Società Chimica Italiana
Sezione Sardegna

XII La Parola ai Giovani

27 Settembre 2013

Aula C Cittadella Universitaria di Monserrato

ABSTRACT BOOK

PROGRAMMA

9:30-10:00	REGISTRAZIONE PARTECIPANTI		
10:00-10:15	INTRODUZIONE LAVORI E SALUTI		
10:15-13:20	Sessione A: Chair Marzia Fantauzzi		
	10:15	O1	M. ATZORI - New BEDT-TTF/$[FE(CL_2AN)_3]^{3-}$ and (*S,S,S,S*)-TM-BEDT-TTF/$[FE(CL_2AN)_3]^{3-}$ Hybrid Systems: Synthesis, Crystal Structure and Physical Properties
	10:40	O2	G. MANZO - TRI-DIMENSIONAL CHARACTERIZATION OF THE IMMUNOMODULATORY PEPTIDE PLASTICIN-L1 AS A TOOL TO INVESTIGATE ITS MODE OF ACTION
	11:00	O3	F. TRUDU - I complessi di Platino nel trattamento dei tumori: una nuova classe con leganti fenantrolinici e imidazolidine-2-tione
	11:20	O4	M. PEANA - The role of Y-PARK9 protein in Preventing Manganese-induced Parkinson's Disease
	11:40	O5	A. RIGOLDI - METODI DI RECUPERO ECO-COMPATIBILI DI METALLI NOBILI DA RIFIUTI HI-TECH: VALORIZZAZIONE E TRASFERIMENTO TECNOLOGICO
	12:00	O6	A. DEPLANO – Derivati dell'Ibuprofene quali inibitori duali di FAAH e COX
	12:20	O7	E. VALLETTA - Nuovi complessi di rame(II) con derivati dell'1,10-fenantrolina: sintesi, equilibri in soluzione, attività citotossica e DNA-Binding
	12:40	O8	V. MELI - NAAOT/C_{12}MIMBR catanionic Vescicles as nanocarrier for fluorescent Chemosensors
	13:00	O9	A. PINTUS - A coarse-grained model for diffusion in zeolites based on clustering of short MD trajectories
13:20-14:45	PAUSA PRANZO / SESSIONE POSTER		
14:45-16:05	Sessione B: Chair Francesco Secci		
	14:45	O10	A. GABRIELI - Development of reliable classical force fields For simulations in microporous materials
	15:05	O11	M. SERRATRICE - Complessi di oro con leganti imidazolici di interesse farmacologico
	15:25	O12	D. PERRA - AL-SBA-15 FOR THE PRODUCTION OF METHYL LACTATE FROM C_3-SUGARS
	15:45	O13	E. SESSINI - Processing of multifunctional materials: conducting PEDOT thin films doped with magnetic complexes
16:05	CONCLUSIONE DEI LAVORI E SALUTI		
16:30	ASSEMBLEA SOCI SCI SARDEGNA		

NEW BEDT-TTF/$[FE(CL_2AN)_3]^{3-}$ AND (*S,S,S,S*)-TM-BEDT-TTF/$[FE(CL_2AN)_3]^{3-}$ HYBRID SYSTEMS: SYNTHESIS, CRYSTAL STRUCTURE AND PHYSICAL PROPERTIES

Matteo Atzori,[a,b] Flavia Pop,[b] Carlos J. Gómez-García,[c] Pascale Auban-Sanzier,[d] Narcis Avarvari,[b] Maria Laura Mercuri [a]

a) Dip. Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, Cagliari (Italy); b) Laboratoire Moltech Anjou, Université d'Angers, Angers (France); c) Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Paterna (Spain); d) Laboratoire de Physique de Solides, Université Paris Sud, Orsay (France)

