone. If the aryl rings in the 1,3 positions, lack of a local C_2 symmetry axis, the non-planar arrangement implies the formation of conformational stereoisomers. Depending on the hindrance of the *ortho*-substituents they could be either stereolabile or configurationally stable (*i.e.* atropisomers).

Stable atropisomers with a cyclopentadienone core can be useful as chiral ligands in organometallic systems as the Shvo catalyst [2]. With this aim this work explores the synthesis and stereodynamic study of new 1,3-diarylphencyclones **1a-e** (**Figure 1**) by means of DFT calculations, Dynamic-NMR, Dynamic-HPLC and ECD [3].

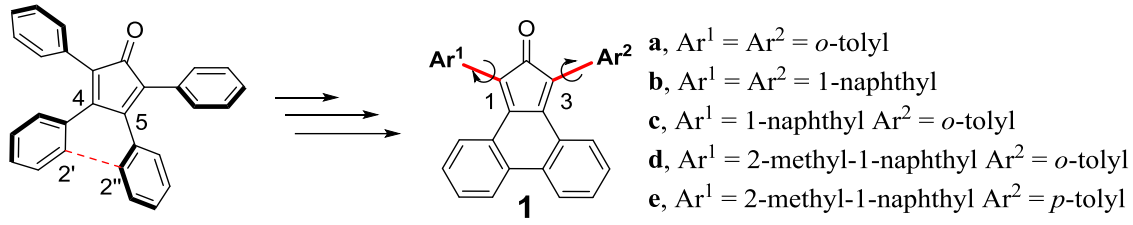

Figure 1: Tetraphenylcyclopentadienone and 1,3-diarylphencyclones studied **1a-e**.

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OR-75

Research communication, dissemination and exploitation: where we are and where we go from here

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Research communication, dissemination and exploitation are three key activities increasingly required to researchers when asking for grant applications (e.g., Horizon2020 [1]).

These requirements include not only traditional publications in peer-reviewed journals or attendance at national and international conferences, but also innovative way of disseminating research including social media, websites, video, public event, and even exhibitions.

In the Italian scenario of the didactic offer in Chemistry, however, students and young researchers are currently in a transition period in which they are asked to prove such new skills indeed, but those skills can be very poorly acquired during traditional undergraduate and postgraduate courses. Moreover, such activities are usually still perceived as unnecessary extra-work that take time away from busy research careers.

To address these issues, the creation of a new group for research dissemination and communication in the contest of the Italian Chemical Society will be proposed. The reasons for the creation of such group will be addressed, and main aims and objectives will be also proposed to inspire further discussion.

Moreover, general guidelines for an effective research dissemination strategy [1, 2] and examples on how to integrate dissemination into a researcher' everyday life will be given, demonstrating that it can turn out to be a unique opportunity to ultimately complete our mission as scientists.

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OR-76

Oxygen-doping of polycyclic aromatic hydrocarbons: insertion of pyrano/pyrylium rings

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Engineered polycyclic aromatic hydrocarbons (PAHs) have enticed great attention as organic semiconductors [1,2]. Specifically, replacing the carbon atoms with other isostructural atoms, *i.e.* doping, is emerging as a powerful approach to control the chemical, supramolecular and optoelectronic properties of PAHs [3].

In this contribution, we present a facile synthesis of O-doped PAHs, which has been achieved through the Cu-mediated Pummerer oxidative cyclization reaction. The novel molecules were extensively characterized, their molecular structure and optoelectronic properties were fully elucidated. Further chemical or electrochemical oxidation readily gave access to pyrylium cations, featuring extended π-conjugation. This is revealed in their visible absorption spectra, which are significantly red-shifted when compared to those of the neutral species. Theoretical simulations indicate that the insertion of pyrano rings in the neutral O-doped PAHs provokes a local antiaromatic perturbation, which experiences a dramatic aromatic evolution upon oxidation, making these cations isoelectronic to their all-carbon analogues.

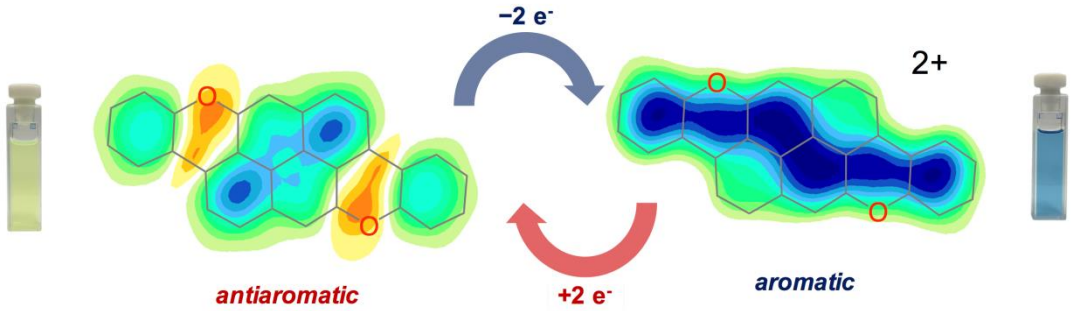

Figure 1: Insertion of pyrano/pyrylium rings into PAHs.

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OR-77

Synthesis of new glycomimetic DC-SIGN ligands with improved metabolic stability

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DC-SIGN (Dendritic Cell-Specific ICAM3 Grabbing Non integrin) is a tetrameric calcium dependent lectin that recognizes highly mannosylated glycoproteins displayed at the surface of several pathogens [1]. In particular DC-SIGN is known to play a key role in HIV-1 transmission. For this reason, the design of DC-SIGN antagonists has aroused great interest in the past decade. In this field, our group has been developing new glycomimetic DC-SIGN ligands based on the structure of the pseudo-dimannobioside **1** [2]. We are now proposing a straightforward one pot synthesis for the creation of a new class of glycomimetic compounds with improved metabolic stability, thanks to the replacement of the pseudo-glycosidic oxygen atom with a sulfur atom (molecules **2** and **3**). The activity and the conformational behavior of the new thio-glycomimetic were found to mimic the corresponding *O*-linked analogue **1** by SPR inhibition assay and NMR analysis supported by computational studies. The stability of **2** towards hydrolysis by an α-mannosidase was investigated and found to be higher than that of **1**. Finally, tethering **2** to an appropriate azido-linker afforded **3**, which allowed the construction of multivalent ligands. Dendrimers and glyconanogels (NGs) both decorated with the pseudo-thiodisaccharide **3** were created as multivalent DC-SIGN ligands.

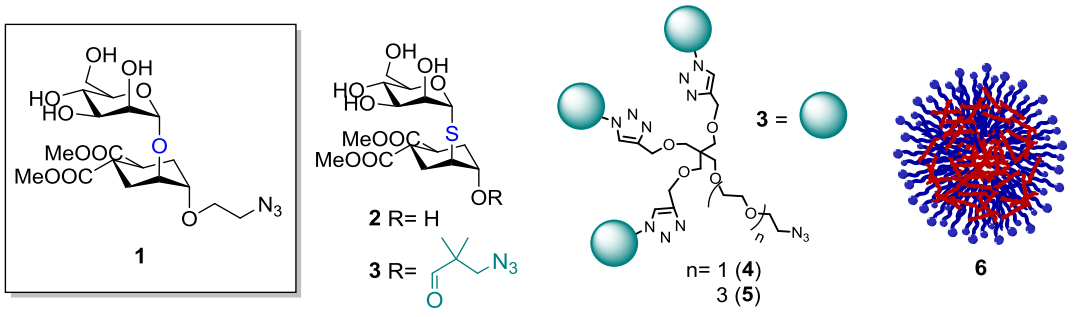

Figure 1: the pseudo-dimannoside **1**; the designed thioglycomimetics **2**, **3**; multivalent scaffolds decorated with **3** as dendrimers (**4**, **5**) and as NGs **6**.

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OR-78

Antibody controlled toehold strand displacement reaction

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The high programmability and specificity offered by the Watson−Crick base interaction make DNA a versatile material for constructing nanoscale devices of varying complexity and functionality. By using simple DNA-based reactions, it is also possible to create dynamic nanodevices, including nanomachines and nanorobots, able to perform a specific function in response to a certain molecular input. One of the most exploited reaction to build such dynamic DNA systems relies on networks of DNA strand-exchange reactions. Specifically, toehold-mediated strand displacement reaction is a process through which two DNA strands hybridize with each other displacing one (or more) prehybridized strands. Such reaction has been mostly employed to control the building of complex DNA nanostructures, but also finds applications in the control of gene transcription, biosensing and signal transduction and amplification. Generally, the entire displacement process is based on an exogenous control by the addition of the invading strand to the reaction mixture and only few examples have been reported that allow to activate strand displacement with small molecules. Thus motivated, we have demonstrated the possibility of employing antibodies as inputs to control the activation of toehold strand displacement reaction. Specifically, we have exploited our previously reported DNA-based nanomachine [1] that can load and release a molecular cargo upon antibody binding. The nanomachine is designed to recognize a cargo strand (invading strand) through the formation of a clamp-like triplex forming mechanism and it's also conjugated at the two ends with a pair of antigens. In addition, the cargo strand contains a portion that recognizes the toehold binding domain of a preformed target duplex. Antibody binding to the two antigen tags in the nanomachine causes a conformational change that allows the release of the invading strand and the following activation of the strand displacement reaction [2]. Given these attributes our approach could represent a new way to control these DNA-based reactions employing molecular inputs.

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OR-79

Enhancement of lipid extraction from microalgae by synergistic pretreatment with deep eutectic solvent under microwaves

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Microalgae are promising alternative sources of several valuable bioactive compounds. Conventional processes typically employ toxic organic solvents (e.g., chloroform and methanol or hexane) for lipids extraction [1].

Herein is presented a new green protocol for a fatty-acids-rich extract from the diatom *Phaeodactylum tricornutum* [2].

A number of choline chloride-based (ChCl) deep eutectic solvents (DESs) were tested, using different hydrogen-bond donors (urea, oxalic acid, sorbitol, *etc.*). The solvent with the highest affinity with the extract has been used to investigate the synergistic effect between DESs and microwaves (MWs) as pretreatment, demonstrating the efficiency of the combined system compared to the separated elements. After prtetretments, extractions were performed with environmental friendly solvents such as dimethyl carbonate (DMC) and supercritical CO_2 ($scCO_2$).

Best pretreatments were achieved with ChCl/carboxylic acids DESs, enhancing both selectivity and total fatty acid (TFA) extraction yield with DMC (by 16% and 80%, respectively). Furthermore, combined pretreatment MW/DES followed by DMC extraction showed yields comparable to the traditional *Bligh&Dyer* method, dramatically enhancing the selectivity (88% vs 35%).

Switching the extraction solvent to $scCO_2$, yield is 20-fold increased, bringing to extracts with highly purified triglycerides profile.

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OR-80

Advanced bioconjugation strategies for engineering the gold nanoparticles surface

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Gold nanoparticles (AuNPs) hold unique physicochemical features strongly dependent on their size and shape which, combined with high biocompatibility, and low toxicity, make them excellent nanomaterials for biotechnological applications. The desired solubility in aqueous environments can be achieved through suitable organic surface coatings and the interaction with the biological interface can be controlled by conjugation of a controlled number of biologically active molecules.

Our research activity focuses on the development of advanced bioconjugation strategies for the functionalization of AuNPs, which are effective under mild conditions, proceed with nearly quantitative yields, and are chemoselective and biorthogonal [1].

In this contribution I will present several bioconjugation strategies that we are currently developing. In particular:

1) Disulfide bridging using next generation maleimides (NGMs)[2];

2) Cu(I)-catalyzed (CuAAC) and strain-promoted (SPAAC) azide−alkyne cycloadditions [3];

3) inverse electron demand Diels–Alder reactions (DAinv) with 1,2,4,5-tetrazines.

Using these strategies, we have been able to conjugate the peptide hormone leptin to PEGylated AuNPs and we have investigated their biological activity in vitro. I will also discuss the immobilization of peptides functionalized with azido groups.

These studies demonstrate the importance of judiciously choosing the bioconjugation strategy to prepare functionalized AuNPs for biological applications.

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OR-81

Improved mayenite features using PMMA as a soft template agent and its application in Cl-VOCs oxidation

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Trichloroethylene (TCE) is a widespread pollutant belongs to the class of chlorinated volatile organic compounds (Cl-VOCs).

Catalytic oxidation is an interesting method since it allows to work at low temperatures (250-550°C) with a great reduction of energetic costs respect to traditional incineration technique [1]. The activity of mayenite in the catalytic oxidation of chlorinated organic compounds was recently investigated obtaining interesting results [2]. In this work mayenite was prepared by a new sol-gel process using PMMA polymer (PMMA Maye) as soft template, and tested in the total oxidation of TCE [3]. Table 1 shows the comparison of PMMA Maye activity in terms of T_{50} and T_{90} respect to others prepared by traditional routes (ceramic CR, sol-gel SG and Hydrothermal HA).

Table 1: Comparison of catalysts activity in the TCE oxidation reaction

Catalyst	T_{50} (°C)	T_{90} (°C)
Maye CR	450	> 550
Maye SG	390	> 550
Maye HA	350	490
Maye PMMA	350	440

As it can be seen, mayenite prepared using PMMA as template agent, shows better performances than the other mayenites. These differences in catalytic activity could be explained by BET surface area and Raman spectroscopy results. As conclusion, we can state that in order to obtain an active catalyst for the TCE oxidation, we need a combination of oxidative properties and high surface area. Those can be obtained preparing a mayenite using PMMA as a soft template agent.

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OR-82

Investigation of mass transfer phenomena in zwitterionic chiral stationary phases

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Zwitterionic chiral stationary phases (CSPs) combine the applicability of both anion and cation exchangers parent chiral ions. For this reason, they can provide direct enantioseparation of a huge range of compounds including chiral acids, bases and zwitterions (such as amino acids and peptides).

ZWIX(+) and ZWIX(-), based on a *Cinchona* alkaloid derived chiral selector, are among the most employed zwitterionic CSPs. The retention mechanism of zwitterions on these CSPs is rather complex and both the two charged sites of the solutes are simultaneously recognized by the charged sites of the chiral selector.

In this work, mass transfer phenomena of these CSPs have been investigated at four different temperatures for the separation of mefloquine (an antimalarial agent) enantiomers. The two mefloquine peaks showed remarkably different shape and behavior. By means of peak parking experiments and a proper model of diffusion in porous media (in this case the parallel model was used [1]), each contribution to band broadening was individually determined [2].

In order to investigate the effect of the adsorption-desorption kinetics, the two peaks were analyzed by means of a microscopic-probabilistic approach to chromatography (stochastic theory). Important information about the heterogeneous adsorption-desorption process (i.e. the residence time of the second enantiomer on both enantioselective and nonselective sites, enthalpy and entropy of adsorption) were obtained starting from the peak shape.

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OR-83

Determination of insects infestation on stored rice by NIR spectroscopy

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Cereals are among the first plants that have been domesticated by human populations, and rice is one of the most widely consumed cereal in the world; a main issue of storing rice is to protect it from animal attacks, in particular, insects infestation. Consequently, the possible presence of food pests must be continuously checked by producers and/or retailers.

Different methods have been developed for the identification of infestation by insects in rice, but they present the limitation of being destructive approaches, leading to an obvious loss of product (and consequently, of profit), affecting farmers, retailers, and finally consumers. For this reason, the aim of the present work is to develop a methodology for the identification of pests infestation in stored rice by NIR spectroscopy coupled with discriminant and class-modelling classification methods. Different samples of rice, both "*infested*" and "*edible*", coming from different farmers located in six different Countries (Cambodia, India, Italy, Pakistan, Suriname and Thailand) have been analyzed by NIR spectroscopy. Two different classification methods, Partial Least Squares Discriminant Analysis (PLS-DA) [1] and Soft Independent Modeling of Class Analogy (SIMCA) [2] have been applied to distinguish between infested and edible samples. 38 parcels of rice (either milled, semi milled or unmilled) have been analyzed: of these, 23 were infested by storage pests, while 15 were suitable for human consumption. Individual grains have been scanned by means of an integrating sphere (Thermo Scientific Inc., Madison, WI) for a total of 1525 spectra. In order to externally validate the predictive models, measurements have been divided into a training (1025 samples) and a test set (500 samples: 181 of "edible" rice and 319 of "infested" rice).

Different pretreatments were applied on the spectra prior to the data analysis. As mentioned, classification models were created applying either discriminant and class-modelling approaches; in both cases the error rate is around 3%.

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OR-84

Investigation of secondary metabolites production by three strains of a human and plant pathogen *Lasiodiplodia theobromae*

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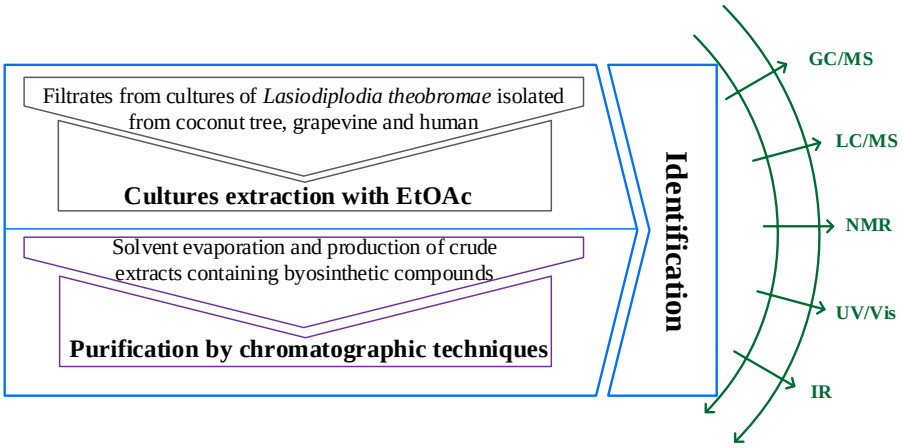
Lasiodiplodia theobromae is a phytopathogenic fungus from the family Botryosphaeriaceae which infects a broad range of hosts causing diverse diseases. In fact, *L. theobromae* synthesizes a variety of lipophilic and hydrophilic metabolites (e. g., lasiodiplodins, jasmonates, melleins, exopolysaccharides, cyclohexenes) which manifest interesting biological activity and which may be involved in fungal pathogenicity and virulence.

The aim of this study is to identify and compare secondary metabolites produced *in vitro* by cultures of three strains of *L. theobromae* isolated from coconut tree, grapevine and human to shed light on their biological activity and toxicity for hosts and environment. To this end, metabolites were isolated and identified by employing an assortment of physical and spectroscopic techniques. From our data, it appears that production of several secondary metabolites by *L. theobromae* may be strain-specific.



OR-85

Glycidol as green feedstock for the synthesis of fine chemicals

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Waste recovery and their utilization as starting material for the synthesis of fine chemicals could be an important step towards the development of environmentally acceptable processes [1].

Recently, we have shown that the production of value added chemicals from glycidol (2,3-epoxy-1-propanol) results very promising if we consider its preparation through the conversion of 2-chloro-1,3-propanediol, a by-product in the bio-based epichlorohydrin production plant (Epicerol® process) [2].

The present work deals with the use of glycidol as green starting material for the synthesis of different products with important industrial applications such as propanediols, glyceryl ethers and polyethers (Figure 1).

In particular: 1,2-propanediol was selectively obtained through hydrogenolysis of glycidol in the presence of Pd/C as catalyst and THF as solvent; polymerization of protected glycidol catalyzed by aluminum alkyls has led to the formation of linear polyethers; glyceryl ethers were easily synthetized by ring opening reaction of glycidol with alcohols catalyzed by Lewis acids based catalysts [3].

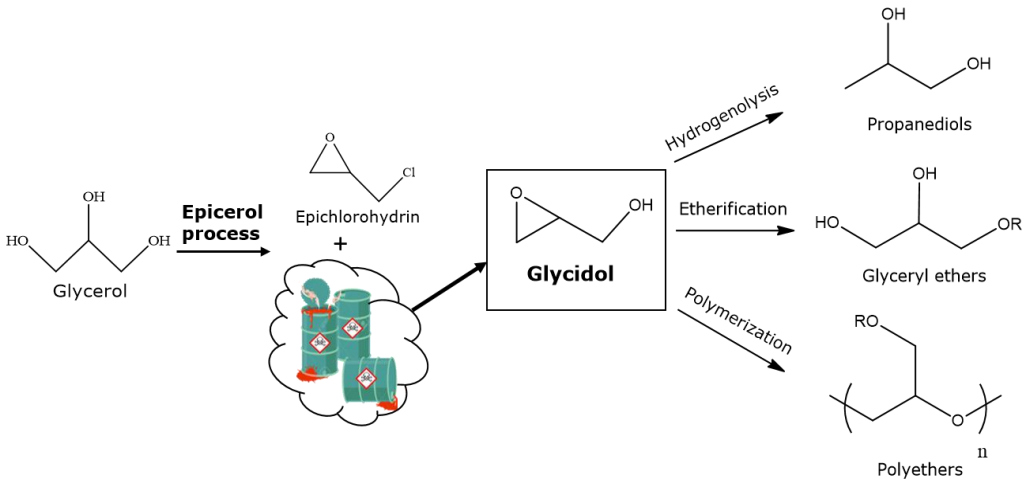

Figure 1: Glycidol production from Epicerol® process wastes and its conversion to value added products.

