

La Parola ai Giovani 2018



Book of Abstracts

Mercoledì 05 Dicembre 2018,
Dipartimento di Chimica e Farmacia
Complesso Didattico, Aula Magna A, Via Vienna 2,
Sassari

Il comitato organizzatore:

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La Parola ai Giovani

Sassari 5 Dicembre 2018

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INV1

CHIMICA VERDE 4.0: LA NUOVA VIA DELLA CHIMICA

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Recentemente il Rapex (Rapid Alert System for dangerous non-food products) sistema comunitario di informazione rapida per i prodotti non conformi e di allerta per i prodotti non alimentari ha posto l'attenzione sulle sostanze chimiche presenti sui vestiti e sui capi di moda, che sembrano essere responsabili del 7-8% delle patologie dermatologiche, questo prevede interventi nei settori dei coloranti, degli inchiostri, delle vernici, dei plastificanti, dei biocidi, dei fissanti, dei reticolanti, ecc., inoltre il regolamento europeo REACH, le ONG ecologiste e la camera della moda sotto la pressione ambientalista hanno imposto dei limiti molto restrittivi di presenza di sostanze chimiche nell'abbigliamento e nelle calzature con il marchio "made in italy", questo comporta un ripensamento nella chimica delle specialità e dell'ausiliaristica che permetta ai formulatori italiani di fornire sostanze compatibili con le nuove regole all'industria manifatturiera. La visione più attuale della Chimica Verde può aiutare a risolvere queste serie problematiche, per cui è necessario considerare la Chimica verde 4.0, in analogia al progetto Industria 4.0, come la via della chimica del futuro. In quest'ottica è necessario impegnarsi nello studio di nuove sostanze "green" in grado di sostituire efficacemente quelle non più compatibili con le nuove tendenze. Il passaggio che potrebbe aiutare in modo sostanziale il traghetamento verso la sostenibilità è, dopo il lancio delle bioraffinerie al posto delle tradizionali raffinerie, la riprogrammazione dell'industria petrolchimica all'industria rinnovochimica, dove le sostanze rinnovabili forniscono una quantità di intermedi chimici naturali già strutturati che possono essere trasformati e adattati alle esigenze necessarie a quanto sopra descritto, questo tipo di trasformazione è in grado di migliorare la sostenibilità dei fine chemicals necessari, ma sarebbe anche molto compiacente con l'attuale situazione socio-politica che vede nel prodotto naturale quanto di più igienico ci sia per l'ambiente e per la salvaguardia della salute umana.

O1

A Brønsted Acid Mediated Cascade Reaction to Access 3-(2-Bromoethyl)benzofurans.

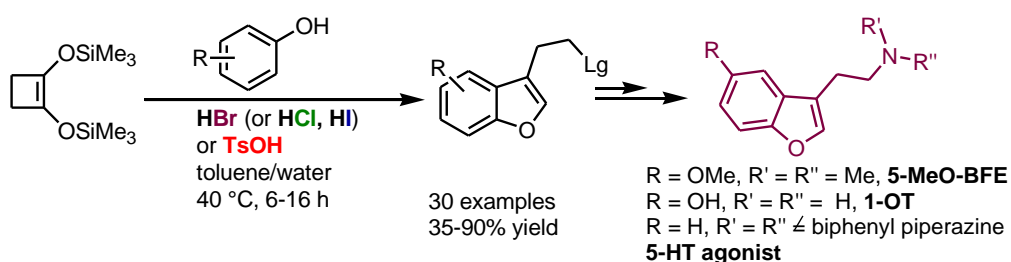
Andrea Cocco,^a Stefania Porcu,^a Stefania Demuro,^a Alberto Luridiana,^a Angelo Frongia,^a David J. Aitken,^b Florence Charnay-Pouget,^b Regis Guillot,^b Giorgia Sarais,^b and Francesco Secci^a

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A unified protocol for the construction of 3-(2-Bromoethyl)benzofurans and 2-(benzofuran-3-yl)ethylamines from bis[(trimethylsilyl)oxy]cyclobutene has been developed [1]. This mild and facile strategy [2] was applied for the synthesis of a series of 5-HT serotonin receptor agonists, underlining its potential for the syntheses of bioactive compounds and natural products [3].



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O2

**Acid-catalyzed Synthesis of Arylthio Cyclopropane
Carbaldehydes and Ketones**

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A general strategy for the synthesis of arylthio cyclopropyl carbaldehydes and ketones via a Brønsted acid catalyzed arylthiol addition/ring contraction reaction sequence has been exploited [1]. The procedure led to a wide panel of cyclopropyl carbaldehydes in generally high yields and with broad substrate scope. Two fundamental challenges have been explored: a) the photochemical synthesis of functionalized cyclobutanone derivatives via Norrish-Young photocyclization reaction of diones, and b) the mechanistic aspects involved in the C4-C3 ring contraction of strained carbocyclic systems [2]. This protocol was also employed for the development of a four step synthesis of a biologically active cyclopropylsulfone carboxylic acid as bradykinin BK1 receptor agonist [3].