Multifunctional molecular materials (MMMs) showing electrical conductivity (semiconduction, conduction and superconduction) and magnetic properties (para-, ferro-, ferrimagnetism) are of great interest in the field of material science for their academic interest as well as for their potential applications in the post-silicon era of molecular electronics. With the aim to prepare novel MMMs, here we report the synthesis, crystal structure and physical characterization of three new magnetic conductors obtained by reacting, via electrocrystallization, the novel paramagnetic anion $[Fe(Cl_2An)_3]^{3-}$ (Cl_2An = chloranilate = dianion of chloranilic acid = 3,6-dichloro-2,5-dihydroxy-1,4-benzoquinone) as magnetic carrier, with BEDT-TTF (bis-ethylenedithio-tetrathiafulvalene) and (*S,S,S,S*)-TM-BEDT-TTF ((*S,S,S,S*)-tetramethyl-BEDT-TTF) as conducting carriers. Combining the organic donor BEDT-TTF with $[Fe(Cl_2An)_3]^{3-}$ we observed the formation of two different structural phases: the salt $[BEDT\text{-}TTF]_3[Fe(Cl_2An)_3]\cdot 2CH_2Cl_2\cdot H_2O$ (**1**) which behaves as a semiconductor, and the salt $\beta\text{-}[BEDT\text{-}TTF]_6[Fe(Cl_2An)_3]\cdot CH_2Cl_2\cdot H_2O$ (**2**) which shows metallic behaviour until ca. 200 K (Figure 1).

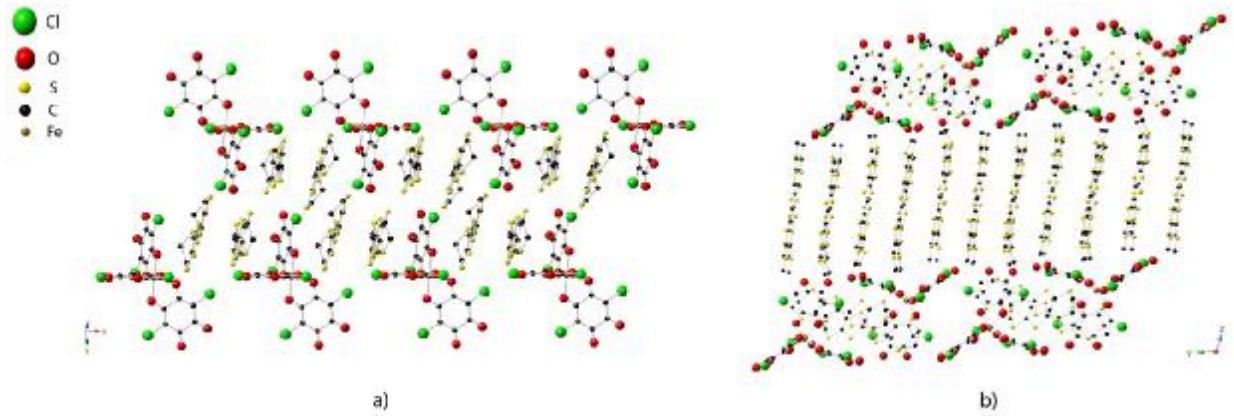

Figure 1: View of a portion of the crystal structure for **1** and **2**: a) **1** along the a axis, b) **2** along the bc plane.

Furthermore, by combination of the chiral donor (*S,S,S,S*)-TM-BEDT-TTF with $[Fe(Cl_2An)_3]^{3-}$ we obtained the chiral salt $\beta\text{-}[(S,S,S,S)\text{-}TM\text{-}BEDT\text{-}TTF]_3[P(Ph)_4]_2[Fe(Cl_2An)_3]_2$ which behaves as a semiconductor. The synthesis of the magnetic carriers and their magnetic properties as well as the electrosynthesis of the hybrid systems and their structural features and physical properties will be discuss in details during this oral communication.

TRI-DIMENSIONAL CHARACTERIZATION OF THE IMMUNOMODULATORY PEPTIDE PLASTICIN-L1 AS A TOOL TO INVESTIGATE ITS MODE OF ACTION

Giorgia Manzo[^], Mariano A. Scorciapino[^], Roberta Sanna[^], Mariano Casu[^], J. Michael Conlon[‡], Milena Mechkarska[‡], Jelena M. Pantic[§], Miodrag L. Lukic[§], Andrea C. Rinaldi[#] (giorgia.manzo@unica.it)

[⊥]Department of Chemical and Geological Sciences, University of Cagliari, I-09042 Monserrato (CA), Italy, [‡]Department of Biochemistry, Faculty of Medicine and Health Sciences, United Arab Emirates University, 17666 Al Ain, United Arab Emirates, [§]Center for Molecular Medicine, Faculty of Medicine, University of Kragujevac, Kragujevac, Serbia, [#]Department of Biomedical Sciences, University of Cagliari, I-09042 Monserrato (CA), Italy.