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OR-86

Development of flavonol and flavanone derivatives as anti-trypanosomatidic drugs

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Trypanosomatid parasites are the etiological agents of neglected tropical diseases, such as Human African Trypanosomiasis and Leishmaniasis. Dihydrofolate reductase (DHFR) is an established target for the treatment of some parasite infections, nevertheless DHFR inhibitors are poorly effective against *Leishmania* and *Trypanosoma* due to the overexpression of pteridine reductase 1 (PTR1) [1]. Since PTR1 is an enzyme unique to these parasites, it represents a promising target to fight trypanosomatidic infections. A library of natural products was assayed using target-based screening on PTR1 and phenotypic screening on parasites. Flavonols were identified as hits, and two libraries of derivatives, having either a flavonol or a flavanone core, were synthesized. Seven crystal structure of PTR1 from *Trypanosoma brucei* (*Tb*PTR1) and *Leishmania major* (*Lm*PTR1) were obtained in complex with different inhibitors [2,3]. The observed structure-activity relationship was rationalized providing the basis for further chemical modifications aimed to generate novel and high affinity anti-trypanosomatidic agents.

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Flash communications

FL-1	Michele ANSELMI
FL-2	Mariateresa BADOLATO
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FL-4	Francesca CARELLA
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FL-1

Peptidomimetics and peptide-NP conjugates for therapy and diagnosis of inflammatory and autoimmune diseases

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Integrins α4β1 are cell surface receptor expressed on most immune cells, that mediates cellular adhesion events crucial to inflammatory processes and autoimmune diseases. Hence, the antagonists of the integrin α4β1 represent potential drugs for pathologies such as rheumatoid arthritis, asthma, or autoimmune diseases such as multiple sclerosis.

In this context, peptidomimetic integrin ligands based on a central heterocyclic scaffold derived from hybrid α/β-peptides, the retro-modification, and macrocyclization [1], showed receptor affinity up to the low nanoM range, high enzymatic stability, and *in vivo* activity [2].

Besides, the peptidomimetics have been equipped with functional linkers useful to connect peptides to dyes, NPs, polymers, or surfaces, for therapeutic or diagnostic applications [3]. These devices were able to discriminate the α4β1 integrin-expressing cells. In perspective, these systems may represent prototypes for the non-invasive diagnosis of inflammatory or auto-immune diseases, from one drop of blood or other fluids easily obtainable from the patients.

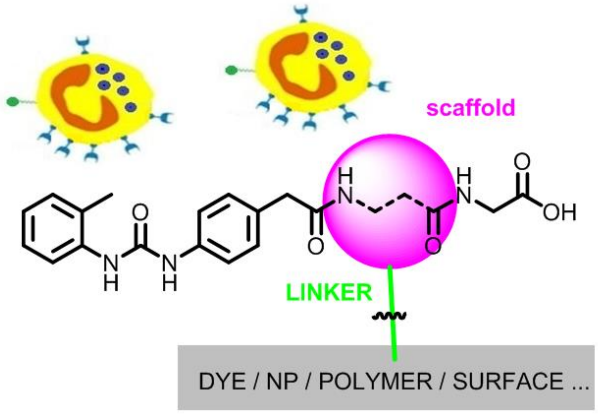

Figure 1: Peptide-conjugate tools for integrin-mediated cell detection.

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FL-2

Glycyrrhiza glabra L. leaves: from agrochemical waste to new potential therapeutic agents

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In Italy, *Glycyrrhiza glabra L.* plants, commonly called licorice, are mainly present in Calabria. Generally, *G. glabra* roots are used in traditional medicine, food and pharmaceutical products. On the contrary, the aerial parts of *G. glabra* are scarcely used and considered agrochemical waste. According to a green chemistry approach, we (re)used the agrochemical waste as source of promising therapeutic agents. *G. glabra* leaves were harvested and, after a classical maceration extraction, an organic (n-hexane) and a methanol fraction were obtained and characterized. Several fatty acids were present in the *n*-hexane fraction, while pinocembrin mainly constituted the methanolic fraction. They showed antibacterial, antioxidant and antiproliferative activities [1]. Increasing evidence suggested that the *in vitro* and *in vivo* studies of pinocembrin are hampered by its instability in biological media and poor bioavailability [2]. In order to overcome these limits, we designed and synthesis new hybrid molecules, merging pinocembrin with a series of fatty acids, by a lipase-catalyzed esterification (Figure 1). A set of biological assays was performed to determine the antibacterial, anti-inflammatory and antioxidant properties of this new class of compounds, compared to the lead compound.

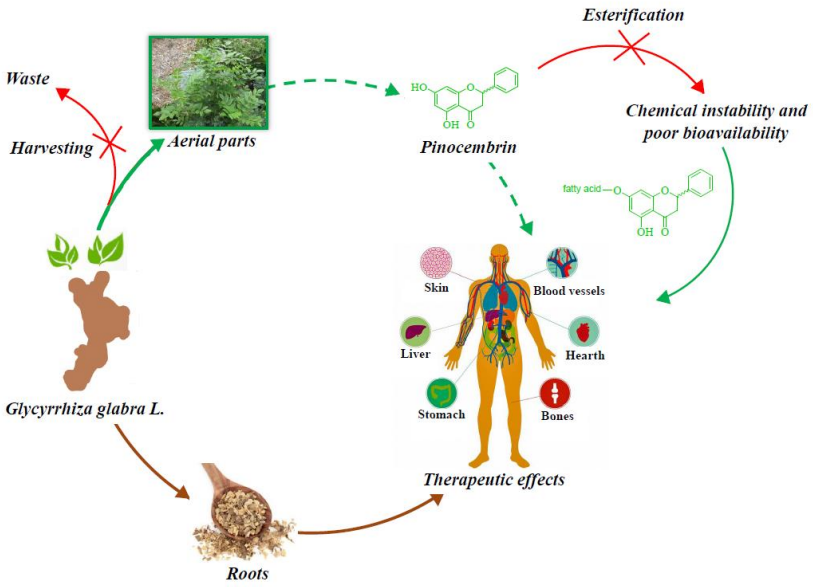

Figure 1: Green reuse of agrochemical waste.

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FL-3

Thermodynamics of binding between proteins and gadofullerenes: a comparative study

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Medical applications of fullerenes are hampered by their tendency to aggregate in aqueous media. Recently, it was shown that proteins can form adducts with fullerenes. These hybrids disperse monomolecularly and are water-soluble [1]. Endohedral gadofullerenes are a possible, efficient alternative to commercial Magnetic Resonance contrast agents. They yield a higher signal at significantly lower concentrations [2].

In order to design stable protein-gadofullerene adducts, it is crucial to understand their mutual interactions. We present a computational study of the thermodynamics of binding of the adduct lysozyme-Gd@C_{60} in comparison to lysozyme-C_{60}, which was the subject of a previous analogous computational study [3]. In both systems, the driving force of binding are van der Waals interactions, while polar solvation and entropy contributions are strongly detrimental. In lysozyme-Gd@C_{60} electrostatic interactions, which are absent in lysozyme-C_{60}, assist the binding despite a decrease of the vdW interactions. The balance between vdW and Coulomb interactions results in a lower binding energy (-18,5 kcal mol^{-1} vs -4,8 kcal mol^{-1}) for the Gd-based system. In addition, while pristine C_{60} locates in the binding pocket of the physiological substrate of lysozyme, Gd@C_{60} binds to a different pocket.

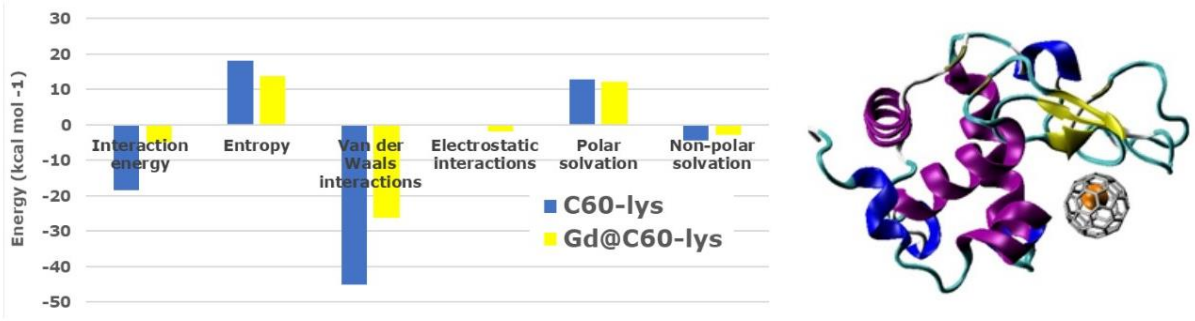

Figure 1: Left: Comparison of the contributions to the binding energy for lysozyme-C_{60} and lysozyme-Gd@C_{60}; Right: lysozyme-Gd@C_{60}.

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FL-4

Calcium phosphate nanoparticles for targeted cardiac drug delivery

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The occidental "modern" lifestyle and the lengthening of life expectancy have led to an increase in the incidence of cardiovascular diseases and despite advancements in its management it remains a major cause of death worldwide [1]. The requirement to overcome the issues associated with the use of conventional pharmacological therapies has led to the development of innovative therapeutic strategies. In this domain, nanoparticles hold great promise for new medical systems and provide alternative strategies for more specific, controlled, and safe drug delivery approaches.

The main aim of this research is to develop novel formulations based on calcium phosphate nanoparticles (CaP-NPs), having excellent intrinsically features including biocompatibility, ease of synthesis, versatility in drug loading and permeability of cell membranes [2]. CaP-NPs were synthesized using a straightforward one-pot inspired biomineralization protocol employing citrate as a stabilizing agent and regulator of crystal growth [2]. CaP-NPs were successfully loaded with microRNA for the management of heart failure. Drug loaded CaP-NPs were administered to cardiac cells *in vitro* and effects of treatments were assessed. CaP-NPs were also labelled with near-infrared fluorophore (Cy7) and administered to healthy mice by inhalation revealing in a rapid delivery of CaP-NPs to the myocardium and a significant targeting to the heart.

These results suggest that CaP-NPs are efficient systems for the therapeutic management of cardiomyocytes. Inhalation administration allows for rapid translocation of CaP-NPs from the pulmonary tree to the blood stream and thus to the myocardium. Our findings open up a new avenue for novel nano-technological approach for cardiovascular disease treatment.

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 720834.

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FL-5

Photodynamic therapy: development of a novel series of strained ruthenium complexes

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Photodynamic therapy (PDT) has recently attracted much attention on the use of light and light-induced chemical reaction for application in medicine for treatment of a wide variety of skin diseases, bacterial infections and cancers [1]. Among the main advantages, the possibility to achieve a temporal and spatial control of the drug-activation ensures a better discrimination between malignant and surrounding healthy tissues. This permits to strongly reduce the dose-limiting side effects, commonly incurred with standard chemotherapies. Many ruthenium (II) polypyridyl complexes have been exploited in PDT due to their strong ability to generate singlet oxygen $^1O_2$, one of the most potent cytotoxic species known, when exposed to visible light. However, in the case of hypoxic tumors, the reliance on molecular oxygen might preclude their application. Thus much interest has been focused on the development of a new class of ruthenium (II) polypyridyl complexes, characterized by a 'distortion feature' in their octahedral coordination geometry. The enhanced strain lowers the triplet metal-centered state (^{3}MC), allowing for thermal population from the triplet metal to ligand charge transfer state (^{3}MLCT), bringing to the loss of one or more ligands upon light activation [2]. The resulting active species are then able to form covalent adducts with DNA, in a 'cis-platin like' fashion.

In this context we present a series of novel ruthenium (II) polypyridyl complexes containing different ancillary ligands, and featuring a peculiar macrocycle unit optimally designed to selectively coordinate Cu(II) ions in physiological media. Thanks to their tunable absorption properties and to the strong ability to produce both oxygen singlet and ligand photo-ejection processes upon light activation, they appear to be optimal candidates for a further development as light-activated drugs in PDT.

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FL-6

Design and synthesis of novel furan-based MbtI inhibitors as potential antitubercular agents

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Tuberculosis (TB) is among the leading causes of morbidity and mortality worldwide. Since the treatment of TB still relies on outdated drugs, compromised by toxicity issues, and drug resistant infections are getting more and more widespread, the discovery of new antitubercular agents has become an urgent need: the impairment of mycobacterial iron acquisition could be a very effective strategy to reach this goal.

Iron works as a redox cofactor, playing a fundamental role in several cellular processes, involved in mycobacterial survival and proliferation. Its acquisition relies on the synthesis of high-affinity iron-chelating molecules. MbtI is a mycobacterium-specific Mg^{2+}-dependent salicylate synthase, which catalyses the double-step conversion of chorismic acid to salicylic acid, the building block of these siderophores; this enzyme has been recently validated as a pharmacological target to develop novel antitubercular agents [1].

Herein, we report on the identification of a competitive MbtI inhibitor (**VS1**) by a structure-based virtual screening analysis. This compound was found to be a promising inhibitor (IC_{50}=21.1 μM, Figure 1); with the aim of improving its activity, chemical modifications were made to the **VS1** structure. This optimisation process led to derivative **MM40** (IC_{50}=7 μM), which is the most potent MbtI inhibitor reported in the literature so far. MIC experiments are currently ongoing.

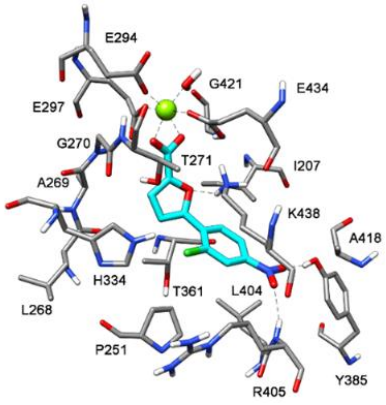

Figure 1: Binding mode of VS1 into MbtI.

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FL-7

Green synthesis of peptides from non-activated amino acids: production of Ser-His dipeptides with potential capability as organocatalyst

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Peptide synthesis interests several aspects of modern chemistry research, from the crescent employment of peptide-based pharmaceutics, the needs for green synthesis, to the implications in the prebiotic chemistry. Catalytic methods represent a promising approach, in alternative to the well-established solid phase peptide synthesis, for the possibility to avoid reagents activation steps and to carry out the reaction using mild conditions. Heterogeneous catalysis has lately withdrawn attention and surface-catalyzed peptide bond formation is of particular interest in synthetic biochemistry and shows great potential in synthetizing different kinds of peptides [1].

On this basis, we report a proof-of-principle study of the production of homo- and heteropeptides produced by sublimating non-activated serine (Ser) and histidine (His) on TiO_2 nanoparticles, exploiting a chemical vapor deposition (CVD) method. The formation of peptide linkages was detected by in-situ infrared spectroscopy in controlled atmosphere, while mass spectrometry of washing solutions was exploited to determine the extent of peptide chains. Homopeptides up to 3-mer of serine and histidine are observed, whilst as heteropeptides are concerned, the method appeared quite selective in producing Ser-His and His-Ser hetero-dipeptides.

The interest towards the possibility to prepare Ser and His containing peptides stems from the presence of these amino acids in the catalytic triad (together with Asp) found in many enzymes. The catalytic activity of Ser-His has been reported with different conclusions on the activity of dipeptide [2,3]. As a contribution to the debate, we tested the hydrolytic activity of Ser-His produced by CVD towards a simple, model oligopeptide, namely hexaglycine (6-Gly). The presence at the end of the incubation of both 6-Gly and monomeric Gly product suggests that these species show a potential hydrolytic activity towards simple peptides.

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FL-8

A molecular hybrid for mitochondria-targeted NO photodelivery

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The design, synthesis, spectroscopic and photochemical properties and biological evaluation of a novel, molecular hybrid that is able to delivery nitric oxide (NO) into the mitochondria are reported. This molecular conjugate unites a tailored o-CF3-p-nitroaniline chromophore, for photo-regulated NO release [1], and a Rhodamine moiety, for mitochondria targeting [2], in the same molecular skeleton via an alkyl spacer. A combination of steady-state and time-resolved spectroscopic and photochemical experiments demonstrate that the two chromogenic units preserve their individual photophysical and photochemical properties in the conjugate quite well. Irradiation with blue light triggers NO release from the nitroaniline moiety and photoionization in the Rhodamine centre, which also retains considerable fluorescence efficiency.

The molecular hybrid preferentially accumulates in the mitochondria of A549 lung adenocarcinoma cells where it induces toxicity at a concentration of 1 μM, exclusively upon irradiation. Comparative experiments, carried out with ad-hoc synthesized model compounds, suggest that the phototoxicity observed at such a low concentration is probably not due to the NO itself but rather to the formation of the highly reactive peroxynitrite that is generated from the reaction of NO with the superoxide anion.

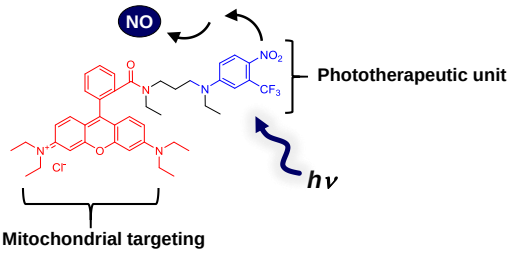

Figure 1: Molecular hybrid structure.

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FL-9

Towards the crystal structure determination of the protein Hsp90 N-terminal domain from Leishmania braziliensis and Homo sapiens sapiens in complex with new in silico identified inhibitors

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Heat shock protein 90 (Hsp90) plays a significant role in the life cycle control of the protozoan parasite *Leishmania braziliensis* and is essential for survival and proliferation of the intracellular mammalian stage, the amastigote. This protein is a promising target for the development of a specific drug therapy against leishmaniasis [1]. In a medicinal chemistry-oriented strategy for identifying small molecule inhibitors of the N-terminal domain (NTD) of *Leishmania braziliensis* Hsp90 [2], we set up a robust structure-based approach boosted by similarity search and docking-based virtual screening studies. This approach led to identify 13 most interesting molecules, showing the highest chemical diversity among them and against nucleotides or well-known Hsp90 inhibitors, to be investigated *in vitro* for anti-protozoan activity. Two compounds emerged as potential ligands of Hsp90, thus representing a valuable starting point of a second virtual screening. Therefore we set up a protocol composed of substructure filtering and docking studies. Finally, 16 molecules were selected, purchased and submitted to *in vitro* testing for anti-protozoa activity. Some of them emerged as potential ligands of Hsp90 showing K_d values in the low micromolar range. To date, the crystallographic structure of *Leishmania braziliensis* NTD (*Lb*NTD) is not available. To provide insight on the selectivity profile displayed by some inhibitors we have planned to determine the crystal structures of protein inhibitors complex with both *Lb*NTD and *human* Hsp90 NTD (*h*NTD). We developed efficient and reproducible protocols for expression and purification of *Lb*NTD and *h*NTD. Crystallization trials for *Lb*NTD are ongoing whereas the native structure of *h*NTD and its complex with substrate ADP were solved (resolution of 1.5 and 2.0 Å, respectively). Structural studies will provide the basis for the rational design of inhibitors having improved inhibitory activities and selectivity profiles.

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FL-10

Fatty acids from sea urchins' shell: a comparison between the species of the Gulf of Naples

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Sea urchins, like other Echinoderms, are extremely interesting as source of bioactive compounds, although most studies focus on the content and properties of edible parts, such as the composition and the nutritional profile of gonads [1]. Instead, the shell is little or nothing investigated with these aims, being considered as waste material.

Paracentrotus lividus and *Arbacia lixula* are two co-occurring sea urchin species (Echinodermata, Echinoidea), abundant on hard substrata in the shallow water of the Mediterranean and very common in the Gulf of Naples. The edible *Paracentrotus lividus* is concurrently an important commercial species for the consumption of its gonads (roe) and a well-known animal model in biology and ecotoxicology fields. *Arbacia lixula* is a non-edible species, which has become more popular for recent studies on bioactive compounds found in its eggs [2].

The aim of this study was to draw attention on the sea urchins' shell composition of these two species. Shell's extracts were obtained by a technology based on Rapid Solid Liquid Dynamic Extraction (RSLDE) implemented via an automated apparatus.

Extracts were submitted to fractionation by column chromatography on silica gel and then analyzed via NMR. NMR data showed the presence of free fatty acids, methyl and ethyl esters of fatty acids and monoglycerides.

In order to identify these compounds, GC-MS analysis was performed and the possible differences between two species were investigated.

[1] I. Martínez-Pita, F. J. García, and M. L. Pita, *Helgol. Mar. Res.* **64** (2009) 135-142.
[2] P. Cirino, C. Brunet, M. Ciaravolo, C. Galasso , L. Musco, T. Vega Fernández, C. Sansone, and A. Toscano, *Mar. Drugs* **15** (2017) 187.