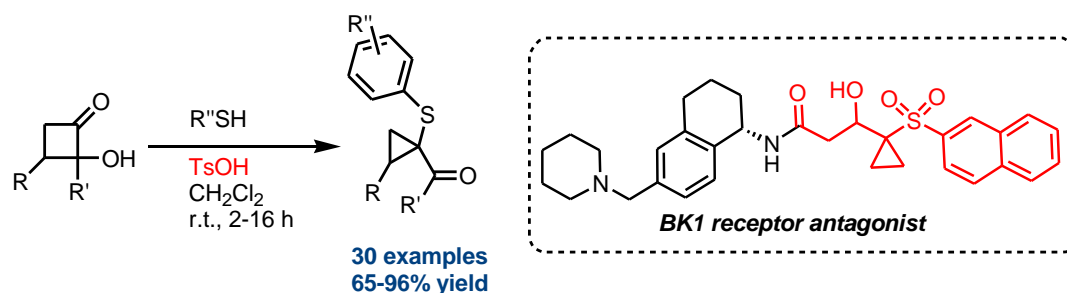


Figure 1: Scheme of acid-catalyzed synthesis of arylthio cyclopropyl derivatives (left) and its potential application as synthetic building block for medicinal chemistry (right).

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O3

Sliding crosslinked thermoresponsive materials: polipseudorotaxane made of poly(N-isopropylacrylamide) and acrylamide- γ -cyclodextrin [1]

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One of the most studied stimuli-responsive polymers is poly(N-isopropylacrylamide) (PNIPAAm), which is a non-toxic, biocompatible, and relatively cheap polymer characterized by a lower critical solution temperature (LCST) at about 30–32 °C. These properties make PNIPAAm suitable for biomedical and pharmaceutical applications. Moreover, the possibility of increasing its LCST up to the physiological range could provide great practical advantages. However, its poor thermal and mechanical properties greatly limit its application. The aim of the present work was to synthesize a novel polipseudorotaxane (PPR) based on PNIPAAm and acrylamide- γ -cyclodextrin (A γ CD). It was found that A γ CD acted as a pendant group and, at the same time, allowed macromolecular PNIPAAm chains to flow through its empty cavity, giving rise to a sliding crosslinking system with peculiar features. The A γ CD influences the thermoresponsive behavior of PNIPAAm hydrogels, by modifying their LCST value that increased with increasing A γ CD amount, up to 38 °C. This result, which approaches the LCST value of classical PNIPAAm to actual human body temperature, widens the practical applications of PNIPAAm in the biomedical field.

Furthermore, A γ CD influenced also the swelling behavior of the resulting hydrogels and their thermal and mechanical properties. In detail, the T_g values of samples increased with increasing A γ CD content. This result was in agreement with the observed increase of the compression modulus E of the hydrogels.

Reference:

[1] G. Malucelli, J. Dore, D. Sanna, D. Nuvoli, M. Rassu, A. Mariani* and V. Alzari*, *Front. Chem.* **2018**, in press, doi: 10.3389/fchem.2018.00585

O4

Medicinal Sponges Based on Extracellular Matrix, Chitosan and Alginate for Regenerative Medicine Applications

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Incorporation of extracellular matrix (ECM) into polymer-based formulations could improve bioscaffold characteristics and promote wound healing. ECM is attractive for regenerative medicine applications due to its similarity with soft tissues, biocompatibility and biodegradability. Natural polymers, such as sodium alginate and chitosan are widely used for regenerative medicine applications due to the wound healing properties [1,2]. The research aims to develop and characterise medicinal sponges based on ECM and natural polymers of marine origin.

Medicinal sponges, composed of decellularized ECM, chitosan and sodium alginate (ECM/Ch/Alg) were developed by using lyophilisation and ionic cross-linking techniques. Medicinal sponges without ECM were used for comparison (Ch/Alg). Lidocaine hydrochloride (2%) was immobilised to serve as a model drug. Porous structure of the prepared sponges (120–400 µm pore size) was confirmed by using scanning electron microscopy (SEM) technique. The results showed rapid mass loss of ECM/Ch/Alg sponges within 7-day stability testing, comparing with Ch/Alg samples: 80–100% and 40–70%, respectively. Moreover, rapid lidocaine hydrochloride release from ECM/Ch/Alg sponges was also influenced by stability of the samples: >50% of the drug was released within 4 h of immersion in phosphate buffer saline. To conclude, incorporation of ECM into the structure of polymer-based scaffolds showed improvement of *in vitro* sponge characteristics and its applicability for accelerated wound healing.