FL-11

The synthesis and biological activity of new 2*H*-benzimidazole 1,3-dioxides

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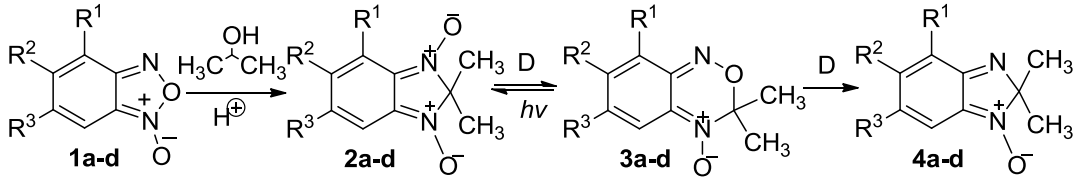
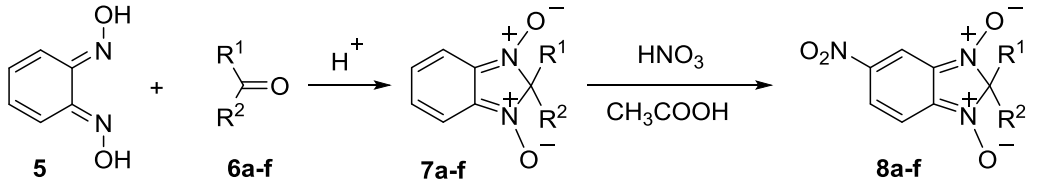
As a result of our work, we have synthesized new 2*H*-benzimidazole 1,3-dioxides (**2a-d**), which according to the literature show high biological activity against the parasites *Trypanosoma cruzi* and *Leishmania spp.* as a result of the interaction of benzo[1,2-*c*][1,2,5]oxadiazole *N*-oxides derivatives (**1a-d**) with isopropyl alcohol in sulfuric acid.



a) R^1=R^3=Cl; R^2= H; **b**) R^1=OCH_3; R^2=H; R^3=Cl; **c**) R^1=NO_2; R^2=R^3=H; **d**) R^1=R^3=Cl; R^2=NO_2

Furthermore, we also proposed a new method for the preparation of 2*H*-benzimidazole 1,3-dioxides (**7a-f**) by the reaction of *o*-benzoquinondioxime (**5**) with ketones (**6a-f**). Further nitration of obtained compounds makes it possible obtainment of a wide range of Sepin-1 analogues with various substituents in the 2-position (**8a-f**).



a) R^1=R^2=CH_3; **b**) R^1=CH_3; R^2=CH_2Cl; **c**) R^1+R^2=-$(CH_2)_4$-;
d) R^1+R^2=-$(CH_2)_5$-; **e**) R^1=CH_3; R^2=CH_2COOCH_3; **f**) R^1=CH_3; R^2=$CH_2CH_2COOCH_2CH_3$

The resulting compounds (**2a-d, 3a-d, 4a-d**) were studied for antimicrobial and hemolytic activities *in vitro*. As a result of the biological tests, it was shown that compounds (**2a-d**) and (**3a-d**) show good biological activity among the classes of compounds, and removal of oxygen atom from the benzimidazole cycle compounds (**4a-d**) worsens the biological activity by several times.

This work was supported by the President of the Russian Federation, grant MK-4838.2016.3.

FL-12

Computational study of the reduction mechanism of platinum (IV) antitumor prodrugs by biological reductants

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There is a growing interest in six-coordinate Pt(IV) complexes because of their anticancer activity. Platinum(IV) complexes are an important class of compounds that can act as prodrugs and can undergo a transformation in vivo to release the active Pt(II) complexes losing the two axial ligands that, in turn, can be chosen to possess improved physiochemical and biopharmaceutical properties.

This requirement, for example, is fulfilled by Asplatin [1] a cisplatin-based Pt (IV) complex with an aspirin in axial position (see Figure 1).

The reduction of Pt(IV) complexes has been the subject of many studies over several decades and several mechanisms were proposed for the reductive elimination such as outer sphere reactions, inner sphere mechanisms and Pt(II) catalyzed reaction schemes.

Here are reported the outcomes of a theoretical investigation of the Asplatin reduction with the aid of density functional theory (DFT) with the purpose at elucidating the mechanism of reduction and rationalizing experimental data [2].

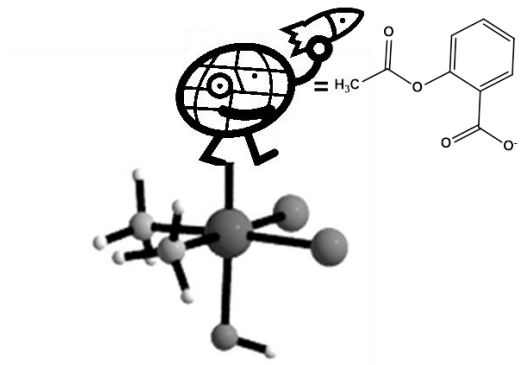

Figure 1. Asplatin.

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FL-13

Excited state proton transfer of a super-photoacid in methanol solution

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The absorption of radiation can hugely increase the acidity of a photoacid molecule, which dissociates at the excited state (ES) by transferring a proton to a nearby solvent molecule, or to a strong base molecule present in solution [1]. Such "super" photoacids have acquired interest in several technologies, like photolithography and polymer synthesis.

The Excited State Proton Transfer (ESPT) elementary steps cover a wide range of time and space scale and the balance of these events finely controls the kinetics and thermodynamics of the overall process. Therefore, unveiling at molecular level the complex aspects of ESPT reactions with solvent molecules acting as proton acceptor is extremely difficult. In this contribution we investigate the mechanism and the driving forces of an ESPT reaction by means of Time-Dependent Density Functional Theory based ab-initio molecular dynamics simulations. An effective hybrid implicit/explicit model of solvation was adopted to consider in an explicit way the solvent coordinate in the ESPT process.

We studied the solvation and photo-reactivity of a cyanine dye, named QCy9, in methanol solution, both in the ground and the excited state. The QCy9 molecule is a super-photoacid, which exhibits the largest k_{PT} value reported in the literature so far, independent on the nature of the solvent [2].

Our calculations revealed that the ESPT event between the QCy9 molecule and the accepting methanol molecule is actually assisted by the oscillations of solvent molecules belonging to the first and second solvation shell of the acceptor. Moreover, the simulated ESPT occurs at times compatible with the experimental rate constant, suggesting that the electronic potential employed and the method are accurate and reliable. Ab initio molecular dynamics combined with a robust hybrid implicit/explicit model for the solvent appears a suitable tool to disentangle such kind of photo-reactivity where methanol solvent molecules are directly involved.

[1] P. Cimino, U. Raucci, G. Donati, M.G. Chiariello, M. Schiazza, F. Coppola, and N. Rega, *Theor. Chem. Acc.* **135** (2016) 117.
[2] R. Simkovitch, S. Shomer, R. Gepshtein, D. Shabat, and D. Huppert, *J. Phys. Chem. A* **118** (2014) 1832-1840.

FL-14

Copper(I)-catalyzed regio- and stereoselective synthesis of cyclopropyl vinylindolines

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The functionalization of indole core is an interesting research field because the indole moiety is present in a huge number of bioactive natural products and pharmaceutical compounds [1]. For this reason, the proposal of new methodologies for indole synthesis and functionalization is still of great interest in synthetic organic chemistry. In the context of our studies on metal-catalyzed cycloaddition reactions of vinylindoles [2] and on functionalization of indole core [3], we decided to investigate the reactivity of 2-vinylindoles with diazo compounds. We envisioned in this way to functionalize these indole derivatives by means of a new reaction pattern. Thus, the reaction between 2-vinylindole and ethyl diazoacetate was conducted in the presence of a copper(I) complex and led to a series of cyclopropyl vinylindolines with satisfactory yields and with complete regio- and diasteroselectivity (Figure 1). Optimization of conditions, scope and proposed mechanism of the reaction will be illustrated in the poster, together with preliminary results on an enantioselective version.

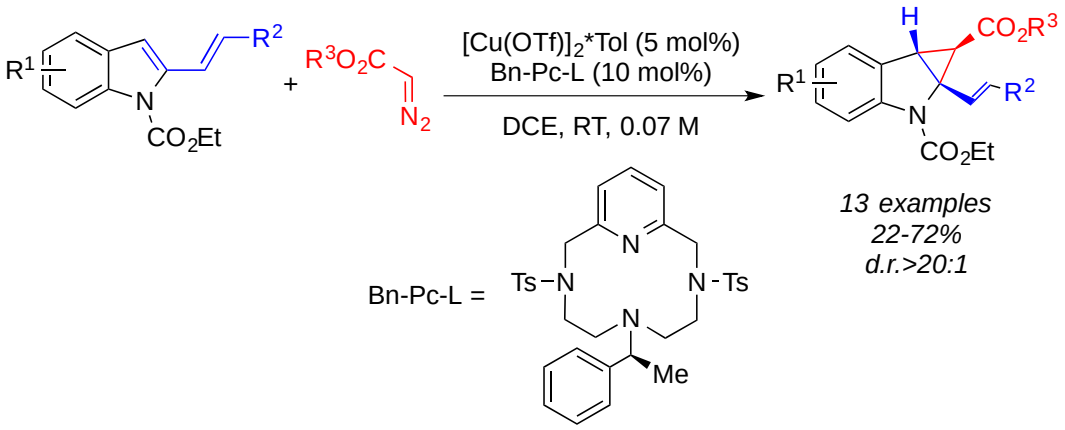

Figure 1: Copper(I) catalyzed synthesis of cyclopropyl vinylindolines.

[1] a) A. W. Schmidt, K. R. Reddy, and H. J. Knölker, *Chem. Rev.* **112** (2012) 3193-3328; b) A. Głuszyńska, *Eur. J. Med. Chem.* **94** (2015) 405-426; c) L. S. Tsutsumi, D. Gundisch, and D. Sun, *Curr. Top. Med. Chem.* **16** (2016) 1290-1313.
[2] E. Rossi, V. Pirovano, and G. Abbiati, *Eur. J. Org. Chem.* **2017** (2017) 4512-4529.
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FL-15

Computational study of the reaction mechanism of deoxyribozyme 9DB1

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9DB1 is a deoxyribozyme with RNA ligase activity. Recently the crystal structure of 9DB1 was obtained. The deoxyribozyme is bound with its substrate in the post-catalytic state [1]. The 9DB1 catalyzes the reaction between the terminal 3'-nucleophilic adenosine, and the 5'-guanosine triphosphate (GTP). The proposed mechanism is an S_N2, where the alcoholic group of the nucleophilic adenosine attacks the alpha-phosphate of GTP.

A quenched molecular dynamics protocol was used to generate the pre-catalytic state. This geometry was used to build a quantum mechanical (QM) model system in order to explore the potential energy surface of the 9DB1 ligase mechanism. The calculations showed that the reaction mechanism for the RNA ligation is a nucleophilic acylic substitution with two reaction steps:

- A nucleophilic addition step of the alcoholic group to the alpha-phosphate of GTP, with a concerted proton transfer;
- A dissociation step of the diphosphate group with a second concerted proton transfer between the alpha-phosphate and the leaving group.

To conclude:

- The reaction mechanism is based on a substrate activation of the nucleophilic entering group.
- The rate determining step is the nucleophilic addition step.
- The calculated activation energy is 22.8 kcal/mol in agreement with kinetic measurements.

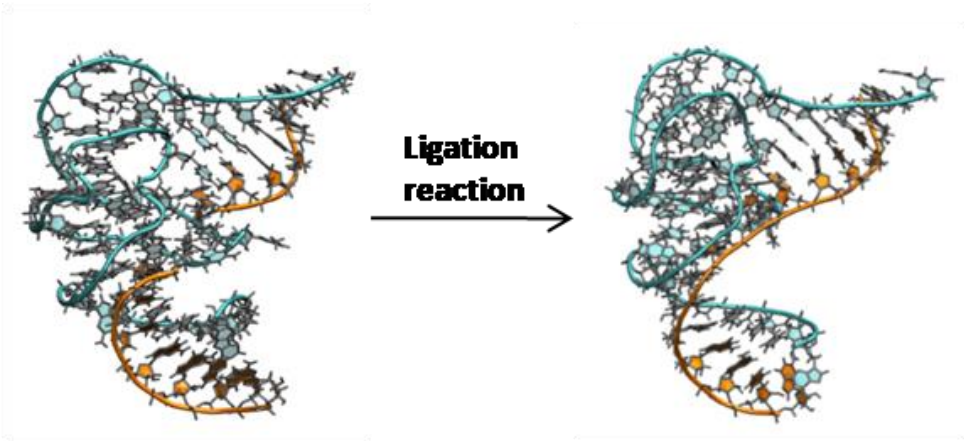

Figure 1: Global view of the ligation reaction catalyzed by 9DB1.

[1] A. Ponce-Salvatierra, K. Wawrzyniak-Turek, U. Steuerwald, C. Hobartner, and V. Pena, *Nature* **529** (2016) 231-234.

FL-16

Dual iminium and Lewis base catalyzed Morita Baylis Hillman reaction on cyclopent-2-one

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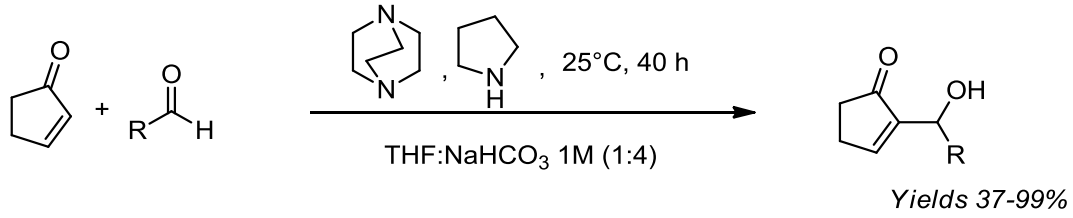
The Morita-Baylis-Hillman (MBH) [1] reaction is an atom-economic carbon-carbon bond-forming reaction between the β position of an electron poor alkene and different carbon electrophiles under the influence of a catalyst or catalytic system. The product of a MBH reaction is a very interesting compound because of its polyfunctional character which can be used in the total synthesis of complex organic molecules or as a building block in diversity oriented Synthesis (DOS) strategies.

Several electron poor alkenes have been used in this reaction such as acrylic acid derivates, nitro alkenes, α-β unsatured ketones, however the cyclic enones in particular cyclic pent-2-enone prove to be challenging substrate as only few examples of efficient catalytic systems on this compound have been reported in the literature [2]. In our work, we proposed a new mild catalytic system based on the concomitant presence of an iminium catalyst, derived from a secondary amine, and a basic water solution of $NaHCO_3$ for the reaction of cyclic pent-2-enone with several aldehydes, obtaining 16 compounds in moderate to excellent yields (37-99%) [3].



Yields 37-99%

[1] D. Basavaiah, A. J. Rao, and T. Satyanarayana, *Chem. Rev.* **110** (2010) 5447-5674.
[2] a) R. Gatri, and M. M. El Gaied, *Tetrahedron Lett.* **43** (2002) 7835-7836; b) K. P. Guerra, and C. A. M. Afonso, *Tetrahedron* **67** (2011) 2562-2569; c) A. Bugarin, and B. T. Connell, *J. Org. Chem*. **74** (2009) 4638-4641.
[3] R. Innocenti, G. Menchi, and A. Trabocchi, submitted.

FL-17

2-piperidine ethanol as building block for the synthesis of alkaloids-inspired compounds

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Alkaloids are a wide class of naturally-occurring compounds, characterized by diverse biological activities, which make them well known targets in medicinal chemistry.

Several alkaloids share a piperidine-containing scaffold, which attracted our interest, prompting us to exploit the commercially available 2-piperidine ethanol **1** as versatile precursor for the synthesis of different alkaloids-inspired compounds, synthesized in our laboratory in the last years.

In particular, **1** was used to a great extent for the total synthesis of plant-derived alkaloids, such as (+)-aloperine, boehmeriasin A, (+)-dumetorine, (-)-coniine, (-)-epidihydropinidine and sedum alkaloids, and for the obtainment of hybrid compounds **2**, which proved to be promising *α*–tubulin binders [1]. Moreover, building block **1** was easily converted in different polycyclic piperidine derivatives **3**, characterized by increased molecular complexity, exploiting a diversity-oriented synthetic approach [2].

The search for new scaffolds which could enrich this collection is still active in our laboratory, and the synthesis of new withanolides-inspired compounds is currently under study.

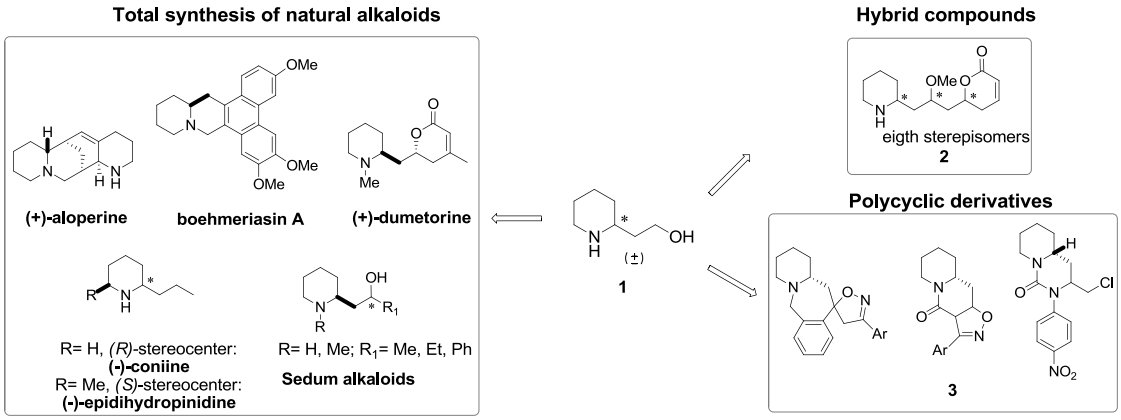

Figure 1: Piperidine-based compounds synthesized from precursor **1**.

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[2] C. Marucci, M. S. Christodoulou, S. Pieraccini, M. Sironi, F. Dapiaggi, D. Cartelli, A. M. Calogero, G. Cappelletti, C. Vilanova, S. Gazzola, G. Broggini, and D. Passarella, *Eur. J. Org. Chem.* **11** (2016) 2029-2036.

FL-18

First-principles study of Co and Cu-based electrolytes for dye-sensitized solar cells

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Since the pioneering work by 'O Regan and Grätzel [1], dye-sensitized solar cells have attracted great academic and industrial interest and are a promising technology in solar energy conversion thanks to their low manufactural costs, eco-friendly materials and high efficiencies even under diffuse light conditions. The chemical complexity of these devices, which is inherent to the electronic processes undergoing at semiconductor/ dye/electrolyte interfaces, represents a great challenge for the effective design and engineering of DSSCs with high photo-conversion efficiency [2]. State-of-the-art devices present record PCEs ~14% with metal-organic dyes on mesoporous ZnO or TiO_2 n-type semiconductors, which are, however, still below to the theoretical efficiencies expected for these devices. Beside the optimization of the dye-electrode interface properties, several research groups are focusing on possible alternatives to the most exploited I_3^-/I^- redox couple. Latest efforts have shown that one-electron redox systems such as Co(II/III) and Cu(I/II) organometallic complexes, can overcome the problems of the two-electrons process of the I_3^-/I^- : corrosiveness, competitive light absorption and large internal potential losses [3]. The aim of this work is provide structural and electronic insights at the dye-electrolyte interface in DSSCs by means of first-principles methods. In particular, we investigated structural and electronic features of several cobalt-based complexes and copper-based complexes, which have recently shown to outperform Co-based ones due to a minimized steric hindrance that overcomes mass-transport limitations [3]. Here we report the computed redox potentials and reorganization energies for each Co(II/III) and Cu(I/II) couple in order to understand how the ligands can tune these important parameters for the electron transfer processes. These results are discussed together with the electronic properties of the push-pull dyes used in n-type and p-type DSSCs in order to predict and assess the most promising combinations of dye-electrolyte couple for the foreseen development of tandem-DSSCs.

[1] B. 'O Regan, and M. Grätzel, *Nature* **353** (1991) 737-740.
[2] A. Hagfeldt, G. Boschloo, L. Sun, L. Kloo, and H. Pettersson, *Chem. Rev.* **110** (2010) 6595-6663.
[3] Y. Saygili, M. Söderberg, N. Pellet, F. Giordano, Y. Cao, A. B. Muñoz-García, S. M. Zakeeruddin, N. Vlachopoulos, M. Pavone, G. Boschloo, L. Kavan, J. E. Moser, M. Grätzel, A. Hagfeldt, and M. Freitag, *J. Am. Chem. Soc.* **138** (2016) 15087-15096.

FL-19

Insight in pillararenes synthesis and applications in catalysis

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Pillar[n]arenes (P[n] n = 5-15) were discovered for the first time by Ogoshi in 2008 [1], and since then the scientific community spent many efforts to improve their synthesis. In this context, our group published a paper focused on the enhancement of P[6] yield, bearing three different alkoxy substituents and templated by a series of small organic and organometallic cations, such as tetramethylammoniumchloride (TMAC) or cobaltocenium and ferrocenium salts [2].

We further investigated through MS spectrometry the reaction templated by TMAC in a DCM/H_2O solution, involving the conversion of P[5] and of the oligomeric by-products into P[6].

Since very few example of catalysis mediated by P[n]s cavity have been yet published [3], our group studied the catalytic effect of P[5] in nucleophilic substitution reactions. The rate of such reactions has been increased between 10 and 20 times in presence of P[5], when the reactants involved where allyl halide and primary amines. Further investigations on a wider range of reactions are currently underway.

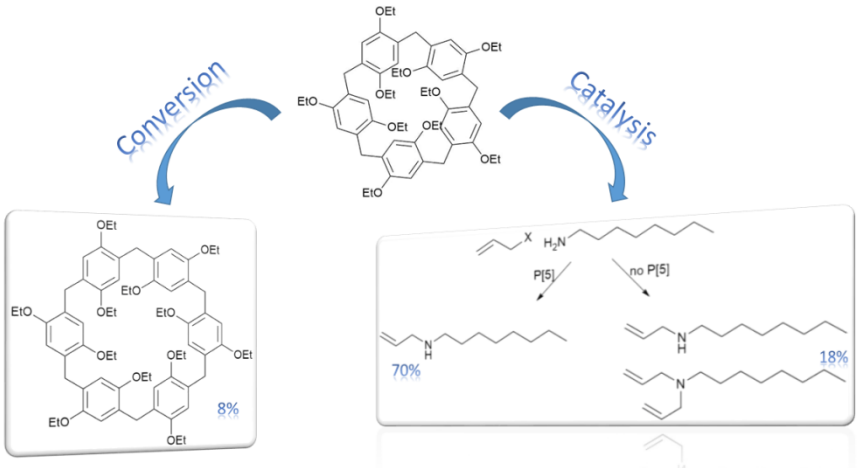

Figure 1: P[5] as starting material for the synthesis of P[6] (left) and as catalysts in a nucleophilic substitution reaction (right).