References:

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O5

Synthesis and antiproliferative activity of variously substituted 2-(5,6-difluoro-1*H*(2*H*)-benzo[*d*][1,2]triazol-1(2)-yl)-3-(4-*R*-phenyl)acrylonitrile derivatives

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Cancer represents the second leading cause of death in Italy. Among the anticancer drug treatments, we should mention mitosis-targeted therapies that cause cell cycle arrest in G2/M phase of the mitosis and, consequently, apoptosis. Antimitotic drugs that are highly validated chemotherapy agents may be grouped into microtubule destabilizing agents (e.g. vinca alkaloids) and microtubule stabilizing agents (e.g. taxanes). Drug resistance and toxicity on normal cells limits their use [1].

This work is part of a long time project initially based on the synthesis of some organic compounds with antitubercular activity. Subsequently, the synthesized compounds showed cytotoxicity against MT-4 cells at lower concentrations, as their antimycobacterial activity was not selective. Thus, the most cytotoxic compounds were evaluated for potentially anticancer activity [2].

A new series of variously substituted 2-(5,6-difluoro-1*H*(2*H*)-benzo[*d*][1,2]triazol-1(2)-yl)-3-(4-*R*-phenyl)acrylonitrile derivatives was synthesized as part of this project. The *in vitro* activity of the derivatives was evaluated on a panel of 60 human cancer cell lines at the National Cancer Institute in Bethesda, Maryland, USA. In this work we report the preliminary screening of the compounds **81a,b,c,e,f,g** and **82a**, which showed an interesting activity at 10 μ M, with a percentage of growth inhibition in tumor cells between 50% and 100%. Some of them, **81a,e,h**, have been selected to be screened on the same 60 tumor cell lines, but at 5 different concentrations down to 0.01 μ M, to obtain their CC₅₀ value. These preliminary data looks encouraging for this class of derivatives.

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O6

**Conversion of Hydroxycinnamic acids into Cholinium salts:
Water solubility studies and evaluation of antioxidant profile**

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Hydroxycinnamic acids (HCAs) are one of the major classes of phytochemicals found in nature [1]. Recently, HCAs received increasing attention for providing wide-ranging beneficial effects on health ascribed to their free radical scavenging, metal chelation and protein binding antioxidants mechanism [2]. However, bioavailability features of HCAs are strongly limited by their poor water solubility which represents the main issue when envisaging their incorporation in water-rich formulations [3]. Since HCAs bearing an ionizable carboxylic group their conversion into cholinium-based ionic liquids (ILs) is the easiest way to significantly increase their solubility and dissolution rate. Herein, a small set of cholinium-based salts, were synthesized and characterized. Contrary to common ILs, the cholinium-salts here presented are biocompatible, non-toxic, and simple to prepare [4]. These salts, are significantly more soluble in water than their precursors, and showed not only similar but even higher antioxidant activity and absence of cytotoxicity in B16-F10 cell line. In this communication, we report synthesis, water solubility studies, antioxidant and cytotoxic profiles. Additionally, cholinium caffeate was also evaluated and compared with its acidic precursor as a substrate for catecholase activity in Mushroom Tyrosinase (MT).

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O7

Development of PROTACs Based on Tubastatin A

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PROTACs are heterobifunctional molecules constituted by a small molecule inhibitor, a linker, and a ligand for an E3 ligase. PROTACs simultaneously bind the E3 ubiquitin ligase and the target protein to promote the degradation of the target protein by Proteasome [1]. Histone deacetylases (HDACs) are an important family of enzymes that regulate protein activity through removal of the acetyl-lysine post-translational modification. Class I and Class IIb HDACs are overexpressed in several cancer forms [2].

Here I report the design and synthesis of a new class of PROTACs based on the Tubastatin A scaffold. In several experimental models of CNS diseases, Tubastatin A has exhibited neuroprotective [3] effects. Developing PROTACs for these well-validated drug targets has the potential to open up new opportunities in targeted cancer.

Four different ligands have been described in the literature which can be used to target PROTACs to different E3 ligases: MDM2, cIAP1, VHL and CRBN. My synthesis efforts to PROTACs bearing E3 ligase ligands targeting both the von-Hippel Lindau protein as well as Cereblon are described.

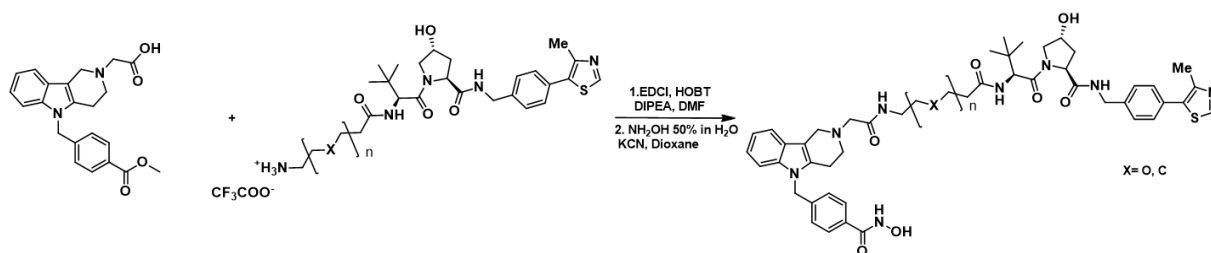


Fig1: Synthesis of final PROTACs

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O8

Discovery of benzothiazole derivatives as Dual DNA Gyrase A/Gyrase B Inhibitors

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Bacterial DNA gyrase is a topoisomerase type II enzyme that is essential for cell viability because it introduces negative supercoils in DNA in front of the replication fork. DNA gyrase, an ATP-fueled heterotetrameric protein is composed of two A subunits (GyrA) and two B subunits (GyrB). The GyrA subunit is the target of fluoroquinolone antibiotics, while the GyrB site is the target of novobiocin. Despite GyrB subunit is an intriguing target, no inhibitor has been introduced into the clinic up to now. In previous works we reported the binding mode of several structural types of pyrrole-2-carboxamide derivatives e.g. 2-((2-(4,5-dibromo-1H-pyrrole-2-carboxamido)benzo[d]thiazol-6-yl)amino)-2-oxoacetic acid with *E. coli* GyrB [1]. Unfortunately, all these inhibitors did not show *in vitro* antibacterial activity, because of insufficient penetration and effluxing. Since fluoroquinolones and gyrase B inhibitors (pyrrole-2-carboxamides) do not share common structural features, we decided to combine ciprofloxacin, through a methylene linker, with our reported benzothiazole-based gyrase B inhibitors, placing a pyrrole-2-carboxamide moiety at position 2 or 6 of the benzothiazole scaffold.

All the synthesized compounds displayed potent bioactivity against Gram negative *E. coli*. Moreover, one compound showed good *in vitro* activity against Gram negative *Shigella flexneri* and *Klebsiella pneumoniae*. The lack of bioactivity change in presence of GyrB E136 mutant and the lack of bioactivity in the case of the mutated fluoroquinolone binding site indicates that the primary binding site of our dual inhibitors is on GyrA. These results provide a good starting point for further optimizations.

References:

[1] M. Gjorgjieva, et al., J. Med. Chem. **2016**, 59, 8941–8954

O9

New complexes of Pd(II), Pt(II) and Au(III) with N-heterocyclic ligands of pyridyl-imidazole type

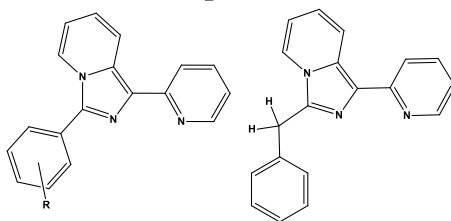
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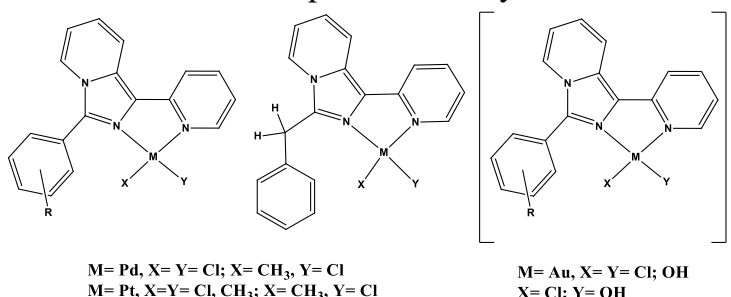
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The cyclometalation reactions of 6-substituted-2,2'-bipyridines with transition metal ions in d⁸ configuration (e.g. Pt(II), Pd(II) and Au(III)), are well known.¹ Here, we report the attempts to obtain cyclometallated derivatives of the same ions with a series of N-heterocyclic ligands of imidazo[1,5-a]pyridynyl type² with formula, with modification of the substituents on the ring or insertion of spacers:



Up to now, only adducts have been obtained, despite the considerable efforts on the ligand design and reaction conditions to promote the cyclometalation reactions:



For some of these derivatives, particularly those of Pd(II) and Pt(II), it was possible to solve the structures by X-Ray diffraction method. Different experimental conditions are under investigation to obtain new cyclometalated species by activation of a C-H bond both that of the substituent in position 3 and that in position 8 of the N-heterocyclic imidazole[1,5-a]pyridynyl ligands. Finally, the survey will be extended to the ion Au^I.

References:

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b) Cocco F., Cinellu M. A., Minghetti G., Zucca A., Stoccoro S., Maiore L., and Manassero M., *Organometallics* **2010**, 29, 1064–1066. [2] Ardizzoia G. A., Brenna S., Durini S., Therrien B. and Veronelli M., *Eur. J. Inorg. Chem.*, **2014**, 4310-4319.

O10

Synthesis of Strongly Fluorescent Carbon Dots

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Water is essential for life and therefore any improvement in the detection or capturing of its pollutants is highly desirable. Carbon dots (CDs) hosting organic-inorganic hybrid materials [1] can help to achieve highly sensitive, luminescence-based detection of contaminants in water.