[1] T. Ogoshi, S. Kanai, S. Fujinami, T. A. Yamagishi, and Y. Nakamoto, *J. Am. Chem. Soc.* **130** (2008) 5022-5023.
[2] M. Da Pian, O. De Lucchi, G. Strukul, F. Fabris, and A. Scarso, *RSC Adv.* **6** (2016) 48272-48275.
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FL-20

Highly efficient synthesis of C_3-symmetric *O*-alkyl substituted triphenylenes and related Mannich derivatives for supramolecular applications

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Triphenylenes (TPs) are class of self-aggregating molecules that can provide columnar aggregates with important optical applications, as well as high charge-carrier transport capacity. [1]

Due to the extensive interest in the preparation of C_3-symmetric hexa-substituted TPs and the lack of straightforward methods, herein we report a simple and efficient method for the preparation of 2,6,10-tribenzyloxy-3,7,11-trihydroxytriphenylene. The strategy is based on the optimization of the reductive ring opening of the benzyl acetal of hexahydroxytriphenylene with diisobutylaluminum hydride, enabling the isolation of the desired product in overall 48% yield. [2] This molecule was further functionalized with alkylating and acylating units and reacted with amines and formaldehyde under Mannich conditions to provide a small library of eleven C_3-symmetric derivatives (Figure 1) obtained in moderate to good yields to be exploited as molecular scaffolds for sensors [3] and for their liquid crystal properties.

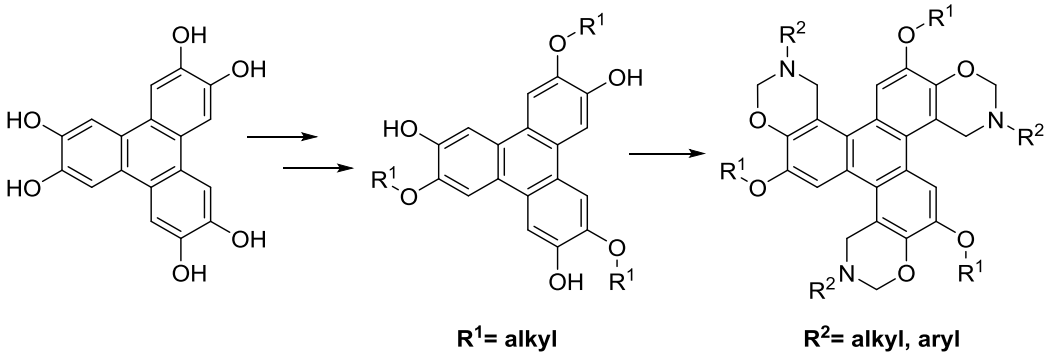

Figure 1: Synthesis of C_3-symmetric *O*-alkyl substituted triphenylenes and Mannich derivatizations leading to a small library of functionalized TPs.

[1] D. Adam, P. Schuhmacher, J. Simmerer, L. Häussling, K. Siemensmeyer, K. H. Etzbachi, H. Ringsdorf, and D. Haarer, *Nature* **371** (1994) 141-143.
[2] S. Takano, T. Ohkawa, and K. Ogasawara, *Tetrahedron Lett.* **15** (1988) 1823-1824.
[3] L. Mosca, J. Ĉejka, B. Dolenský, M. Havlĵk, M. Jakubek, R. Kaplánek, V. Král, and P. Anzenbacher, *Chem. Commun.* **52** (2016) 10664-10667.

FL-21

[2+2] photocycloaddition in crystalline molecular salts of 4-amino-cinnamic acid, an XRD study

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The description of solid state [2+2] photoreactions in cinnamic acid derivatives dates back to the 60s with the pioneering works of Schmidt and Cohen [1]. As a rule-of-thumb, when the molecular arrangement found in the crystal packing satisfies the Schmidt's criterion - *i.e.* double bonds are parallel and at a separation of less than 4.2 Å. Although, scientific community has devoted great attention to the control of the reactivity by using templating units *via* noncovalent interactions such as hydrogen bond [2], a deep knowledge about the factors and reaction pathways are still somewhat enigmatic, especially when they are carried out in the solid state [3].

Crystalline state offers a suitable medium where to study these transformations because it allows to follow the fate of the reacting species by means of X-Rays Diffraction techniques (XRD), thus not only from a molecular point of view but also from a crystallographic one, giving precious information about crystal phases evolution *vs.* irradiation.

Here we report our findings on the crystal-to-crystal photoreactivity of molecular salts of cinnamic acid derivatives which have been monitored by means of polarized light microscopy, powder and single crystal X-ray diffraction. Following the structural response to UV *via* powder XRD and Rietveld analysis at various irradiation intervals, it has been possible to construct a conversion model for such transformations.

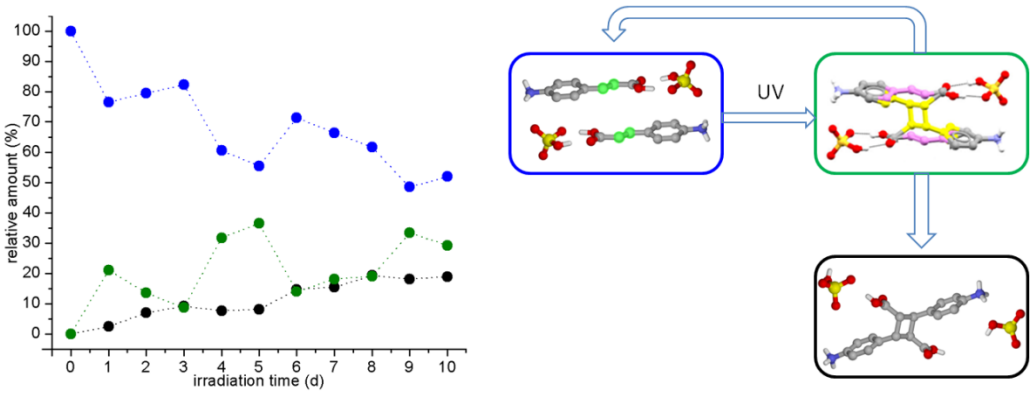

Figure 1: Relative amounts (%) of crystal phases *vs.* irradiation time.

[1] M. D. Cohen, G. M. J. Schmidt, and F. I. Sonntag, *J. Chem. Soc.* (1964) 2000-2013.
[2] D. Braga, S. D'Agostino, and F. Grepioni, *Cryst. Growth Des.* **12** (2012) 4880-4889.
[3] S. D'Agostino, P. Taddei, E. Boanini, D. Braga, and F. Grepioni, *Cryst. Growth Des.* **17** (2017) 4491-4495.

FL-22

Alkyl carbonates as non-toxic reagents for the selective gas-phase alkylation of phenolics

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Alkyl carbonates are readily biodegradable and non toxic compounds characterized by good solvent power towards organic molecules and adjustable reactivity as a function of temperature, substrate nature and catalyst type [1]. In the presence of a basic catalyst, organic carbonates can react either as carboxymethylating or methylating agents; the yield of these reactions is strongly affected by the nature of the nucleophile: stronger nucleophiles mainly attack on the carbonyl C-atom of the carbonate while weaker nucleophiles (e.g. PhOH) mainly attack on one of the two alkyl C-atoms [2].

Diethyl carbonate was used as a non-toxic and effective reagent for PhOH alkylation. The chemo-selectivity with MgO catalyst is strongly directed towards the phenolic O-atom to give phenetole with no C-alkylation. The modulation of catalyst basicity by substituting part of Mg with Al atoms in the mixed Mg/Al oxide results in a bifunctional catalyst capable of selective O-alkylation of PhOH to give phenetole at low temperatures, and selective O-alkylation at higher temperatures together with isomerization of the O-alkylated products on Al-sites. This cascade effect directs the overall selectivity of phenol alkylation with DEC to C-alkylated products, allowing the use of organic carbonates for both C-alkylation and O-alkylation of aromatic substrates.

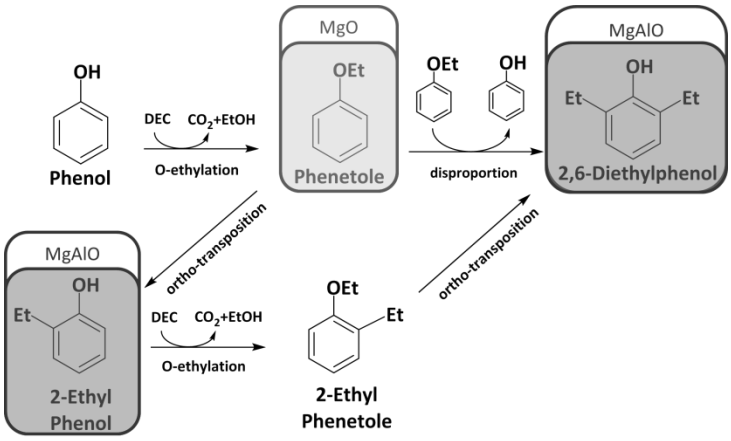

Figure 1: Reaction pathway for PhOH ethylation with DEC over MgO and MgAlO.

[1] P. Tundo, and A. Perosa, *Chem. Rec.* **2** (2002) 13-23.
[2] F. Arico, and P. Tundo, *Russ. Chem. Rev.* **79** (2010) 479-489.

FL-23

Anabolic androgenic steroid doping: development and application of an analytical procedure for determination of urinary sulphate steroid metabolites

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The World Anti-Doping Agency (WADA) includes anabolic androgenic steroids (AAS) among the substances and methods prohibited in sport [1]. The process of steroid detection undertaken by the WADA accredited laboratories is based on GC-MS(/MS) or LC-MS(/MS) analysis of urinary samples collected from male and female athletes. The methods routinely used in steroid screenings mainly focus on substances that are excreted unconjugated or as glucuronides and for this reason common procedures includes enzymatic hydrolysis with β-glucuronidase from *Escherichia Coli* or *Helix Pomatia*. Despite this, for doping control purposes, the development of a confirmation procedure to determine the endogenous (i.e. dehydroepiandrosterone or androstenedione) and exogenous steroids and their metabolites excreted primarily as sulphates could be of interest.

In this work we have first evaluated the performances of different preparations of sulphatases from *Helix pomatia* and *Pseudomonas aeruginosa* compared to chemical hydrolysis of sulphate steroids. Then we have studied different approaches for the selective isolation of steroids conjugates from urine matrix.

Our results show that chemical hydrolysis is preferable to enzymatic methods as it results in quantitative cleavage of the sulphate moiety and that ion paired extraction is the more reliable method for direct isolation of sulphate steroids from urinary matrices.

[1] The World Anti-Doping Code, WADA 2017 List of Prohibited Substances and Methods, The World Anti-Doping Agency, Montreal, September 2016.

FL-24

Synthesis and photovoltaic properties of polymer containing both electron-donor and -acceptor units

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There is a remarkable level of interest in the development of π-conjugated polymers (ICPs) which are being employed, thanks to their promising optical and electronic properties, in numerous applications including photovoltaic cells, light emitting diodes and thin-film transistors. Poly(3-alkylthiophenes) (P3ATs), due to their high solubility, film-forming ability and structural versatility, are surely the most studied and promising class of ICPs [1].

Among the various possible techniques for fabricating organic photovoltaic cells, bulk heterojunction (BHJ) architecture has been studied intensively in recent years for its potential to obtain high efficiency at low costs. With the aim of producing optimal phase contact between the donor and acceptor molecules for charge generation, while maintaining a continuous path in each phase for the efficient transport of electrons and holes, the synthesis of both donor and acceptor containing polymers appears particularly intriguing [2].

New 4,7-bis(3-alkylthiophen-2-yl)benzo(2,1,3)thiadiazole monomers, functionalized with different alkyl chains, have been synthesized through a palladium-catalyzed Suzuki cross-coupling reaction and then polymerized by oxidative coupling using $FeCl_3$. The newly synthesized polymers (PTRBTZ) have been characterized by common analytical techniques, such as ^{1}H-NMR, gel permeation chromatography (GPC), thermal analyses (DSC, TGA) and UV-Vis and PL spectroscopy; the PTRBTZ derivatives were also tested as active media in air-processed single material organic solar cells, and as blends with $PC_{61}BM$ (1:1 w/w) as additional acceptor material.

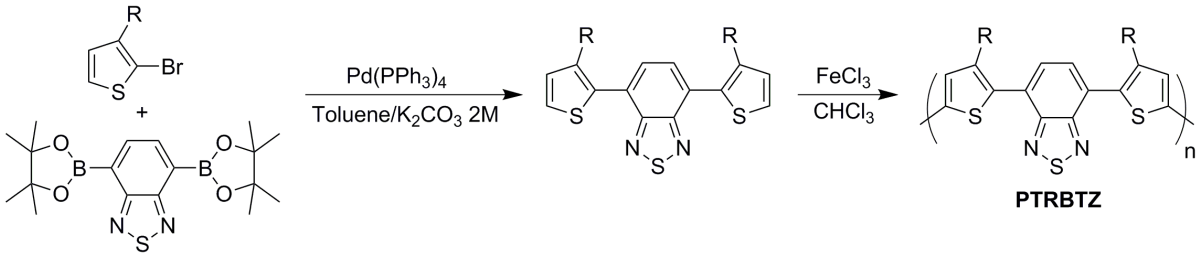

Figure 1: Synthesis of PTRBTZ.

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[2] Z. Tan, J. Hou, Y. He, E. Zhou, C. Yang, and Y. Li, *Macromolecules* **40** (2007) 1868-1873.

FL-25

From jelly to ion liquid for CO_2 capture

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The rapid global climate change has induced academes and industries to develop novel technologies for the efficient and reversible capture of CO_2.

In the last decade more researcher lines had focused their interest on the use of Ion Liquids (ILs) for CO_2 capture. In the last few years a new approach has been developed through chemical interaction, particularly was important the discovery of environmentally friendly ion liquid made with using Amino Acids as anion and Choline as cation [1].

Choline is a soluble vitamin usually grouped within the b-complex vitamin. The use of Cholinium cation with amino acid has given good result for the CO_2 capture. Both substances are easy to obtain in large quantities at high purity, have low environmentally impact and high biodegradability.

In this work a further step was performed: Amino Acids-Choline ILs were prepared directly using food-grade fish gelatine as Amino Acids source. This food product formed by collagen, a protein composed of repeated sequence of proline, glycine and hydroxyproline, collagen can be found in animal's bones and cartilages. The alpha amino acid were extracted from fish jelly with three different approaches for maximize the yield: Acid hydrolysis, Basis Hydrolysis an enzymatic catalysis.

The obtained Amino Acids mixture have been studied as green and low cost stating materials to prepare ILs. The chemical and physical properties of ionic liquids prepared from the former amino acids mixture and choline were investigated. The obtained ionic liquids were also tested for the CO_2 capture.

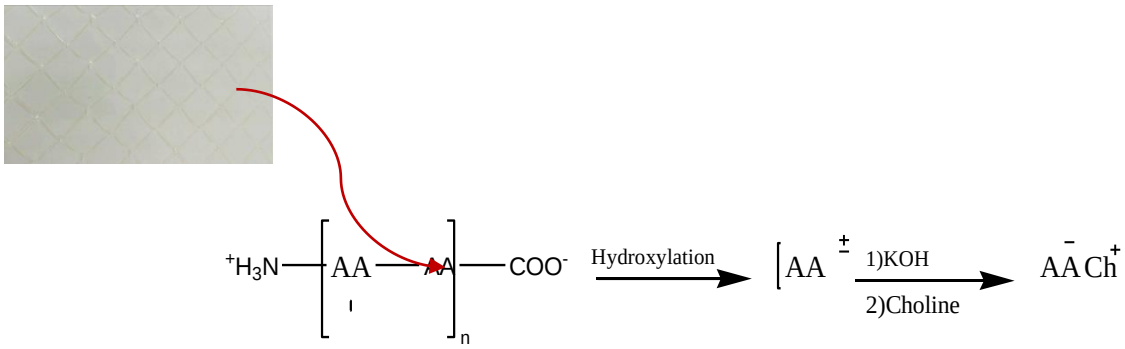

Figure 1: Synthesis ILs from jelly.

[1] S. Bocchini, S. Hernandez, S. Bianco, A. Chiappone, G. Saracco, and C. F. Pirri, *Proceedings of the Merck Young Chemists Symposium 2016*, ISBN: 978-88-86208-92-5.

FL-26

Ethanol steam reforming process: lanthanum oxide effect in ceria and zirconia based catalysts

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Looking at the global energy scenario, biomass utilisation is becoming increasingly popular, thanks to its high intrinsic potentiality [1]. This work is focused on the development of heterogeneous catalysts for the valorisation of one promising product obtained from lignocellulosic waste: bioethanol. This component can be exploited for hydrogen manufacturing. Finding a green and sustainable way to produce hydrogen is a great challenge because it is employed for widespread applications, from chemicals to fuels. Nowadays hydrogen is mainly produced by methane steam reforming process that is linked to the use of fossil fuels, and for this reason, can't be considered suitable anymore. The attention was focused on the synthesis of an active, selective yet resistant catalyst to maximize H_2 production. The focus is the stabilization of nickel active phase in order to suppress side reactions and reduce coproducts such as methane, acetaldehyde and ethylene, which are coke precursors. A preliminary screening on the support was carried out, and in particular zirconia and ceria based materials were considered. Ceria was chosen for high redox properties, while zirconia for its elevated mechanical and thermal stability [2]. In particular, knowing the limitations of those systems, lanthanum oxide was added into the system as structural promoter. Those catalysts were prepared using different preparation methods, and in particular, lanthanum oxide introduction method was studied. It was found that lanthanum oxide is a good promoter both for ceria and zirconia catalysts. Lanthanum oxide acts with ceria in order to increase redox properties; this quality was confirmed by XRD analysis that affirms that La^{3+} substitutes Ce^{4+} in ceria lattice improving CeO_2 reducibility and thus redox pump. On the contrary, lanthana has a different effect on zirconia support. It reduces zirconia acidity limiting ethanol dehydration; CO_2-TPD verifies this property. At the same time, it was observed that co-precipitation method is the best technique to introduce the promoter into the support, in particular for ceria catalyst. This experimental approach allowed to maintain a stable conversion of 100 % for 18 hours in ESR.

[1] X. Zhao, H. Zhou, V. S. Sikarwar, M. Zhao, A. A. Park, P. S. Fennell, L. Shenf, and L. Fan, *Energy Environ. Sci.* **10** (2017) 1885-1910.
[2] W. Li, Z. Zhao, and Y. Jiao, *Int. J. Hydrogen Energy* **41** (2016) 17907-17921.

FL-27

Cyclic reforming of ethanol: reactivity study of mixed oxide with spinel structure

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Pollution and global warming, linked to the increasing of the world's population and, therefore the energy demand, had in the last decades highlighted the necessity of finding new sources of renewable energies. However, it will be also important to find a new way to carry the energy and hydrogen is one of the most eco-efficient solutions. In this context, this work deals with a study on the feasibility of a new process, aimed at the production of hydrogen from water and ethanol (a compound obtained starting from biomasses), with inherent separation of hydrogen from C-containing products. The strategy of the process includes a first step, during which a metal oxide is contacted with ethanol at high temperature; during this step, the metal oxide is reduced and the corresponding metallic form develops. During the second step, the reduced metal compound is contacted at high temperature with water, to produce molecular hydrogen and with formation of the original metal oxide.

In overall, the combination of the two steps within the cycle process corresponds to *ethanol reforming*, where however CO_x and H_2 are produced separately. Various mixed metal oxides were used as electrons and ionic oxygen carriers, all of them being characterized by the spinel structure typical of M-modified ferrites: $M_{0,6}Fe_{2,4}O_4$ (M = Co, Mn or Co/Mn). The first step was investigated in depth; it was found that besides the generation of the expected CO, CO_2 and H_2O, the products of ethanol anaerobic oxidation, also a large amount of H_2 and *coke* were produced. The latter is highly undesired, since it affects the second step, during which water is fed over the pre-reduced spinel at high temperature. The behaviour of the different spinels was affected by the nature of the divalent metal cation[1].

The new materials were tested in terms of both redox proprieties and catalytic activity to generate hydrogen.

Still the problem of *coke* formation remains the greater challenge to solve.

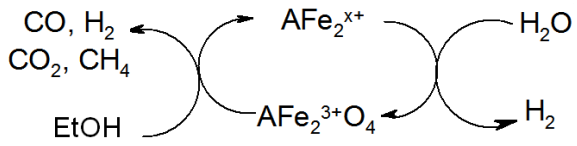

Figure 1: The chemical-loop reforming of ethanol over M-modified ferrospinels.

[1] N. Ballarini, F. Cavani, S. Passeri, L. Pesaresi, A. F. Lee, and K. Wilson, *Appl. Catal., A*. **366** (2009) 184-192.

FL-28

Triazine-based 2D-covalent organic frameworks enhances electrochemical performance of enzymatic biosensors

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Well-ordered two dimensional porous materials such as zeolites, covalent organic frameworks (COFs) and metal organic frameworks (MOFs) have impressed remarkable attention thanks to their great numbers of existing and potential applications. While researchers have utilized from these materials for the purpose of energy storage, optoelectronics or even drug delivery, there have been only a couple studies dealing with biosensor applications of organic frameworks [1, 2], yet, best to our knowledge, there have not been a study that uses COFs as biosensor matrix. In this study, we have focused on the synthesis and characterization of triazine based COFs (CTF-1), followed by application towards electrochemical enzymatic biosensors. We firstly modified screen-printed carbon electrode surface with gelatine-CTF-1 gel, and immobilized superoxide dismutase (SOD) enzyme, that catalyzes the dismutation reaction of superoxide radicals ($O_2^{-}\cdot$) into H_2O_2. Electrochemical impedance spectroscopy measurements showed that the charge transfer resistance (R_{ct}) of gelatine-CTF-1 modified electrode was nearly 21.7% lower than that gelatine modified electrode (Figure 1A). The amperometric spectrum demonstrated that the gelatine-CTF-1-SOD electrode showed an amperometric response that was 25.4% higher than that gelatine-SOD modified electrode (Figure 1B). These findings suggest that CTF-1 is a promising candidate to be used as electrochemical enzymatic biosensor component.

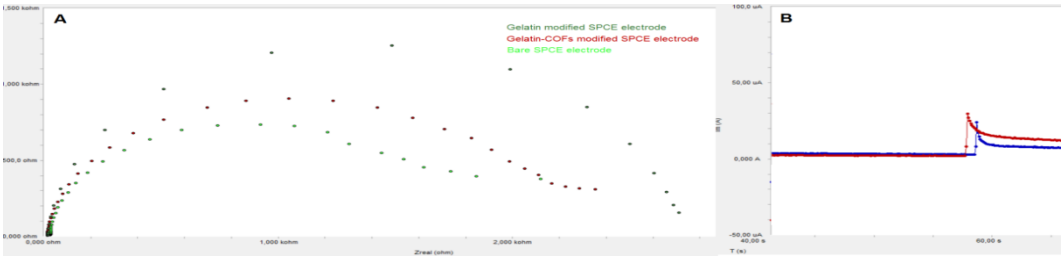

Figure 1: (A) EIS spectra, and (B) Amperometric spectra of gelatine-CTF-1-SOD biosensor.

[1] S. E. Miller, M. H. Teplensky, P. Z. Moghadam, and D. Fairen-Jimenez, *Interface Focus* **6** (2016) 20160027.
[2] X. Q. Wu, J. G. Ma, H. Li, D. M. Chen, W. Gu, G. M. Yang, and P. Cheng, *Chem. Commun.* **51** (2015) 9161-9164.

FL-29

Advanced nanomaterials and nanoparticles for SERS applications

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The SERS (*Surface Enhanced Raman Spectroscopy)* technique has already been applied in the field of Cultural Heritage to study organic substances present in different samples taken from several artistic objects. Various types of silver and gold NPs can be employed as SERS substrates. In particular, Ag nanostars (AgNSs) are prepared using the one-pot synthesis method which involves the reduction of the metallic precursor ($AgNO_3$) by a reducing agent (hydroxylamine) in the presence of a capping agent (trisodium citrate) and additives (NaOH) [1]. Particular attention is given to the pH of the colloid: an acidic pH (≈6.6) prevents the formation of NSs, a slightly basic pH (≈8.1) represents the optimum condition, while a strongly basic pH (≈11.4) generates a polydisperse system composed by NSs and nanospheres. The morphology and size of the NPs are checked through TEM analyses and the optical properties are studied by UV-Vis absorption spectroscopy. Ag nanospheres present one absorption maximum at ≈430 nm while AgNSs absorb in two spectral regions (≈380 and 750 nm) thanks to their starry shape composed of a central core and many tips. Due to this, a stronger enhancement of the Raman effect (≈10^8) is produced. In principle, an even more intense enhancement can be obtained by using hierarchical structures of nanomaterials. To this aim we are studying the possibility to deposit AgNSs on gold nanowire electrodes (AuNWs) to use them as new SERS substrate. The AuNWs can be obtained by templated synthesis in track-etched polycarbonate membranes [2]. After the electroless deposition of gold, the membranes are chemically etched. In this way, it is possible to get 3D structures of AuNWs on which the subsequent deposition of the AgNPs results easier. The final objective of this research project is the detection of protein materials (*e.g.* egg tempera [3]) using special SERS nano-tags*;* these ones should be composed by AgNPs bound to the specific antibody for the target antigen and to a Raman-probe by means of functional thiols.

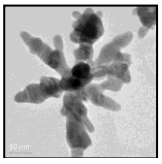

Figure 1: TEM image of one Ag nanostar.

[1] A. Garcia-Leis, J. V. Garcia-Ramos, and S. Sanchez-Cortes, *J. Phys. Chem.* **117** (2013) 7791-7795.
[2] M. De Leo, A. Kuhn, and P. Ugo, *Electroanalysis* **19** (2007) 227-236.
[3] F. Bottari, P. Oliveri, and P. Ugo, *Biosens. Bioelectron.* **52** (2014) 403-410.

Posters

PO-1	Silvia BALDUCCI	**PO-22**	Luca LAVAGNA
PO-2	Serena BARALDI	**PO-23**	Elena LENCI
PO-3	Jennifer BARTOLI	**PO-24**	Federica LEONE
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PO-5	Ginevra BERARDI	**PO-26**	Roberto MANDRIOLI
PO-6	BORGINI / RONZINI	**PO-27**	Marco MASTRODDI
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PO-10	Gabriele CARULLO	**PO-31**	Maria Giulia NIZI
PO-11	Valentina CAUDA	**PO-32**	Nastasja PALOMBI
PO-12	Nicola CHINAGLIA	**PO-33**	Maria Laura PATI
PO-13	Raffaele CUCCINIELLO	**PO-34**	Alessandro PORCHETTA
PO-14	Vito D'ASCANIO	**PO-35**	Emanuele PORRU
PO-15	Mattia DI MARO	**PO-36**	Annalisa REALE
PO-16	Francesco DISTANTE	**PO-37**	Francesco SPINELLI
PO-17	Lucia FALSITTA	**PO-38**	Claudia STEVANIN
PO-18	Placido FRANCO	**PO-39**	Barbara TICCONI
PO-19	Massimiliano GAETA	**PO-40**	Sebastiano TIEULI
PO-20	Alessia GIORDANA	**PO-41**	Leonardo TRIGGIANI
PO-21	Leire IRALDE LORENTE	**PO-42**	Danny ZANARDO

PO-1

Snapshot of ruthenium–carbene–resorc[4]arene complex in an olefin metathesis reaction

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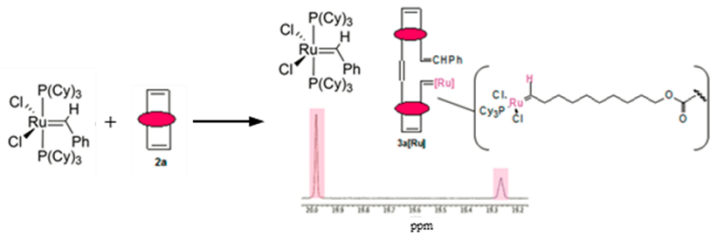
Previously, we envisaged the synthesis of resorc[4]arenes featuring eleven carbon side chains ending with a vinylidene group, in order to incorporate *via* metathesis reaction the macrocycles into polymeric architectures with intriguing mechanical properties[1]. Undecenyl resorc[4]arene **1a**, which featured the simplest pattern of substituent, was submitted to olefin metathesis using the second generation Grubbs complex as the catalyst. Depending on the reaction conditions, different products were isolated: a bicyclic alkene **2a**, a linear dimer **3a**, and a cross-linked homopolymer **P1a** [2]. With regard to the mechanistic pathway, we were able to detect for the first time the formation of a ruthenium-carbene-resorc[4]arene complex during the metathesis reaction of resorc[4]arene olefin **2a** with the first generation Grubbs catalyst in $CDCl_3$, by using high-resolution (600 MHz) ^{1}H, ^{31}P NMR and DOSY spectroscopy [3]. We developed an NMR analytical protocol, which proved capable of yielding both qualitative and quantitative information. In the first case, we were able to identify the complex **3a[Ru]** as a key intermediate in the ROM-CM sequence of reactions, giving us a definitive proof of the previously hypothesized mechanism. As a further feedback of the pathway, we performed a quantitative analysis using benzene in the place of $CDCl_3$, due to the poor stability of the catalyst in such a solvent. The reaction allowed the isolation of decomposition products of the **2a[Ru]** complex, which, due to the presence of still reactive alkene functions, proved to behave as propagating alkylidene species leading to further decomposition products.



[1] C. W. Bielawski, and R. H. Grubbs, *Prog. Pol. Sci.* **32** (2007) 1-29.
[2] F. Ghirga, I. D'Acquarica, G. Delle Monache, S. Toscano, L. Mannina, A. P. Sobolev, F. Ugozzoli, D. Crocco, R. Antiochia, and B. Botta, *RSC Adv.* **3** (2013) 17567-17576.
[3] F. Aiello, F. Balzano, F. Ghirga, I. D'Acquarica, B. Botta, G. Uccello-Barretta, and D. Quaglio, *Eur. J. Org. Chem.* **17** (2017) 2407-2415.

PO-2

Continuous-flow asymmetric benzoin-type condensations in enzymatic microreactors

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The synthesis of (*S*)-phenylacetyl carbinol (PAC) derivatives through enzymatic benzoin-type condensations under batch conditions has been recently reported by our group [1]. Herein we describe the continuous-flow production of PAC and of its analogue phenylpropionyl carbinol (PPC) (Figure 1) using the same enzyme [2] immobilized into a packed-bed microreactor.

The use of enzymes under continuous-flow operational conditions can lead to several advantages, joining the typical sustainability of biocatalyzed processes with the ease of automation and direct scalability of the flow-chemistry reactions. Furthermore, often the covalent immobilization of the enzymes on solid supports and the flow regime preserve the enzymatic activity over time.

After optimization of the process parameters (temperature, reagents molar ratio, flow rate) by means of a design of experiment (DOE) approach, the condensations of benzaldehyde (**1**) with the two different acyl-anion donors **2a** and **2b**, proceeded with complete conversions, high enantioselectivities (>97%) and good productivities (up to 0.32 mmol/day) with a considerable operational stability of the reactor (up to 100 hours).

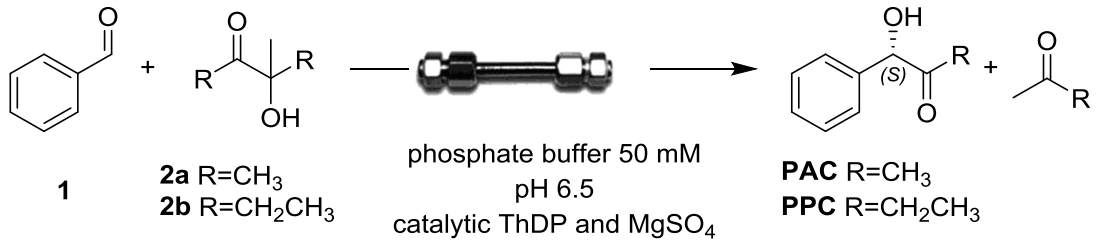

Figure 1: Biocatalyzed cross-benzoin like condensation of benzaldehyde with two different donors in flow mode.

[1] P. P. Giovannini, L. A. Lerin, M. Müller, G. Bernacchia, M. De Bastiani, M. Catani, G. Di Carmine, and A. Massi, *Adv. Synth. Catal.* **358** (2016) 2767-2776.
[2] Acetoin:dichlorophenolindophenol oxydoreductase from *Bacillus Licheniformis*.

PO-3

Bis-vanillin thiosemicarbazones: evaluation of antifungal and anti-aflatoxigenic activity

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Mould contamination of cereals is considered a social emergency. Food deterioration is principally caused by the presence of fungi: Aspergillus genera is in particular the major producer of aflatoxins, secondary metabolites with high carcinogenic potential [1]. Here we present the synthesis of a panel of thiosemicarbazones derived from the bis-vanillin scaffold. The compounds were tested for their antifungal and antiaflatoxigenic activity towards A. Flavus, revealing promising activity. Best hits were also evaluated for their toxic and mutagenic activities on bacteria, human and plants cells.

[1] V. H. Tournas, *Critical Rev. Microbiol.* **31** (2005) 33-44.

This work is supported by Fondazione Cariplo - Project N. 2014-0555, www.aflatox.it

PO-4

Lignocellulosic and biosourced materials for electrochemical energy conversion and storage

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In the last 20 years, the Li-ion battery market has rapidly grown thanks to the extensive diffusion of mobile electronics devices; at the same time, dye-sensitized solar cells emerged as promising low-cost alternatives to silicon devices. In order to lower the cost and reduce the environmental impact of these energy storage and conversion devices, efforts must be devoted to reduce the amount of inactive components in the cell, to substitute synthetic polymer binders/separators and organic solvents with low-cost and biosourced materials and to develop new eco-friendly processes for the manufacture of cell components (both electrodes and electrolyte).
Here we review the use of biosourced materials for manufacturing:

- Bio-inspired all-paper Li-ion polymer cells, constituted by NMFC-binded paper-electrodes, and NMFC reinforced polymer electrolytes. The use of NMFC as filler/binder leads to produce high performing, safe and extremely flexible electrolytes for LiBs. No organic solvents or synthetic polymer binders are used during the entire electrode/electrolyte/cell preparation process.
- Paper-based flexible electrodes and electrolytes for third generation solar cells, useful to lower oil-derived components and typical temperatures used to electrodes processing.

This materials platform is promising not only for the sustainable manufacture of energy devices components [1-3], but also for their processability at the end of life. For example, the all-paper lithium cell can be easily re-dispersed in water by simple mechanical stirring, as well as common paper handsheets and battery materials can be recovered using well-known water-based recycling process.

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[3] L. Zolin, J. R. Nair, D. Beneventi, F. Bella, M. Destro, P. Jagdale, I. Cannavaro, A. Tagliaferro, D. Chaussy, F. Geobaldo, and C. Gerbaldi, *Carbon* **107** (2016), 811-822.

PO-5

Antimicrobial activity of magnetic nanoparticles coated with Syringomycin E

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Bacterial secondary metabolites often show high antimicrobial activity that make them promising drugs to overcome the problem of multidrug resistant pathogens [1]. Moreover, the development of new strategies for drug administration, for instance using nanotechnology, can lead to a more efficient treatment of infections [2].

Syringomycin E (SRE) is an amphiphile compound belonging to the class of lipodepsinonapeptides produced by the phytopathogenic bacterium *Pseudomonas syringae* pv *syringae*. SRE is characterized by a strong antifungal activity against pathogens such as *Candida Albicans* and *Aspergillus Niger* [3].

For the first time, we have functionalized polymer-coated magnetic nanoparticles (MNPs) with this antimicrobial agent. The biological activity of nanosystems was tested against the non-pathogenic fungus *Rhodotorula pilimanae*. Our results demonstrate that SRE-MNPs inhibit fungal growth while bare MNPs don't show any toxic effect. Moreover, the immobilization onto nanosystems does not affect the biological properties of SRE, rather it improves its antifungal activity as compared to that of free SRE.

This approach can pave the way to new efficient treatments of resistant fungal infections.

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[2] L. H. Reddy, J. L. Arias, J. Nicolas, and P. Couvreur, *Chem. Rev*. **112** (2012) 5818-5878.
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PO-6

Design and synthesis of new HIV-1 Reverse Transcriptase dimerization inhibitors

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Since HIV-1 Reverse Transcriptase is an enzyme whose catalytic activity depends on its heterodimeric structure, this system could be a target for inhibitors that perturb the interactions between the protein subunits. We previously demonstrated that the small molecule MAS0 reduced the association of the two RT subunits p51 and p66 and, at the same time, inhibited both the Polymerase and the Ribonuclease H activities [1].

Starting from MAS0 structure we applied docking studies with the aim of exploring *tetrahydropyrimido[2,1-f]purinedione* derivatives as potential leads for developing new HIV-1 RT activity inhibitors. As a result, two compounds showed an improved activity profile against RDDP and RNase H with respect to the starting compound confirming that this chemical family is of interest for the development of novel inhibitors [2].

Based on this result, several derivatives were synthesized in order to improve the biological activity and to extend our SAR knowledge. This study led the basis for the rational design of more potent inhibitors of RT dimerization.

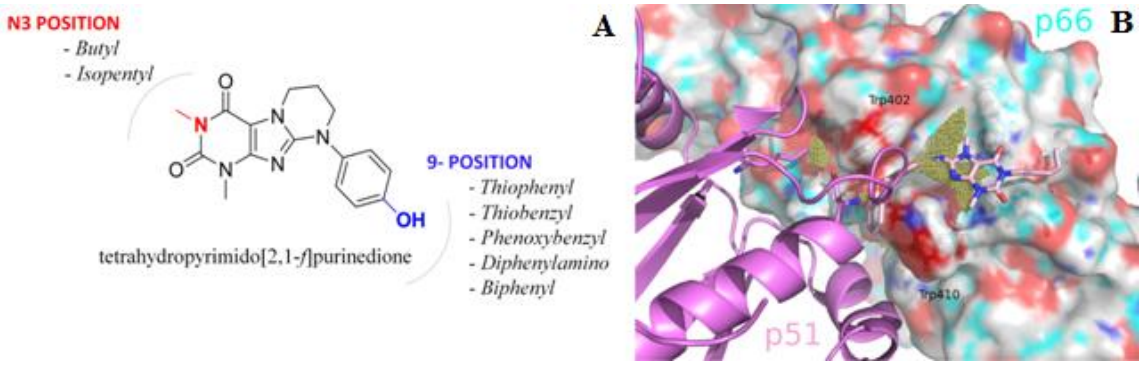

Figure 1: (A)Derivatives of MAS0 and (B) their predicted binding mode.

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PO-7

Pristine, defective and reduced cerium oxide: a hybrid DFT study

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Cerium Oxide (CeO_2) is well known for his oxygen storage capability, which is a consequence of the feasibility of the interconversion between the Ce(IV) and Ce(III) states. The extraction of an Oxygen atom from the solid lefts behind two electrons, which are observed to localize into atomic like 4f states of two Cerium atoms in the proximity of the vacancy: standard DFT approaches fail in describing reduced Cerium Oxide, due to prediction of metallic conducting states instead of localized 4f states [1].

Among the many ways to correct this problem, Hybrid DFT methods are the most promising: PBE0, B3LYP,B1-WC and HSE06 have shown promising results in describing several properties of these oxides [2].

In the last decade a large amount of new hybrid functionals has been developed but, due to the difficulty of an efficient implementation in plane wave based codes, only few of them have been used for solid state applications. In this work we have investigated several structural and properties of CeO_2 and Ce_2O_3 with 26 different Hamiltonians (including 9 Global Hybrid, 8 Range Separated Hybrid, 6 meta-Hybrid, 1 meta-GGA, 1 GGA and Hartree-Fock) to unveil their performance over the two valence states of Ce.

Few selected functionals have then be used to compute the energy of formation of a single vacancy on the most stable surface 111 of CeO_2.

[1] T. Montini, M. Melchionna, M. Monai, and P. Fornasiero, *Chem. Rev.* **116** (2016) 5987-6041.
[2] J. Paier, C. Penschke, and J. Sauer, *Chem. Rev.* **113** (2013) 3949-3985.

PO-8

Internalization of magnetic nanoparticles into macrophages

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Multitasking nanoparticles are promising tools in medicine both in diagnosis and therapy of different diseases [1]. The main problem related to their in vivo administration is the surface coverage with proteins in physiological environment, that lead to a rapid clearance, limiting the activity of nanosystems [2]. In order to overcome this issue, it is possible to use immune-cells as carriers of those nanoparticles, exploiting their natural ability to reach pathological area thought specific cell signaling. In this manner, nanoparticles can be focused in the close proximity of damaged tissues thus allowing a more efficient therapeutic treatment [3].

Our research plan involves the use of macrophage cells to encapsulate and carry different types of functionalized magnetic nanoparticles. The experimental data obtained show that the internalization process takes place efficiently, providing a biologically compatible system for drug delivery.

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PO-9

Laser printed conductive track on biochar-based polypropylene

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Metal free conductive tracks were obtained on Biochar-Polypropylene composites by laser printing technology. Laser printing is an innovative technique that has been exploited for creating conductive paths on the surface of polymeric materials containing a conductive filler like carbon nanotubes (CNTs) [1-3]. To date CNTs are the most established fillers able to enhance the conductive properties of polymeric materials. However, the possibility to replace CNTs with low cost and/or environmental friendly materials is nowadays an attractive field of research from both academic and industrial point of views. Biochar is a solid bio-product derived from the thermochemical decompositions of biomass and it appears as a fine-grained charcoal rich in carbon with graphitic phase. Starting from the biochar characterization, different PP-based nanocomposites have been developed and laser treated according to the laser printing technique. The resulting material contained several distinct and not-interacting conductive tracks embedded on the polymers surface, which demonstrates the possibility of replacing CNTs with cheaper conductive fillers.

Figure 1: Laser treated PP-based composites.