Carbon dots [2] are a class of fluorescent nanomaterials, which recently aroused a growing interest of the scientific community. Simple synthetic methods applied to easily accessible carbon sources [3] can produce strongly fluorescent, non-toxic CDs to be used as optical probes in aqueous samples.

Any increase in the fluorescence intensity potentially lowers the detection limit of a pollutant, so an extensive study of the reaction parameters is required to carefully design the CDs structure and properties.

The cheap and environmentally-friendly citric acid is frequently used as a CDs source. This compound, however, allows achieving weak fluorescence, therefore it is often reacted in the presence of nitrogen-containing molecules. We introduced tris(hydroxymethyl)aminomethane and urea in the CDs synthesis in order to enrich the nitrogen content of the core in the nanoparticle. The obtained nanoparticles were characterized with UV-Vis, fluorescence and FTIR spectroscopies. We found that a simple pyrolysis process is capable of producing highly fluorescent CDs in short reaction times (15-60 min).

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O11

Thiophene-based conducting polymers and metal-polymers: biosensors applications

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Recently, conducting polymers and metal-polymers have attracted the interest of scientists, in particular in sensing and biosensing fields.

These materials are in fact known to possess several suitable features for the development of (bio)sensors: they offer an appropriate surface (which can properly be functionalized) to immobilize biomolecules with different techniques, and due to their excellent conductivity they allow rapid electron transfer.

Here, we report a comparison between different thiophene-based conducting polymers (poly(3,4-ethylenedioxythiophene, poly(2,2'-bithiophene) and poly(4,4'-diethynyl-2,2'-bithiophene)) and conducting metal-polymers (poly[(TAT)Ru(TpyCOOH)] [1] and poly[Ru(TAT)₂] [2] TAT = 4'-[(2,2':5,2''-terthien-3'-ethynyl)-2,2':6,2''-terpyridine; TpyCOOH = 4,4',4''-tricarboxylate-2,2':6,2''-terpyridine) used as modifying agents for electrode surfaces to obtain amperometric (bio)sensors for histamine detection.

On each of these polymer films, diamine oxidase (DAO) from *porcine kidney* (E.C. 1.4.3.6) was immobilized using different techniques (entrapment and cross-linking).

The obtained biosensors were tested both in presence of a redox mediator (working as a second generation-biosensors) and without a redox mediator (according to the scheme of more common first generation-biosensors).

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O12

Synthesis, structure and optical behaviour of $\text{Sr}_2(\text{Ge}_{(1-x)}\text{Si}_{(x)})\text{O}_4$

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The present thesis aims at advancing the fundamental knowledge on luminescent materials based on a suitable planned experimental investigation. The activity carried out during the internship period at the "Nanophasic Materials Laboratory for Energy and Environment and Mechanochemistry" at the University of Sassari and at the laboratory of "Luminescent Materials" at the University of Wrocław focused on the synthesis and characterization of luminescent materials. The set of data obtained by XRD and PL demonstrates the satisfactory properties of $\text{Sr}_2(\text{Ge}_{0.75}\text{Si}_{0.25})\text{O}_4:\text{Pr}^{3+}$ with regard to the excellent thermal stability and high workability range.[1]

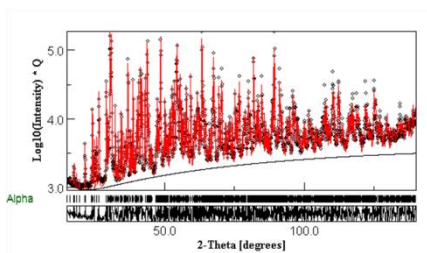


Figure 1: XRD pattern of $\text{Sr}_2(\text{Ge}_{0.75}\text{Si}_{0.25})\text{O}_4:\text{Pr}^{3+}$

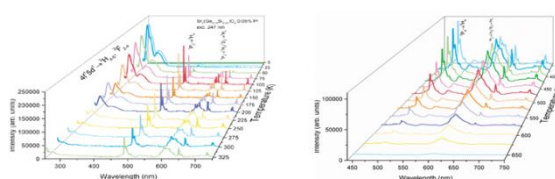


Figure 2: Emission spectra of $\text{Sr}_2\text{GeO}_4:\text{Pr}^{3+}$ (excited at 247 nm) in the low range of temperature

As far as fabrication is concerned, the classic ceramic method has shown significant reliability. In particular, it has allowed synthesizing materials free of undesired impurities.

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O13

MgCr₂S₄: a new compound for multivalent battery cathode applications

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New materials for energy applications are requiring combination of electrochemical and magnetic properties. As was reported in several studies [1] these features may be typical of spinels and sulfur-spinels. MgCr₂S₄ compound was suggested to be an interesting candidate as multivalent battery cathode. The well-known potential of Mechanical Alloying to overcome the strong physical limitations of immiscibility has stimulated our attempts for a solid state synthesis route starting from magnesium or magnesium hydride, chromium and sulphur powders. The course of such mechanically induced reaction as a function of processing time was checked by XRD and it was evidenced the occurrence of a mechanically induced self-propagating reaction, MSR. The analysis of the reaction products shows the MgCr₂S₄ (space group Fd-3m, a=10,137 Å) partially occurs.