[1] F. Cesano, I. Rattalino, D. Demarchi, F. Bardelli, A. Sanginaro, A. Gianturco, A. Veca, C. Viazzi, P. Castelli, D. Scarano, and A. Zecchina, *Carbon* **61** (2013) 63-71.
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PO-10

After wine: typical white Calabrian grape pomaces as useful source of functional foods

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Vitis Vinifera *L.* is abundantly cultivated in Italy, and mainly used for wine production. The byproduct of wine-making process is grape pomace that is still a rich source of bioactive compounds, exploitable for several uses such as pharmaceutical, cosmetic and nutraceutical ones [1,2].

In this context, selected white Calabrian grape pomaces (derived from indigenous cultivars Pecorello and Mantonico) have been extracted using two different procedures, refluxing with ethanol and ultrasound-assisted extraction. The phytochemical profile of all the extracts was carried out by spectroscopic methods.

The antioxidant capacity of the extracts, was evaluated by DPPH and ABTS assays, and the best samples were used to be incorporated into a pectin polymer, further used to enrich a pear jam.

Stability studies are ongoing to evaluate jam shelf life and *in vivo* assays will be performed to identify promising nutraceutical employments.

Figure 1: An intelligent waste road.

[1] W. P. de Oliveira, A. C. T. Biasoto, V. F. Marques, I. M. Dos Santos, K. Magalhães, L. C. Correa, M. Negro-Dellacqua, M. S. Miranda, A. C. de Camargo, and F. Shahidi, *J. Food. Sci.,* DOI: 10.1111/1750-3841.13841.
[2] V. Georgiev, A. Ananga, and V. Tsolova, *Nutrients* **6** (2014) 391-415.

PO-11

In-vitro evaluation of bioactive and biodegradation properties of mesoporous ZnO architectures

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Currently there is strong interest in the development of smart piezoelectric biomaterials for tissue engineering, where piezoelectricity may actively promote the growth, proliferation and differentiation of cells [1]. Piezoelectric Zinc Oxide (ZnO) materials may be easily prepared in high-surface area structures by several techniques, and captured considerable attention due to their biocompatibility and antibacterial properties [2]. Despite being widely investigated for sensors and energy harvesting applications [3], the study of ZnO-based materials for tissue engineering is still in its infancy. Herein, we propose a preliminary investigation on the in-vitro bioactive and biodegradation behavior of high-surface area mesoporous ZnO layers, after soaking in Simulated Body Fluid (SBF) solution for different times. The ZnO samples were obtained by thermal oxidation of Zn layers sputtered on silicon substrates. The morphology, crystal structure, and chemical composition of the ZnO samples were studied before and after in-vitro tests. Our results show the rapid formation of CaP structures after soaking in SBF for few hours, then resulting into the formation of a CaP-rich layer onto the whole ZnO surface for prolonged soaking times. The mesoporous ZnO architecture was preserved during the overall in-vitro experimental analyses, with negligible release of biodegradation products from the ZnO structure.

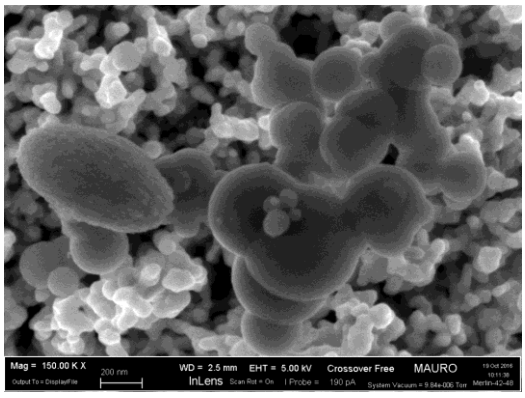

Figure 1: CaP structures formed on the ZnO surface after soaking in SBF.

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PO-12

Functionalization of polystyrene support for solid phase synthesis of oligonucleotides with bile acid moiety

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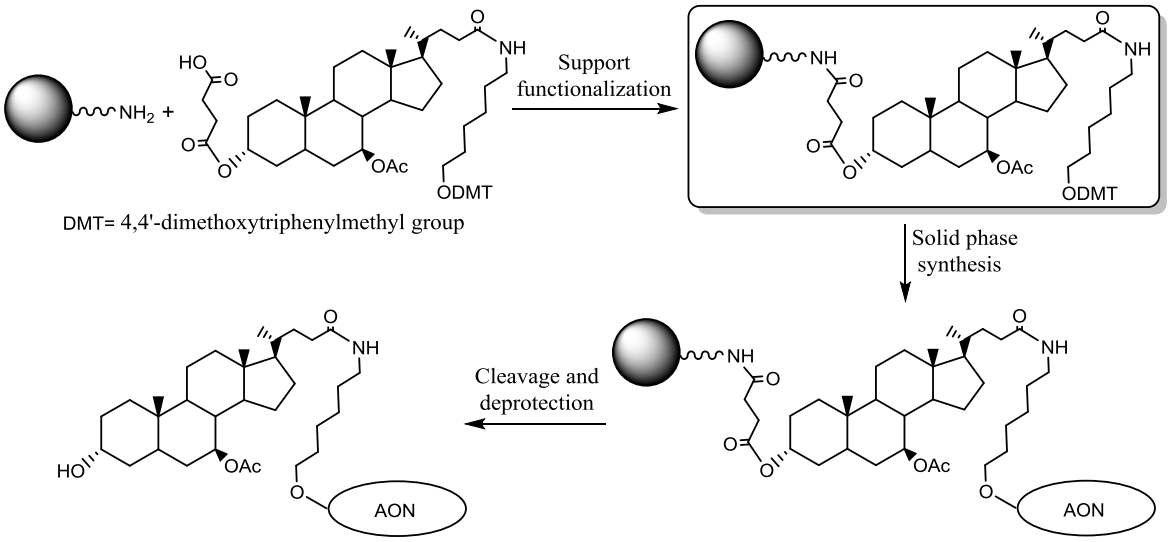
Various approaches are known to conjugate a lipophilic moiety to antisense oligonucleotides (AONs), for increasing some of their properties such as cellular and nuclear uptake, in solution. These methods, however, need industrious multistep synthesis and get low yields [1]. Solid phase synthesis is advantageous respect to in solution one for the easier purification, the higher yield and the possibility to automate the process [2].

In this work, we have functionalized a commercially available polystyrene support with a lipophilic moiety (the opportunely modified ursodeoxycholic acid [3]) and used it for the oligonucleotide solid phase synthesis. Experimental details will be discussed in the poster presentation.



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PO-13

Oxigenated fuel additives from glycidol valorization

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The use of bio-based chemicals and fuels is expected to surpass the products from non-renewable fossil source, as confirmed by recent studies. As a matter of fact, in the last two decades, the development of a green and sustainable chemical industry for the production of bio-based feedstocks has engendered a growing interest of the scientific community that resulted in the impetuous rise of the number of publications in the field.

In this scenario, one of the most investigated field concerns the conversion of glycerol into value-added compounds through catalysis. Indeed, glycerol condensation with acetone to produce solketal (2,2-dimethyl-1,3-dioxolane-4-methanol) represents a promising strategy to obtain a green fuel additive [1].

In this work, we show the preparation of solketal using glycidol instead of glycerol as green starting material. Glycidol is a very reactive molecule with several industrial applications and recent papers refer about its preparation from renewable sources [2,3].

Herein, solketal is prepared with high conversion and selectivity through glycidol reaction with acetone under mild reaction conditions, using several heterogeneous catalysts.

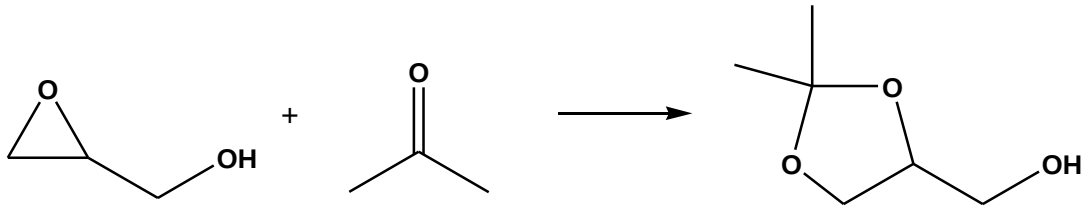

Figure 1: Solketal preparation from glycidol.

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PO-14

Development and *in vitro* efficacy assessment of a new multi-mycotoxins adsorbing additive

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The use of feed additives that reduce animal exposure to mycotoxins is regarded as an effective way to improve animal welfare. According to the European Regulation No.386/2009, mycotoxin adsorbents are intended as nutritionally inert feed additives, which when incorporated into contaminated feeds diminish the absorption of mycotoxins from the gastrointestinal tract, thus preventing or reducing mycotoxicosis in livestock and poultry and carryover of mycotoxins into animal products [1]. Various materials have been tested as mycotoxin adsorbents, and several studies have shown that these materials have high affinity for mycotoxins by the formation of stable linkages which can occur in several liquid systems. However, the main drawback in the use of these additives is that most mycotoxin adsorbents appears to bind to only a limited group of mycotoxins while showing very little or no binding to others. The aim of this work was the development of a new mineral-based material showing multi-mycotoxin adsorption efficacy. Twenty materials including smectites, humic substances (humates), leonardite coals, organic polymers obtained from agricultural by-products were tested for their ability in binding simultaneously AFB_1, ZEA, OTA, FB_1 and DON from liquid buffers simulating gastric and intestinal pH values. Under restrictive experimental conditions, i.e. low adsorbent dosage (0.1% w/v) and high mycotoxin concentration (1 µg/mL), materials adsorbed the mycotoxins of interest with different extent depending on their source and medium pH. All of them did not bind DON. Three materials (an organic polymer and two Na-smectites) adsorbed significant amounts (>70%) of AFB_1, ZEA, OTA and FB_1 at different pH values. Thereof, a two-component mixture containing a sodium smectite and a bio-polymer was prepared and analyzed by equilibrium adsorption isotherms to determine the extension of the adsorption for each mycotoxin/material combination, the strength of the binding, and the equilibrium adsorption parameters (maximum adsorption capacity, adsorption affinity and heterogeneity of the adsorption mechanism). In addition, the effect of adsorbent dosage, pH, and gastrointestinal digestion were assessed. This is the first time that a smectite-based product was found effective in adsorbing *in vitro* several mycotoxins and in reducing the bioaccessible fraction of toxins in the chyme obtained after digestion of a multi-mycotoxins contaminated feed meal.

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PO-15

Preparation and characterization of HDPE/chitosan composites for bone replacement applications

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A study carried out in the Netherlands has reported that the mean rates of infections related to surgery that involves implants are in the range of 1.5% in the case of total knee implantation and 6.8% for femur head replacement, where polyethylene is widely used as cotyle. Such infections result in disease for the patient and prolongation of hospital stay, then increasing cost of care [1]. Chitosan is the second most abundant polysaccharide found in nature after cellulose and it is the most promising bio-based polymer for tissue engineering. Chitosan is nontoxic and shows biocompatibility and antimicrobial properties [2].

In view of preventing the disease arising from infections, this work investigates the study of HDPE composites containing chitosan in different shapes and compositions. The HDPE composites have been prepared by melt extrusion with the aim to achieve materials with good mechanical properties and antimicrobial activity for bone replacement applications. Their thermal behavior has been investigated by means of Thermogravimetric and Differential Scanning Calorimetry analyses. Dynamic-Mechanical Analysis and Scanning Electron Microscopy have provided information about mechanical behavior of the composites and the distribution of the filler within the polymer matrix, respectively.

The authors acknowledge the support from the "Ministero degli Affari Esteri e della Cooperazione Internazionale-MAECI", Joint project n. PGR000701 (2016/2017) and from the Egyptian Science & Technology Development Fund (STDF), Egypt-Italy joint cooperation project no. 25997.

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PO-16

Ring opening polymerization (ROP) of *vic*-disubstituted lactones

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For this work, at first we have studied the acid catalysed lactonization of several γ-hydroxyesters, bearing methyl substituents at different positions.

A ^{1}H-NMR kinetic study of this set of monomethyl and/or gem-dimethyl substituted esters in $CDCl_3$ was carried out. We evaluated the effect of the leaving group (ethyl vs. *i*-propyl ester) and the catalyst efficiency. We found that *i)* a monomethyl substitution produces a lowering of the energy barrier similar to that of a *gem*-dimethyl substitution (Thorpe–Ingold effect), *ii)* the ring closure of *i*-propyl esters is slower than that of ethyl esters, *iii)* strong acids are more efficient than weak acids according to the Brønsted relationship, and iv) the Thorpe–Ingold effect is not just an intrinsic feature of the linear precursor but it depends on the catalyst as well [1,2].

Now, we would like to give an explanation and clarify three issues: *i)* how is the cyclization affected by the vicinal substitution? *ii)* is the effect stereospecific, that is to say, dependent on the diastereomeric relation (*syn* or *anti*) between the two vicinal substituents? *iii)* is it possible to observe a stereospecific effect in the Ring Opening Polymerizaion (ROP) of lactones as well? Preliminaries studies on model compounds indicate that the *vic*-disubstituent effect is not only stereospecific, since the *anti* linear precursors undergo to the cyclisation reaction much faster than the corresponding *syn* diastereoisomers, but it is more efficient than the above mentioned Thorpe-Ingold effect.

Indeed, the *anti* vicinal substituted adduct is faster than the *gem*-disubstituted of about 4 times in the lactonization reaction.

Interesting results are obtained in the ROP process too, in which *vic*-disubstituted δ-lactones show a stereospecific polymerization (in a ratio of around 1 to 5), dependently of the diastereomeric configuration of the monomer.

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PO-17

Human DDX3 protein: a new valuable target to develop broad spectrum antiviral agents

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Targeting a host factor essential for the replication of different viruses, but not for the cells, offers a higher genetic barrier to the development of resistance, may simplify therapy regimens for co-infections and facilitates management of emerging viral diseases. DDX3 is a human host factor required for the replication of several DNA and RNA viruses including some of the most challenging human pathogens currently circulating such as HIV-1, HCV, DENV and West Nile virus. DDX3 has multiple enzymatic activities (ATPase and RNA helicase) and functional domains that may be targeted by potential inhibitors. The first small molecules designed to inhibit the ATPase activity of DDX3 has been identified by our research group [1]. However, the major drawbacks of such ATP-mimetics may be represented by the low selectivity for in vivo treatment, even if some degree of selectivity has been found in in vitro experiments. In a recent work [2], we designed and validated the first small molecule DDX3 inhibitors specifically targeting its RNA binding site. Pursuing this research line, a structure-based optimization process was prosecuted, resulting in the identification of a new family of more potent DDX3 inhibitors [3]. We demonstrated for the first time that the inhibition of DDX3 by a small-molecule could be successfully exploited for the development of a broad spectrum antiviral agent.

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PO-18

Development of supercritical fluid chromatography-atmospheric pressure ionization-mass spectrometry methods for the lipidomic analysis within archaeological finds

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There is an increasing amount of evidence showing that Organic Residue Analysis (ORA) is able to address many archaeological questions about past diets, ancient practices, early use of natural substances, but also vessel production and related use [1]. Most of the organic residue analysis have been performed on absorbed material recovered from archaeological finds, like pots and vessels [2]. Ceramic materials represent an ideal environment for the survival of residual organic matter, because its absorption into the microporous structure prevents from long-term degradation and minimize contaminations [3].

On these basis, this project aim is to develop chromatographic/mass spectrometry methods to identify the organic pyrolysis products that reside within hearths following the cooking of different foodstuffs.

Different instrumental approaches and protocols have been developed to determine the optimal chromatographic and/or mass spectrometric approaches to study a range of expected lipid families.

The developed methods proved to be accurate (bias%<15%), precise (CV%<10%) and with high detectability (down to 1 ng/ml), thus suitable for the analysis of trace level compounds in archeological matrices. The combined use of the SIR detection mode and the high resolution ensured high selectivity and the possibility to discriminate isobaric compounds, species having the same retention time but different m/z ratio and identify molecules whose the corresponding analytical standard is not available.

These protocols have been tested successively for the analysis of residual organic materials produced from a cooking hearth, allowing us to identify food related chemicals whose quali-quantitative composition may represent a biomarker able to provide information related to past human activity.

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PO-19

Polylysine wrapping effect on demetallation-aggregation pathway of ZnTPPS

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Porphyrins are interesting macrocycle due to their intriguing photophysical behaviours in terms of nonlinear optical properties [1]. Nevertheless, their properties can be tuned through the introduction of peripheral substituent groups in meso-positions or the insertion of metals in the core, which are responsible of their aggregation state in aqueous solution [2].

In this respect, Zinc(II) meso-tetrakis-(4-sulfonatophenyl)porphyrin (ZnTPPS) is a metallo-porphyrins widely studied for research field in photocatalysis and solar cells, biochemistry and sensing.

Therefore, water solutions of ZnTPPS are not steady under strong acidic conditions (pH < 4.5) leading to related demetalated/protoned forms (H_2TPPS^{4-}, H_4TPPS^{2-}). In fact, we have previously reported the behavior of ZnTPPS solutions at different pH values, highlighting the role played by polyelectrolytes on the aggregation step after protonation in acid. In particular, we observed that the polylysine affects the overall demetalation/protonation process catalyzing at the same time the formation of J-aggregates [3].

Herein we report a systematic investigation concerning the role of the polylysine chain length on the demetallation-aggregation pathway of ZnTPPS. We anticipate that the increasing of polyelectrolyte length acts as a wrapping for porphyrins, thus affecting the proton transfer kinetic and the self-assembly. Moreover, upon increasing the polylysine chain length, the enhanced interaction between anionic porphyrin and the chiral cationic template is able to induce supramolecular chirality in protonated porphyrins and related J-aggregates.

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PO-20

Microwave-assisted synthesis of tetragonal zirconia

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Zirconia is a versatile and useful inorganic material. We report about a novel microwave-assisted synthesis. ZrO_2 was prepared by sol-gel method starting from Zr propoxide solution, ethanol as solvent and HNO_3 as catalyst: the gel obtained was then dried in a microwave oven. The product has been calcined in a microwave oven using graphite as susceptor.

Zirconia obtained so far is highly crystalline as confirmed by different experimental techniques, such as Raman and FT-IR spectroscopies and X-Ray diffraction. Work is in progress to determinate both BET specific surface area and porosity, as well as the investigation of the morphology by means of HR-TEM.

Tetragonal nanoparticles of ZrO_2 have been obtained by a quick and green procedure assisted by microwave radiations. As already mentioned, ZrO_2-based catalysts can be employed in many different reactions as simple metal oxide, as sulfated oxide or as support for noble metal catalysts, in particular for the transformation/valorisation of lignocellulosic platform chemicals.

PO-21

Human 14-3-3 inhibitors showing interesting activity against Trypanosomatid parasites

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Trypanosomatid parasites are the responsible of some of the most important neglected tropical diseases, including the human African trypanosomiasis (sleeping sickness) and Chagas' disease caused by the parasitesTrypanosoma brucei and Trypanosoma cruzi, respectively. Pentamidine, suramin, melarsoprol and eflornithine are the recommended drugs for the treatment of the sleeping sickness, whereas there are only two drugs available for the treatment of the Chagas disease: nifurtimox and benzidazole.

Currently, there are no vaccines for these diseases and the available drugs are far from ideal, due to lack of efficacy, specificity, acquired drug-resistance and a high toxicity that leads into common side-effects [1]. This makes the need for the identification of novel targets and the development of new, effective drugs even more urgent.

14-3-3 are a family of highly conserved and ubiquitous proteins involved in multiple regulatory activities by interacting with more than 300 cellular partners through an amphipatic binding groove that preferentially recognizes the phosphorylated motifs RSXpS/TXP [2].

In the last few years, a number of small-molecule modulators of the 14-3-3 PPIs have been discovered and characterized. In the Botta group, a compound known as KLDS47 was developed that demonstrated interesting activity as inhibitor of 14-3-3 PPIs [3]. This compound was screened against the intracellular amastigote stage of T. cruzi showing significant potency with low cytotoxicity against mammalian host cells. These findings suggest that 14-3-3 proteins may be exploitable drug targets in these parasites. Here, we report the development of additional analogues of the inhibitor KLDS47 that demonstrate promising anti-trypanosomal activity.

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PO-22

Multiscale composites based on carbon fibers and carbon nanotubes

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The observation of hierarchical structures in nature has shown how great mechanical performances can be achieved by relatively weak constituents if the matter is distributed along multiple length scales [1]. In order to reproduce a biomimetic multiscale material in laboratory [2] pure carbon material have been chosen both for of the intrinsic strength of such materials and for the availability of carbon materials with different length scales (micro and nano). The chemical grafting was performed by dispersing the oxidized nanotubes (CNTs) in acetone by mean of an ultrasound probe, and by pouring the obtained dispersion over the carbon fibers (CFs) drop-by-drop, allowing the solvent evaporation. Then the CF-CNT system was heated in order to create the chemical bonding, finally the thermally treated fibers were washed with water and dried. The composite preparation was done by tape casting technology using a polyvinyl butyral matrix and modifying the type and content of the fillers: at first, only CFs or CNTs in different concentrations in order to asset the properties of the single filler; secondly, a physical mixture of CFs and CNTs; finally, the mixture of CFs and CNTs with hierarchical structure. The composite tapes were cut into specimens that underwent tensile testing. Further characterizations were done by optical microscopy and SEM observation of the fracture surfaces.

The work allowed the assessment of mechanical properties and the collection of a wide and statistically sound range of data that is possible to consider reliable for modelling purposes, both because of the rigorous methodology followed in preparation and testing and because of the matching between the collected data and the ones expected by theory.

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PO-23

Design and synthesis of Beta Secretase (BACE-1) inhibitors for the diagnosis and treatment of amyloid plaques in the Alzheimer's disease

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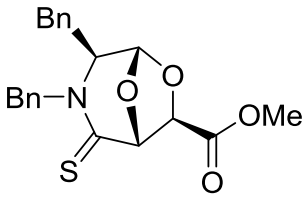
Alzheimer's Disease (AD) is the most common cause of dementia in older people, consisting of a chronic and progressive neurodegenerative disorder. Much of Alzheimer's Disease (AD) research has investigated the amyloid cascade hypothesis, which postulates that AD is caused by changes in amyloid beta (Aβ) stability and aggregation. Blocking Aβ production by inhibiting the first protease required for its generation, Beta Secretase (BACE-1) may be effective in blocking AD progression [1].

Taking advantage of the structural similarity between aspartic proteases, a library of bicyclic acetal thiolactams, containing the 6,8-dioxa-3-azabicyclo[3.2.1]-octane peptidomimetic scaffold, were synthesized and assayed towards BACE-1 enzyme. This study allowed for the identification of compound **1** (Figure 1) with potency in the low micromolar range, thanks to the interaction of the acetal moiety with the catalytic diad of the enzyme and through C@S hydrogen-bond with the flap region [2]. Even if this compound will need further investigation and structure refinement, these results are promising for the development of novel BACE-1 inhibitors based on this peculiar molecular scaffold.



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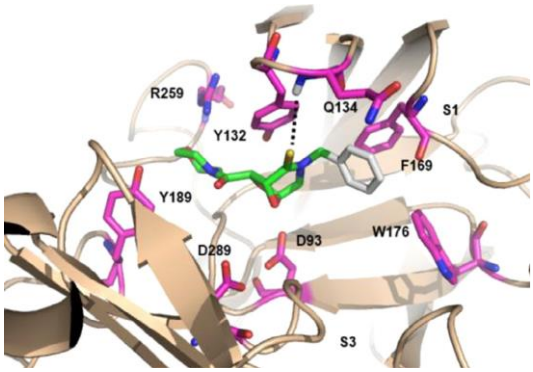

Figure 1: Bicyclic acetal thiolactam **1** docked into the active site of BACE-1.

[1] Y. Luo, B. Bolon, S. Kahn, B. D. Bennett, S. Babu-Khan, P. Denis, W. Fan, H. Kha, J. Zhang, Y. Gong, L. Martin, J. C. Louis, Q. Yan, W. G. Richards, M. Citron, and R. Vassar, *Nat. Neurosci.* **4** (2001) 231-232.
[2] R. Innocenti, E. Lenci, G. Menchi, A. Pupi, and A. Trabocchi, *Bioorg. Med. Chem.* **25** (2017) 5077-5083.

PO-24

An organic-solvent-free route to obtain nanostructured zinc oxide-based reservoir of clotrimazole

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An organic-solvent-free route to obtain nanostructured zinc oxide (NsZnO) reservoir of clotrimazole was studied. Two different NsZnO materials were synthesized, selecting wet chemical approaches without any organic solvents: chemical bath deposition and a soft-template sol-gel method.

For the first time, loading of clotrimazole (CTZ) in a ZnO carrier by impregnation using supercritical CO_2 as solvent was studied. The NsZnO materials were characterized, before and after drug loading, by FESEM, XRD, nitrogen adsorption isotherms, TGA, DSC, in order to elucidate their morphological and physico-chemical properties.

CTZ was dispersed in the NsZnO carrier in amorphous form, with a maximum loading of 17 % w/w. In vitro drug-release was investigated, revealing that the NsZnO carriers can deliver clotrimazole, ensuring a fast release of a larger drug amount when compared to the solid crystalline drug. This might play a key role in several biological applications where the bioavailability of poorly-water-soluble drugs is still a challenging issue.

PO-25

Alendronate doped diatoms as bone regeneration scaffold

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Bisphosphonates are drugs used to treat pathologies characterized by bone destruction such as osteoporosis, Paget's syndrome and bone tumors [1]; despite their use is frequent in industrialized countries, there are several side effects associated to bisphosphonate uptake such as cancer and osteonecrosis. Therefore a delivery in situ, on the damaged area, would reduce the drug dose needed to have an effect and consequently the side effects. Various scaffolds, especially mesoporous materials, are proposed as bone fillers, also conjugated with drugs [2].

In this work sodium alendronate, a second generation bisphosphonate, bone disruption inhibitor, is immobilized on natural silica nanostructures from diatoms algae with an in vivo feeding process. Diatom are unicellular eukaryotic microalgae, able to produce a hierarchically organized nanostructured and mesoporous biosilica shells (frustules).

It has already been shown how frustules can be easily conjugated to drug molecules [3]. Here we demonstrate the in vivo alendronate functionalization frustules, via FTIR, SEM-EDX and TGA; it is also shown that the presence of alendronate on the biosilicica nanostructure makes it an attractive biomaterial capable of increasing the vitality of osteoblast-like cells while inhibiting osteoclastic ones.

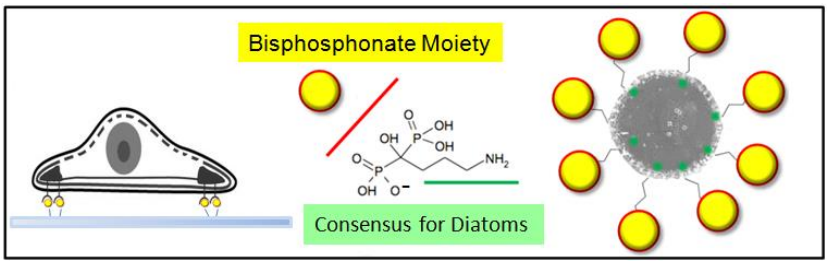

Figure 1: Schematic representation of doped diatoms and osteoblast adhesion.

[1] R. G. G. Russell, *Bone* **49** (2011) 2-19.
[2] P. Tengvall, B. Skoglund, A. Askendal, and P. Aspenberg, *Biomaterials* **25** (2004), 2133-2138.
[3] S. R. Cicco, D. Vona, E. De Giglio, S. Cometa, M. Mattioli-Belmonte, F. Palumbo, R. Ragni, and G. M. Farinola, *ChemPlusChem* **80** (2015) 1104-1112.

PO-26

Application of microsampling techniques to the enantioselective determination of asenapine in human blood and plasma

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Microsampling represents a significant improvement in biosampling, in particular for clinical analysis and Therapeutic Drug Monitoring (TDM). Haematic dried micromatrices are highly stable even when stored at room temperature, safer to handle and less invasive than traditional ones (whole blood and plasma). This aspect results in an attractive and patient-friendly option towards vulnerable population groups such as psychiatric patients. In this work, four different dried micromatrices were studied, two based on dried matrix spots (DMS) – dried blood spots (DBS) and dried plasma spots (DPS) – and two based on volumetric adsorptive microsampling (VAMS™) – VAMS-blood and VAMS-plasma. The former ones consist in the blotting and drying of blood or plasma on dedicated paper supports, while the latter ones use a recently conceived device whose porous polymeric tip absorbs a fixed sample volume (10-20 µL). The microsampling, drying and extraction procedures were optimised for each matrix (absolute recovery > 75%, precision RSD < 6.8%), to be applied for the quali-quantitative determination of asenapine, one of the most recent antipsychotic and anti-bipolar drugs [1]. Being asenapine a chiral compound, an enantioselective analytical method based on LC-DAD-MS/MS was developed to determine the plasma and blood levels of each enantiomer. A cellulose-based column with a tris(3,5-dimethylphenylcarbamate) selector was used as the stationary phase, while the mobile phase was a mixture of aqueous ammonium bicarbonate and acetonitrile, obtaining complete enantiomer resolution (R_s > 1.0). The analytical method is being applied for TDM purposes to microsamples from patients undergoing therapy with asenapine, and the results are compared with those obtained from traditional matrices (blood, plasma), with satisfactory results: analyte levels found in DMS and VAMS are in the 92-104% range when compared to those in the corresponding macrosamples.

[1] R. Mandrioli, M. Protti, and L. Mercolini, *Curr. Drug Metab.* **16** (2015) 141-151.

PO-27

Biological effects of RF-WiFi irradiation on gluthatione redox reactions

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In recent years, data on the connection of organic causes with chronic oxidative damage have progressively increased and can be a key factor in the induction of the functional syndromes found in patients affected by multiple chemical sensitivity (MCS) and electromagnetic hypersensitive (EHS) [1]. Alterations in enzymatic catalysis of glutathione oxidase and/or glutathione reductase is related to changes in glutathione concentration in the blood, that could plausible cause an insufficient detoxification from free radicals, resulting in an increase of the oxidative stress. The chronic exposure to RF could be correlated to modifications of enzymatic activities [2], [3].

As already demonstrated in animal studies [1], our in vitro experiments have shown that RF Wi-Fi exposure modify the structures of these enzymes and their kinetics of red-ox processes, involving both the oxidized and reduced forms of glutathione. These experimental evidences could suggest that the exposure to RF Wi-Fi could affect glutathione concentrations and consequently increase free radicals damages.

These preliminary results on simple models could be useful for a better understanding of the effects of RF exposure at molecular level.

[1] C. De Luca, J. C. S. Thai, D. Raskovic, E. Cesareo, D. Caccamo, A. Trukhanov, and L. Korkina, *Mediat. Inflamm.* **2014** (2014) 924184.
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[3] M. Barteri, A. Pala, and S. Rotella, *Biophys. Chem.* **113** (2005) 245-253.

PO-28

Physical-chemical characterization of sea-silk and its crafting phases

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The sedentary mollusc *Pinna nobilis* L. produces fine but strong filaments of fibre beard called "byssus". This fibre has the task of fixing itself to the sea grass and withstand the flow. Byssus was the basic raw material used to make Sea-silk, but this Mediterranean species is protected since 1992 [1] and production of its iridescent golden textile is therefore impossible. In the history of textile, Sea-silk constitutes a very small part, it is proven that the use of Sea-silk dates back to at least the Roman age while, today, Sardinia and Apulia (Taranto), are the production centres of Sea-silk and keep their importance. We studied samples of sea-silk kept at Commodity Science Museum of Bari University, where one valve, some pearls and all the different phases of crafting of this textile are represented, starting from the raw byssal threads up to the woven textile. The aim of this research is to characterize the threads from a morphological and chemical point of view considering above all the evolution and changing of the material with the different working phases. Due to the samples uniqueness, the smallest amount possible is taken from the byssal threads (about 20 mg). We used different techniques like optical microscopy (OM) and Scanning Electron Microscopy coupled with Energy Dispersive Spectroscopy (SEM-EDS) aimed to the observation of the morphological changing of the fibers examined in their different handmade production steps and ICP-MS for the determination of metal composition in some fibers after their mineralization and in deionized water, observing the metal lost characteristic of the desalination process. The results obtained show how the metal concentrations analysed, decrease after the different crafting steps, and the fiber of the Sea-silk change its microscopic aspect until to obtain the golden "soul of the sea".

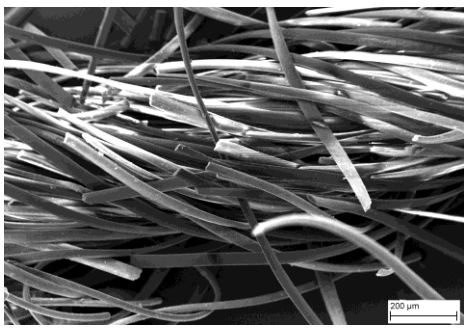

Figure 1: SEM-SE photomicrograph of spun byssus fiber.

[1] http://www.muschelseide.ch/it/biologie/byssus/faseranalyse.html

PO-29

Theoretical insights into the switch off/on $^1O_2$ photosensitization in chemicontrolled photodynamic therapy

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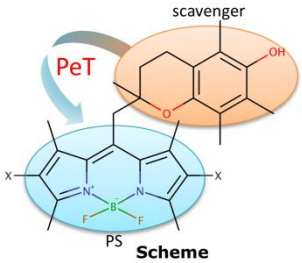
PDT is emerged in the last years as promising cancer therapy for its efficiency in cell death induction and high selectivity for tumour cells. However, several strategies have been proposed to further minimize undesired side effects and increase the specificity to target cells controlling at different levels the photosensitization of $^1O_2$. In this field, the chemical activation of the photosensitizer (PS) selectively in the target tissues has recently emerged as effective control of highly reactive species production demanded to achieve the cells death [1]. This strategy provides the administration of an activatable-photosensitizer (aPS) that can be turned on directly in the target tissues by a wide variety of molecular stimuli. Generally, an aPS increases singlet oxygen generation upon activation and irradiation, while does not display significant toxicity in their dormant state when irradiated. Therefore, only when the photosensitizer reaches the diseased cells, where its molecular activation occurs, and when light is locally applied, the singlet oxygen can be generated and target cells selectively destroyed.

Recently a ROS-aPS has been synthesized by combining the free radical scavenging action of the chromanol ring of α-tocopherol with the photosensitization ability of a Br-substituted BODIPY dye (Scheme). In order to get more insight into the processes that could take part in the deactivation/activation of the $^1O_2$ photosensitization, a systematic theoretical study of the photophysical properties has been undertaken. For this purpose, DFT and TD-DFT methods have been used to characterize ground and excited states properties [2].



Scheme

[1] A. M. Durantini, L. E. Greene, R. Lincoln, S. R. Martínez, and G. Cosa, *J. Am. Chem. Soc.* **138** (2016) 1215-1225.
[2] J. Pirillo, G. Mazzone, and N. Russo, *submitted*.

PO-30

Mo doped TiO_2 nanoparticles for photocatalytic dye degradation

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TiO_2 anatase is a very promising photocatalyst and has been extensively studied. Transition metal ions doping not only affects the band gap, increases the optical absorption in visible range, but also leads to change in the oxidation state and redox potentials as well as structural parameters, which play a primary role in the photocatalytic activity [1]. Among them molybdenum based catalysts have shown promising activity because of the low oxidation potential and high Lewis acidity in the highest oxidation state [2]. Inverse micelle sol-gel method was used to produce mesopourus MoO_x-TiO_2 nanoparticles (~20 nm) of multiple compositions (1, 5 and 10 %w Mo/(Mo+TiO_2)) with a surface area of around 100 m^2/g. The photocatalyst material was characterized by means of diffuse reflectance (DR-UV−Vis spectroscopy), X-ray photoelectron spectroscopy, X-ray diffraction, Raman spectroscopy, N_2 adsorption measurements, temperature-programmed reduction and electron microscopy. Photocatalysis experiments were conducted using a model rhodamine-B (Rh−B) dye reaction using visible irradiation source. Results shows that fast photodiscoloration of this dye can be achieved using the synthetized nanomaterial under visible light (Fig. 1).

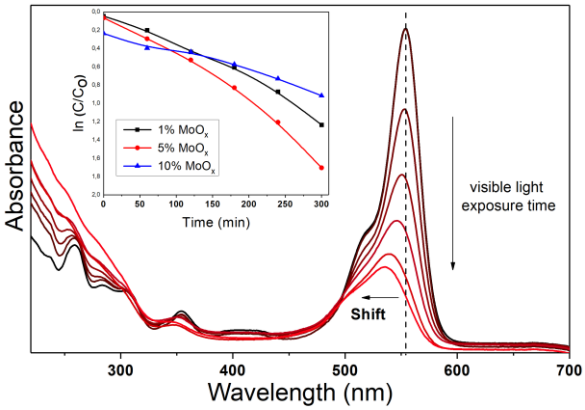

Figure 1: Photoabsorbance spectra of Rh-B *vs* time; inset kinetic curves.

[1] M. R. Hoffmann, S. T. Martin, W. Choi, and D. W. Bahnemann, *Chem. Rev.* **95** (1995) 69-96.
[2] J. Tang, B. Kong, Y. Wang, M. Xu, Y. Wang, H. Wu, and G. Zheng, *Nano Lett.* **13** (2013) 5350-5354.

PO-31

2-phenylquinoline C-6 position functionalization by alkoxyamino chains to obtain new *Staphylococcus aureus* NorA efflux pump inhibitors

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Antimicrobial resistance is nowadays one of the most important health threat owing to the large misuse of antibiotics in controlling bacterial infections. Focusing our attention on Gram-positive bacteria, *Staphylococcus aureus* strains resistant to various classes of antibacterials are arising, thereby making *S. aureus* infections difficult to treat [1].

Since discovery of new antibacterials is hampered by a rapid insurgence of resistance, breaking the resistance mechanisms with a helper compound could be a good strategy to restore drug sensibility in resistant strains.

Among the resistance mechanisms, the overexpression of efflux pumps plays an important role. NorA, the most common efflux pump in *S. aureus*, is responsible for the extrusion of common antibacterials. Therefore, NorA efflux pump inhibitors (EPIs) could restore antibiotic activity.

Previously, we reported a series of 2-phenylquinoline derivatives as potent NorA EPIs [2] and recently, we optimized them by the introduction of a methoxy group in C-6 position of 2-phenylquinoline scaffold. To further improve this class of NorA EPIs, in this work, we explored the introduction of different chains at C-6 position of the quinoline nucleus.

Thus, we obtained 2-phenylquinoline derivatives bearing on the "oxygen" in C-6 position different alkylamino chains (Figure 1). Derivatives were tested in ethidium bromide (EtBr) assay in *S. aureus* strain overexpressing *norA* gene. Compounds with no antibacterial effect and endowed with an EtBr efflux inhibition ≥80% were then assayed in synergism with ciprofloxacin against different resistant *S. aureus* strains. Results of this study will be presented.

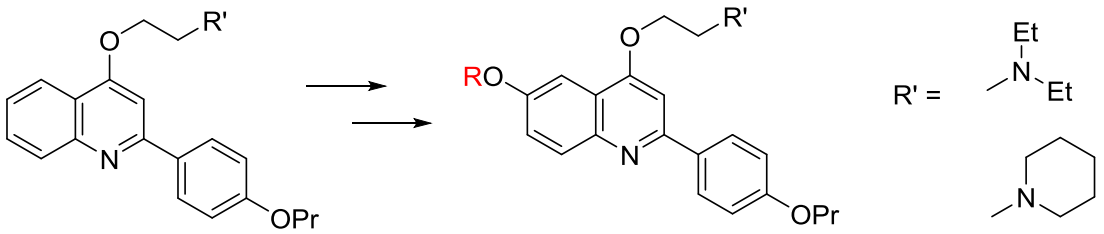

Figure 1: Optimization of 6-methoxy-2-phenylquinoline derivatives.

[1] L. J. Piddock, *Lancet Infect. Dis*. **12** (2012) 249-253.
[2] S. Sabatini, F. Gosetto, N. Iraci, ML. Barreca, S. Massari, L. Sancineto, G. Manfroni, O. Tabarrini, M. Dimovska, G. W. Kaatz, and V. Cecchetti, *J. Med. Chem*. **56** (2013) 4975-4989.

PO-32

Targeting both the hydrophobic pocket and the *N*-terminus domain of HIV-1 Nucleocapsid protein: synthesis and optimization of new inhibitors

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The Nucleocapsid protein (NC) is a highly conserved protein in HIV-1 several subtypes that play a pivotal role in virus replication, mainly by interacting with conserved nucleic acid sequences. NC is considered a highly profitable target, able to inhibit multiple steps in the HIV-1 life cycle with just one compound, a unique property not shown by any of other antiretroviral classes [1,2].

From a multidisciplinary strategy based on molecular simulations, NMR studies, antiviral assays and organic synthesis a validated NC inhibitor, targeting the NC hydrophobic pocket, (AN3) has been identified and has been modified in order to discover new NC inhibitors able to interact both with the hydrophobic pocket and the N-terminus domain [3].

A chemistry oriented approach led to the identification of compounds that showed an increase of the *in vitro* antiviral activity with IC_{50} values in the micromolar range and sustained NC inhibition.

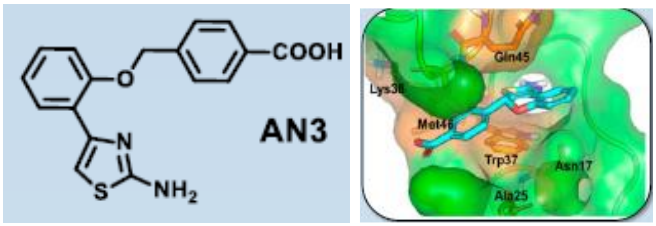

Figure 1: AN3 structure and binding of AN3 to NC.

[1] R. J. Gorelick, T. D. Gagliardi, W. J. Bosche, T. A. Wiltrout, L. V. Coren, D. J. Chabot, J. D. Lifson, L. E. Henderson, and L. O. Arthur, *Virology* **256** (1999) 92-104.
[2] M. Mori, L. Kovalenko, S. Lyonnais, D. Antaki, B. E. Torbett, M. Botta, G. Mirambeau, and Y. Mély, *Curr. Top. Microbiol. Immunol*. **389** (2015) 53-92.
[3] M. Mori, A. Nucci, C. Dasso Lang, N. Humbert, C. Boudier, F. Debaene, S. Sanglier Cianferani, M. Catala, P. Schult Dietrich, U. Dietrich, C. Tisné, Y. Mely, and M. Botta, *ACS Chem. Biol.* **9** (2014) 1950-1955.