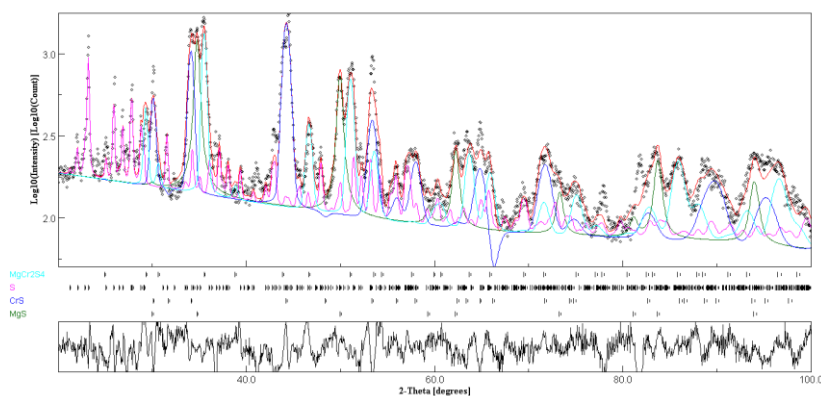


Figure 1: XRD pattern diffraction that showed the new phases MgCr₂S₄ (sky blue line)

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P1

Solid lipid nanoparticles: an interesting approach for oral delivery of Genistein

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Introduction

Genistein (GEN) is a phytoestrogen characterized by antioxidant, antiproliferative and anticancer properties [1]. However, GEN has demonstrated low oral bioavailability due to poor aqueous solubility. The aim of the present study was to develop and evaluate GEN-loaded solid lipid nanoparticles (SLN) to improve oral bioavailability.

Materials and Methods

SLN were prepared using a hot homogenization process [2]. The formulations were characterized *in vitro* by assessing: SLN Size and Polydispersity Index; Zeta potential; Stability test; Morphology; GEN Content and dissolution test. Furthermore, intestinal uptake of fluorescein marked-SLN was evaluated *ex-vivo* using portions of pig duodenum.

Results and Discussion

GEN-loaded SLN, characterized by a spherical morphology, have a mean diameter of 280 nm, a PDI of 0.27 and Zeta Potential of -18.47. The SLN were stable within one month and the GEN loading efficiency was beneath 100%. The dissolution test revealed that the SLN release more GEN compared to drug dispersion used as control. For *ex-vivo* permeation test the suitable conditions of intestine conservation were assessed (3h at room temperature). Moderate to mild fluorescence signal was observed in both the intestinal samples treated with SLN and with a fluorescein solution used as control suggesting a widespread uptake of both free fluorescein and labeled SLN by enterocytes.

Conclusion

On the basis of these results GEN-loaded SLN can be considered promising systems to improve oral delivery of phytoestrogen. Further studies are currently underway in order to better evaluate the intestinal uptake of formulation.

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P2

Ossidazione fotocatalitica di metilareni

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L'ossidazione di metilareni variamente sostituiti suscita elevato interesse in quanto i prodotti che si ottengono sono largamente utilizzati in campo farmaceutico, agricolo ed in vari altri ambiti industriali.[1] Le metodologie di sintesi classiche prevedono l'impiego di reattivi spesso tossici, costosi e dannosi per l'ambiente.[2] Per ovviare a tali problematiche stiamo investigando la possibilità di sviluppare una metodologia alternativa attivando la reazione di ossidazione tramite una fonte rinnovabile come la luce visibile.

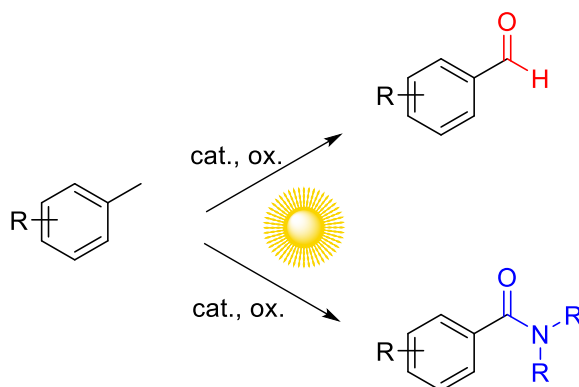


Figura 1: Ossidazione fotocatalitica di metilareni

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P3

Novel benzimidazoles as potent anti Coxsackievirus B5 agents

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Coxsackievirus B5 (CV-B5) is an icosahedral positive single-stranded RNA (ssRNA+) virus. It belongs to the Enterovirus specie within the Picornaviridae family [1]. Although most of the enterovirus infections commonly seen are relatively mild and result in complete recovery of the patient, these viruses can also cause severe and sometimes fatal illnesses or chronic autoimmune diseases. Among the largely studied coxsackievirus B, CV-B5 is representative for its specie and it is one of the most importantly associated with human diseases, mainly affecting infant (neonatal sepsis) or central nervous system (e.g. meningitis, encephalitis) and the myocardium (myocarditis) [2].