PO-33

The concomitant effect of anti-MM drugs in combination with COX inhibitors

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Two cyclooxygenase (COX) isoforms produced by different genes have been identified, COX-1 and COX-2. Starting from arachidonic acid (AA), this enzyme is responsible for the bio - synthesis of prostaglandins (PGs) important mediators implicated in inflammation, angiogenesis and solid tumors growth [1,2]. The involvement of COX in tumorigenesis is ascertained but their role in hematologic malignancies, particularly, in Multiple Myeloma (MM), an incurable plasma cell cancer, has been little investigated. COX inhibitors have shown to be immunotherapeutic agents in several malignancies, including hematological tumors and MM. Some study proven the usefulness, in the treatment of MM, of non-steroidal anti-inflammatory drugs (NSAIDs) with a different grade of selectivity in the inhibition of the two COX isoforms. Therefore, in order to clarify the role of cyclooxygenase in MM, we investigated the expression at the protein levels of COX-1 and -2 in in six different human myeloma cell lines (KMS-12-BM, MM1R, NCI-H929, RPMI-8226, SK-MM-2, and U-266). Furthermore, we evaluated growth inhibitory effects of selective COX inhibitors (SC-560, Mofezolac, as selective COX-1 inhibitors, Celecoxib, as a selective COX-2 inhibitor, and Aspirin, Ibuprofen with a different grade of selectivity towards COX isoforms, Fig. 1) on myeloma cells as chemotherapeutic agents in combination with usual anti-MM drugs (i.e., dexamethasone, bortezomib and thalidomide).

The work here presented is financially supported by First AIRC Grant-MFAG2015 (Project Id. 17566).

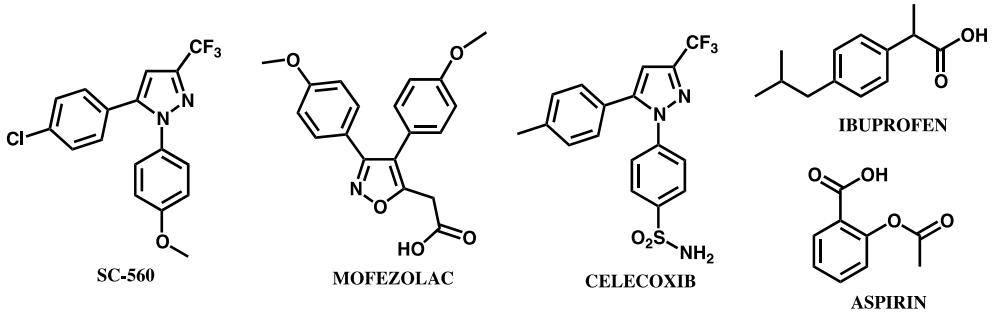

Figure 1: COX inhibitors.

[1] R. Salcedo, X. Zhang, H. A. Young, N. Michael, K. Wasserman, and W. H. Ma, *Blood* **102** (2003) 1966-1977.
[2] M. G. Perrone, A. Scilimati, L. Simone, and P. Vitale, *Curr. Med. Chem.* **17** (2010) 3769-3805.

PO-34

Supramolecular antibody-templated assembly of an RNA mimic of green fluorescent protein

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A synthetic RNA aptamer, called Spinach, has been recently proposed as an alternative to Green Fluorescent Protein for real-time imaging, detection of cellular metabolites, and tracking of dynamic bio-processes [1]. Such RNA GFP-mimic aptamer is able to specifically bind to a synthetic copy of the natural GFP fluorophore, which leads to displaying of GFP-like fluorescent properties. Here we demonstrate for the first time a supramolecular mechanism in which antibodies are used to template the assembly of a split Spinach aptamer. To do this, we have employed two antigen-tagged RNA strands that, upon binding to a specific target antibody, are co-localized in a confined space and re-assemble into the functional Spinach aptamer, yielding a measurable fluorescence signal emission as function of the templating antibody concentration. We have demonstrated the generality of our approach using two different antigen/antibody systems and found that both platforms are sensitive, specific and selective enough to work in crude cellular extracts.

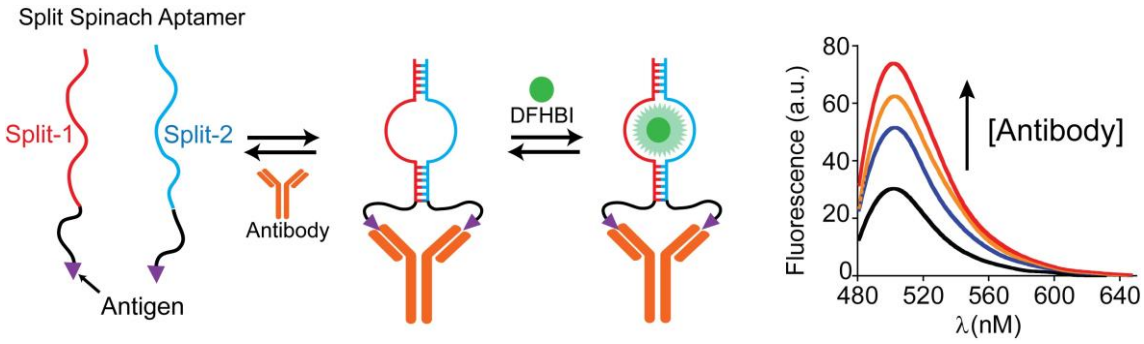

Figure 1: Inspired by complementation-based assay mechanism we report here an antibody-templated assembly of the Spinach aptamer, an RNA-mimic of GFP. In this strategy the spinach aptamer is ideally cut into two segments, (red and blue in the figure) and each of the two fragments is conjugated with a recognition element (antigen) specific for a target antibody. Only in the presence of the antibody the two fragments are co-localized in a confined volume and assemble into the functional Spinach aptamer, which, by binding the fluorophore DFHBI, provides a GFP-like fluorescence signal.

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PO-35

Determination of bile acids by LC-ES-MS/MS in permeability studies through biological membranes using Franz cell model

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Bile acids (BAs), in particular chenodeoxycholic acid (CDCA) and cholic acid (CA), can regulate the expression of genes involved in their synthesis, thereby, creating a feed-back loop. The intestinal adsorption of BAs plays a key role on their homeostasis. It is generally considered that the BA physico-chemical characteristics are the most crucial factors contributing to their partition, permeation and diffusion. BAs as detergent-like compounds self-aggregate to form micelles with phospholipids and cholesterol and therefore BAs could be present in the biological fluids and compartments as distinct species, such as neutral/ionized monomer, simple BA micelles, mixed micelles, monomer-protein complex, monomer-receptor complex, all of these equilibria modulated by the pH and ionic strength. Moreover, additional thermodynamic interactions with binding proteins and specific receptor, for example the farnesoid X receptor (FXR) for which the BAs are physiological ligands, are involved in the net permeation process. To define the species involved, a previously developed HPLC-ESI-MS has been applied to the permeation study through porcine ear skin membranes of BAs with different physico-chemical properties [1]. These studies have been performed using Franz diffusion vertical cells, which allowed the measurement of the BA permeability as a function of the pH, initial concentration and ionic strength. Data show that a BA with a high LogP, such as deoxycholic acid (DCA) and CDCA, present a delayed clearance from the tissue due to a strong interaction with its lipid domain. An intermediate LogP, such as for CA, allows a more efficient and faster permeation process. Modeling, understanding and characterizing the permeation process of BAs with different structure and physicochemical properties through various biological membrane barriers and tissue is essential to predict the *in vivo* behavior and to explain their absorption mechanism.

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PO-36

Syinthesis of imidazole-binding cinnamic derivatives with fluorogenic properties

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In biochemistry, fluorogenic labeling methods emerged as more promising approach to study protein interactions and function [1].

In order to obtain new fluorophores potentially useful in imidazole labeling, a small series of Morita-Baylis–Hillman acetates (3a-c) was synthesized and made to react with imidazole to obtain the corresponding Imidazole-Binding Cinnamic Derivatives (IBCD) 4a-c, which were characterized by the point of view of their optical properties.

Interestingly, the introduction of the electron donor methoxy groups in the cinnamic scaffold of 4c should increase the push-pull character of the scaffold [2], showing emission intensity higher in the solid state than in solution, as it generally occurs in a typical aggregation-induced emission (AIE) phenomenon [3].

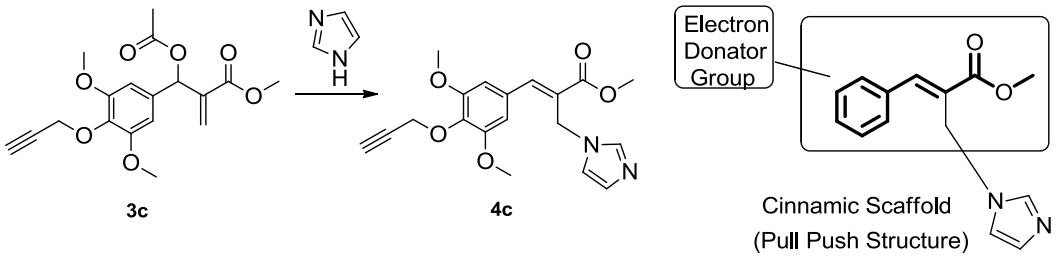

Figure 1: Design of IBCD 4c. The bold lines highlight the common cinnamic scaffold in the fluorophores.

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PO-37

In vitro and in vivo evaluation of [^{11}C]PB212 as radioligand for PET imaging of sigma-1 receptors

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Sigma-1 receptor (σ_1) is a chaperon protein expressed both in the central nervous system and in the periphery and mainly localized at the endoplasmic reticulum, but also at the plasma membrane and nuclear envelope [1]. It regulates the function of a plethora of proteins, enzymes and ion channels, and many endogenous (e.g., steroids) and exogenous ligands (e.g., neuroleptics, drugs of abuse, etc.) have been found [1]. Taken all these features together, σ_1 is a *pluripotent modulator* involved in many physiological pathways with pivotal roles also in some central and peripheral pathological disorders [1]. For instance, knocking-down of σ_1 has been associated with neurotoxic effects and neurodegeneration [1]. Furthermore, σ_1 overexpression has been found in several tumor cell lines and tumor tissues [2]. Although this important information, much remains still unclear regarding σ_1 involvement in physiological and pathological conditions, and PET imaging could be a powerful tool in this regard.

On these bases, we performed the carbon-11 radiolabelling of PB212 (1-(4-(6-methoxynaphthalen-1-yl)butyl)-4-methylpiperidine), a high-affinity and selective σ_1 ligand developed by our group (K_i = 0.030 nM, SI $_{\sigma2/\sigma1}$ = 597) [3], and *in vitro* and *in vivo* experiments were carried out to evaluate the suitability of [^{11}C]PB212 as radioligand for PET imaging of σ_1 both in the CNS and in the periphery. *In vitro* autoradiography on brain tissues showed binding of the radioligand both in WT and σ_1 KO mice, indicating that the binding to brain tissue is mainly nonspecific. Contrariwise, [^{11}C]PB212 binding to the spleen (one of the peripheral tissues where σ_1 is highly expressed) was confirmed to be specific both in *in vitro* autoradiography and *in vivo* PET imaging blocking experiments using two well-known σ_1 ligands as blockers (haloperidol and fluspidine). This result, that deserves to be deepened (for example in animal models of cancer), suggests [^{11}C]PB212 as a probe for σ_1 detection in peripheral organs by PET imaging.

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PO-38

Photocatalytic degradation of organic pollutants in aqueous solution by heterogeneous sodium decatungstate

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In view of the rising world industrialization paralleled by the increment of world population, the re-use of wastewaters will be necessarily an increasing practice, bringing potential health risks due to the presence of highly toxic organic pollutants. In particular, the contaminants of emerging concerns, were proved challenging for conventional wastewaters and recycled water depuration treatments.

This work is focused on photocatalytic method for photodegradation of organic contaminants from water. The photoactive species is decatungstate anion, having light absorption properties similar to those of TiO_2. An important advantage in the use of the polyoxoanion is that it can be immobilized on different solid supports with tunable and desired characteristics, such as hydrophobicity, pore size, surface areas, etc [1].

The target molecules were selected for being some of the most representative contaminants: atenolol and propranolol, levofloxacin, trimethoprim and sulphametoxazol, carbamazepine. The main aim of this work is twice: i) exploitation of the adsorption ability of the solid support that transfers the pollutant from water to a new solid phase that contains also the photocatalyst; ii) estimation of the degradation efficiency of the pollutant concentrated in the solid matrix by the photocatalytic activity of decatungstate. Different kinds of solid supports have been employed: silica particles modified with aminopropyl-silane groups and microporous silicas, ion-exchange resins.

Heterogeneous photocatalysts are stable and can be recycled several times without a significant loss of efficiency, thus opening the possibility of developing new solid materials with interesting photocatalytic performance.

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PO-39

Importance of π-stacking interactions in the hydrogen atom transfer (HAT) reactions from benzylic C-H bonds to short-lived *N*-oxyl radicals

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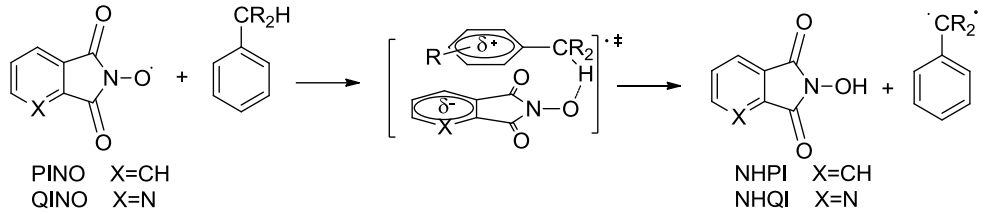
Hydrogen atom transfer (HAT) from benzylic C-H bonds to short-lived *N*-oxyl radicals such as the phthalimide-*N*-oxyl radical (PINO) and the quinolinimide-*N*-oxyl radical (QINO) are characterized by a significant degree of charge-transfer deriving from π-stacking interactions between the substrate and the *N*-oxyl aromatic rings in the transition state [1].



An increase of the HAT reactivity by addition of Brønsted or Lewis acids was observed with both PINO and QINO in the reactions with a series of benzylic substrates, as a result of the stabilizing interaction of the □ -stacked HAT transition state with PINO and by effect of protonation or complexation of the pyridine nitrogen with QINO.

These examples show that reactivity and selectivity in the aerobic oxidations catalyzed by *N*-hydroxyimides can be controlled by changing the structure of the *N*-oxyl radical or the reaction medium thus widening the synthetic versatility of the HAT process.

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PO-40

"ELPIS" - Enhancement of Lignocellulose Processing for Innovation and Sustainability

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Wood has high potential as a raw material for biorefineries as it is one of the most abundant renewable sources of lignocellulosic materials in the world. Cellulose, hemicelluloses, and lignin are the main macromolecular structural components of wood and, among these, lignin holds the greatest potential to be transformed into lower molecular weight compounds, which possess high potential to replace fossil resources [1]. Bearing this in mind, the aim of this study is the development an effective and sustainable process for abundant grapevine wood waste biomass valorisation (not yet exploited for this goal) to obtain biodiesel or fuel additives.

The work was devoted to optimize efficient, sustainable and scalable hydrotreating processes of hydrolysed lignin. The attention was focused on non-noble metal (e.g. Ni or/and Co) catalysts supported on high surface area solid acid materials. Metal particles promoted on Sulphated Zirconia (ZrO_2/SO_4^{-2}) were introduced on ordered mesoporous silica supports, such as SBA-15, with different synthetic approaches.

To identify the most efficient catalyst (best compromise between activity, ability, and recyclability) in depolymerisation of lignin, initially catalytic tests in the hydrodeoxygenation (HDO) of anisole, common lignin model compound, was conducted. Catalysts physicochemical properties were investigated by several analytical techniques. Synergetic effect of support's acid sites and metal's active phase on lignin hydrotreating process was considered and proved to be pivotal for this reaction. Also temperature, reaction time and solvent effects were investigated.

The next step will be carried out at Åbo Akademi University (Turku, Finland) in December and it will concern lignin isolation from the other components, by Accelerated Solvent Extraction (ASE) technique using diluted alkali solutions [2]. Different concentrations of alkali and different extraction protocols will be studied. The effect of preliminary hot-water extraction on lignin isolation with alkali will be also investigated. Finally, the best catalyst in hydrodeoxygenation of anisole will be tested on hydrolysed lignin thus obtained.

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PO-41

Ultrafast spectroscopy and semiconductor nanocrystals: a tale of two charge carriers

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The exploration of charge carrier dynamics in a semiconductor is an ineludible step in the full comprehension of the material's intimate nature. This is especially true for nanocrystalline matter, for which surface chemistry plays a crucial role in determining the ultimate performances. In such systems, once charge carriers are photoexcited, they can migrate toward the surface of the nanoparticle where reduction or oxidization of surrounding species can occur, as long as they possess adequate potentials and live long enough to avoid recombination. For applications in photocatalysis, this picture is the *conditio sine qua non* for the actual exploitation of the charges [1].

Femtosecond Transient Absorption spectroscopy (TAS) has indeed earned the name of a paramount and robust technique to unravel the ultrafast dynamics in nanomaterials, being able to follow elementary processes such as solvation, chemical reactions, exciton formation, to name but a few [2].

We report here a pump-probe TAS investigation optically clear colloidal dispersions of anisotropic TiO_2 nanocrystals (nanorods) in different excitation conditions. The samples were excited using a pump beam tunable in the UV-Vis range and probed by a white light beam in the visible. The temporal evolution of photoinduced absorption changes, probed with sub-picosecond time resolution, was found to be strongly dependent on the excitation wavelength, both at short and long time delays.

Such results suggest the formation of long-lasting exciton-like bound states in these nanocrystals when excited near or below the optical band gap, which is an important step towards the elucidation of the peculiar reactivity of TiO_2 in photocatalytic applications [3].

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PO-42

CuO promoted TiO_2 catalysts for ethanol photoreforming

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Photoreforming is a promising technology to obtain hydrogen from biomass in very mild conditions and using light as energy source. Up to now, this reaction has been studied more in the liquid solutions than in gas phase, although it offers higher hydrogen yield [1], and the most commonly used photocatalysts are promoted by noble metals [2]. Throughout this work, some titanium dioxide based materials promoted with an inexpensive co-catalyst, namely copper oxide, were developed for the photoreforming reaction. Two pristine materials was used: Evonik P25 and a lab-made TiO_2. Then copper was introduced through two techniques: incipient wetness impregnation and deposition-precipitation (DP) [3]. Photocatalysts were then tested on a lab-made rig using alcohol-water vapor mixture as reactants and UV light as energy source. Ethanol was chosen as biomass-like model substrate. It was seen that pristine titanium dioxides yielded hydrogen through a purely dehydrogenation reactions and lab-prepared material shown better activity than P25. X-Ray Diffracyion (XRD) and N_2 physisorption analyses were done on these pristine materials, showing that better performance of lab-prepared TiO_2 can be attributed to pure anatase crystalline phase and higher surface area than P25. Copper promoted samples showed higher hydrogen yield and quantum yield with respect to pristine ones, higher than those reported in literature too [2]. It was also seen DP method gave better results with a ten-fold improve of hydrogen yield in respect to P25, due to higher CuO reducibility, as confirmed by Temperature Programmed Reduction (TPR) analysis. This could be correlated to an easier capability to separate photogenerated electrons from holes, thus improving both hydrogen yield and quantum yield. Concluding we developed a cheap and easily prepared photocatalyst to efficiently produce hydrogen from ethanol on gas phase.

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Società Chimica Italiana

The Italian Chemical Society (Società Chimica Italiana, SCI), founded in 1909 and erected as a Legal Institution with R.D. n. 480/1926, is a scientific association that includes more than 3400 members. SCI members carry out their activities in universities and research institutes, schools, industries, public and private research and control laboratories, or as freelancers. They are joined not only by the interest in chemical sciences, but also by the desire to contribute to the cultural and economic growth of the national community, improving the quality of human life and the protection of the environment.

For new members

All Merck Young Chemists Symposium participants are (or have just become) SCI members.

Those who, before reaching Milano Marittima, were not yet SCI members will be contacted shortly (by e-mail) to complete the membership procedure and indicate the preferred SCI division.

Those who have chosen to become members for a year will be enrolled until 31/12/2018; those who chose the two-year membership will be SCI members up to the end of 2019.

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Tutti i soci SCI con meno di 35 anni fanno parte del Gruppo Giovani. Si tratta di un gruppo interdisciplinare che propone svariate iniziative ai suoi membri: il Merck Young Chemists Symposium, i premi Levi e Reaxys, diversi workshop come Y-RICh, CV Clinic Day e Design Your Future, utili alla preparazione di progetti europei per giovani ricercatori, la creazione di network di collaborazione, lo sviluppo di soft-skills individuali, e molto altro ancora.

Società Chimica Italiana
Gruppo Giovani

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SCI Giovani: il Consiglio Direttivo 2016-2018

Ogni tre anni, ciascuna Divisione elegge un socio giovane come proprio rappresentante nel **Consiglio Direttivo** della SCI Giovani, organismo responsabile della pianificazione e organizzazione delle attività rivolte ai soci under-35. Il Consiglio Direttivo 2016-2018 è composto da:

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Assemblea Ordinaria dei Soci del Gruppo Giovani

Martedì 14 Novembre 2017 – h 18.50

Ordine del giorno

1. Nomina del Presidente dell'Assemblea
2. Relazione del Coordinatore del Gruppo Giovani
3. Relazione del Tesoriere del Gruppo Giovani
4. Proposta di istituzione del Gruppo Interdivisionale di "Diffusione della Cultura Chimica"
5. Programmazione delle attività future del Gruppo Giovani
6. Varie ed eventuali

ISBN 978-88-86208-89-5