Nowadays there are no approved vaccines or effective drug treatment for Coxsackievirus B infectious disease, this motivated our research of potent and selective anti Coxsackievirus B compounds.

We designed and synthesized a series of new variously substituted benzimidazole derivatives that has been tested against a panel of representative virus of different families of virus and most of them showed interesting values of EC₅₀ in a range of 1.5-9.9 µM against Coxsackievirus-5 (CV-B5). The compound 2-(4-(*tert*-butyl)phenyl)-5,6-dichloro-1*H*-benzo[*d*]imidazole turned out as the most active derivative against CVB-5 with a EC₅₀ value of 1.5 µM and it is now the lead compound for a future synthetic project that aim to obtain a more potent and less cytotoxic derivative.

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P4

Metodi a confronto per la determinazione di carbonio ed azoto nel suolo

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Negli ultimi anni le analisi agrochimiche del suolo e dei vegetali hanno acquisito un valore rilevante grazie a una nuova cultura agronomica volta alla razionalizzazione delle produzioni e a un maggiore rispetto ambientale. Le indagini analitiche sono uno strumento fondamentale per l'elaborazione di un corretto piano di concimazione collegato alla massima resa della produzione con conseguente riduzione dei costi.

In Italia sono presenti delle metodiche ufficiali di analisi del suolo (D.M. n. 79 del 11/05/1992 e D.M. n. 185 del 13/09/1999) che consentono di uniformare i metodi di analitici di tutti i laboratori in modo da ottenere valori interpretabili con oggettività. In questo lavoro focalizzeremo l'attenzione su metodi tradizionali quali walkley- black per la determinazione del carbonio organico, conseguentemente della sostanza organica, e il metodo Kjeldahl per la determinazione dell'azoto totale. Le determinazioni in oggetto sono di fondamentale importanza sia nei suoli che nei vegetali in quanto determinano il grado di fertilità nei terreni e la qualità dei prodotti vegetali ottenuti. Dal punto di vista ambientale le analisi sopra descritte oltre ad essere mediamente pericolose e poco performanti, producono degli esausti fortemente inquinanti e quindi molto costosi nella filiera dello smaltimento dei rifiuti tossici. Per il carbonio si utilizza il Cr esavalente e si ha una produzione di esausto di circa 500ml a campione con un costo di smaltimento di circa 3euro/l. Nell'azoto Kjeldahl si usa dell'acido solforico e soda caustica con produzione di circa 250ml di esausto per campione con costo di smaltimento di circa 2,5 euro/l. A questo quadro si può mettere a confronto l'utilizzo di una metodica alternativa più efficace come quella che prevede l'utilizzo di un analizzatore elementare CHN.

P5

A Mechanochemical-Assisted Oxidation of Amines to Carbonyl Compounds and Nitriles

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The oxidation of amines is a powerful method to produce various important synthetic intermediates such as carbonyl compounds and nitriles [1]. The classical methodologies suffer of many drawbacks [2] such as use of toxic metal-containing reagents, toxic solvents and overoxidation of carbonyl compounds. To overcome these problems we have investigated a new mild, efficient, metal-free and solvent-free oxidation of primary amines to aldehydes, ketones and nitriles under ball-milling conditions at room temperature [3]. This approach is simple, convenient and uses inexpensive and commercially available reagents. In addition this method is compatible with various functional groups and requires easily accessible starting materials. Simple filtration of the reaction mixture through pad of silica gel affords pure aldehydes, ketones and nitriles products.

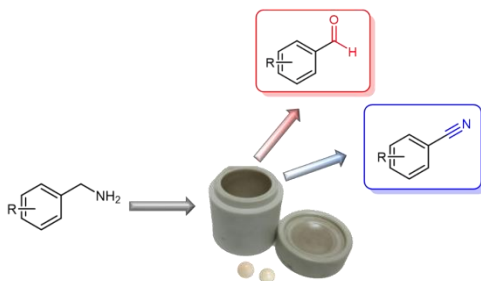


Figure 1: Oxidation of amines to carbonyl compounds and nitriles by ball milling

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P6

An “heretical” irrigation approach aimed to minimize the amount of harmful elements in rice grain

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Among the factors affecting the bioaccumulation of toxic elements (like As and Cd) in rice, a key role is played by the nature of irrigation methods. The sprinkler irrigation method, optimized for rice in Sardinia, Italy, applied to several rice genotypes over a number of crop years has produced no significant differences in yields, exhibiting also many environment-friendly features. In addition, our previous studies show that the adoption of sprinkler irrigation causes, in comparison to data obtained using continuous flooding irrigation, an extraordinary As reduction (ca. -98%) [1], a meaningful Cd reduction (-20%) on rice grain [2]. In this contribution we show the outcomes of our recent studies on the effects of the different methods of irrigation (i.e. continuous flooding irrigation, sprinkler irrigation and saturation irrigation) on the bioaccumulation of a wide number of elements of health concern (i.e. Al, As, Cd, Cr, Cu, Fe, Hg, Mn, Mo, Ni, Pb, Sb, Se, Tl and Zn) in rice (grain, roots, stems, leaves and panicles) at varying of the soil composition and its pollution level, of the rice genotype and of the most representative phenological phases of the rice plant. ICPMS, GFAAS and FAAS methods of analysis have been specifically developed and validated for the measurements in all biotic matrices.

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P7)

Spatial coarse-graining of adsorption and diffusion

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Nowadays, multiscale modelling techniques hold great promise for the representation of physical systems in relatively broad spatial and temporal scales. Starting from a microscopic model, reaching larger scales often requires performing a coarse-graining procedure in order to obtain a simpler but more computationally efficient model. This approach is necessary for the representation of adsorption and diffusion occurring in macroscopic scales, such as industrial gas-separation involving microporous materials.

In this work, we introduce the Interacting Pair Approximation (IPA) method to obtain a coarse-grained model by employing a mean field approximation of the reference system [1,2]. Such representation is based on the definition of a local-density-based potential function which accurately yields the thermodynamic properties of the reference system. Comparing with previous methods, IPA provides a more accurate and more versatile framework for the development of spatially coarse-grained models [3].

References:

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P8

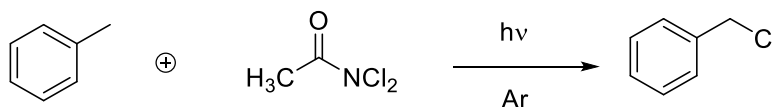
Sintesi di Alfa Cloro Metil Areni Mediante Attivazione Fotochimica

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In questo lavoro è stata testata la possibilità di sintetizzare il benzil cloruro a partire da *N,N*-dicloroammidi mediante attivazione fotochimica. Il benzil cloruro è un composto di notevole importanza e dalle numerose applicazioni a livello industriale come intermedio per la produzione di coloranti, precursore per la produzione di aromatizzanti e profumi e come precursore per la sintesi di farmaci di classe anfetaminica [1]. Viene sintetizzato partendo dall'alcool benzilico o tolueni, utilizzando spesso reagenti costosi, tossici e difficili da maneggiare [2]. Per ovviare a tali problematiche abbiamo sviluppato una nuova metodologia sintetica che prevede la reazione di metil areni con *N,N*-dicloroammidi, impiegando fonti energetiche sostenibili come la luce solare.



Sono stati utilizzati metil areni variamente sostituiti ottenendo delle rese medio alte.

References:

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P9

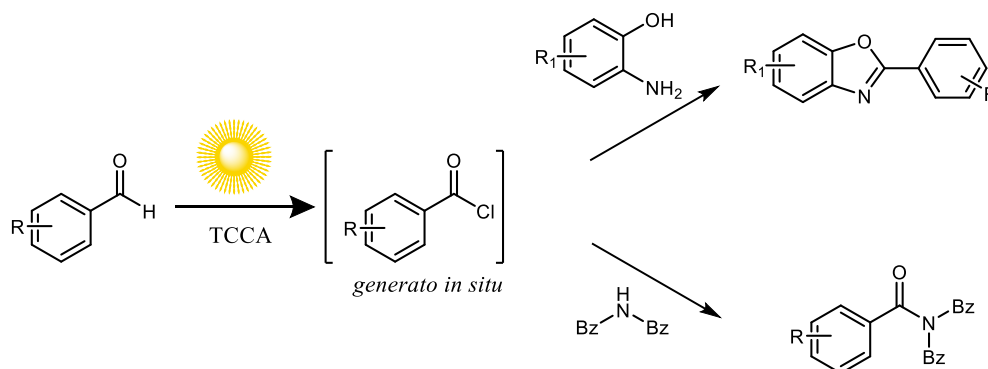
Sintesi di benzossazoli e ammidi mediante attivazione fotochimica

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Le sintesi che portano alla formazione di benzossazoli e ammidi sono importanti nel mondo della chimica organica, poiché sono molecole che trovano numerose applicazioni a livello farmaceutico [1] ed industriale [2]. Per questo motivo si è deciso di investigare delle strategie sintetiche innovative per ottenere benzossazoli sostituiti e la dibenzilbenzammide. Entrambe le strategie sintetiche studiate sono one-pot a due step. Vengono impiegati reattivi di partenza facilmente reperibili, solventi a basso impatto ambientale e fonti energetiche eco-compatibili quali la luce solare. In questo modo è stato possibile ottenere un'ampia varietà di benzossazoli variamente sostituiti e ammidi con buone rese.



Schema 1 Sintesi di benzossazoli variamente sostituiti e ammidi

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RINGRAZIAMENTI

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