The skin of different species of frogs and toads is rich in biologically active peptides. Some of them, named antimicrobial peptides, are endowed with a broad-spectrum antimicrobial activity against bacteria, virus, fungi, etc., while others, which have recently attracted researchers' attention, are devoid of antibiotic power but act as immunoregulatory agents. Experimental studies confirmed that microorganisms' plasmatic membrane is the primary target of most of AMPs but, at present, very little is known about immunomodulatory peptides and their mode of action [1]. An example of such interesting peptides is Plasticin-L1, originally isolated from norepinephrine-stimulated skin secretions of the South-American Santa Fe frog *Leptodactylus laticeps*. It is constituted of 25 residues, mostly leucines and glycines [2]. The lack of net positive charge and the high content of hydrophobic residues are probably responsible for the absence of a 'direct' antimicrobial activity. However, recent biological studies performed by our team revealed that Plasticin-L1 is an immunomodulatory agent, since it stimulated the release of cytokines by mice macrophages. Currently, the only structural information available on this peptide comes from an initial characterization performed through circular dichroism, which revealed a marked solvent-dependent conformational plasticity of Plasticin-L1 [1].

Then, in the attempt to clarify the behaviour of this interesting peptide, and thus to obtain some hints on the mode of action of immunomodulatory peptides, we determined a detailed structural model of Plasticin-L1. We applied liquid state nuclear magnetic resonance (NMR) and molecular dynamics (MD) simulations to characterize the 3D structure of Plasticin-L1 when bound to lipid membrane models, namely pure DPC and DPC/SDS (1/1) micelles. NMR analyses showed a folding into two distinct amphipathic helices encompassing the first and the last residues of the peptide sequence, separated by an unstructured loop in between, where the highest number of glycines is localized. The experimental data in combination with MD simulations led to a detailed peptide 3D structure. When in the presence of both DPC and DPC/SDS, it was found to be located at the micelle/water interface, and its insertion depth and orientation with respect to the micelle's surface resulted to be comparable and in agreement with results obtained by NMR paramagnetic enhanced relaxation experiments. These findings suggested a marked affinity of Plasticin-L1 for biological membranes models, either neutral and anionic ones, and indicate that Plasticin-L1 does not discriminate between eukaryotic- and bacterial-type membranes. Although, the present work surely cannot draw any conclusion about the possible implications of membrane affinity in peptide's immunomodulatory activity, it represents an interesting starting point to address further investigations [3].

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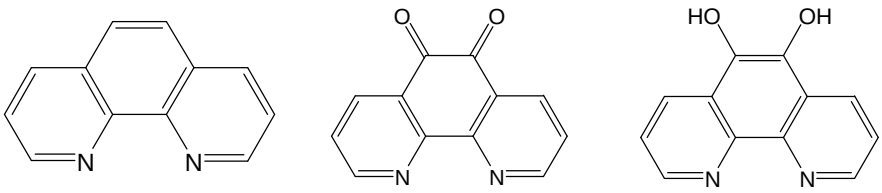
I complessi di Platino nel trattamento dei tumori: una nuova classe con leganti fenantrolinici e imidazolidine-2-tione

Federica Trudu[a], Elisa Valletta[a], Francesco Isaia[a], Sarah Vascellari[b], Elisa Carta[b], Alessandra Pani[b], Tiziana Pivetta[a] (f.trudu@unica.it)

[a]Dipartimento di Scienze Chimiche e Geologiche, [b]Dipartimento di Scienze Biomediche, Università degli Studi di Cagliari, 09042 Monserrato (CA)

L'utilizzo di composti di platino nella terapia antitumorale è iniziato negli anni 60' con la fortuita scoperta delle proprietà antitumorali del cisplatino [$Pt(Cl)_2(NH_3)_2$] [1]. Questo composto presenta un'alta attività citotossica su diversi tipi di tumori come per esempio tumore ai testicoli, al polmone, alla testa e al collo. Numerosi complessi di platino(II) sono stati testati allo scopo di ottenere farmaci attivi su altri tipi di tumore e di limitarne gli effetti collaterali; attualmente solo carboplatino e oxaliplatino [2] sono stati approvati per l'uso clinico. Alcuni tipi di cancro sono intrinsecamente resistenti ai farmaci a base di platino oppure sviluppano resistenza al farmaco o a intere classi di farmaci, anche non strutturalmente correlate. Gli effetti collaterali e la resistenza limitano l'utilizzo di tali composti in chemioterapia. La ricerca è quindi indirizzata a trovare complessi con attività citotossica simile a quella del cisplatino anche su tumori resistenti e con minore tossicità sistemica.
Nell'ambito di questo tema di ricerca sono stati sintetizzati dei complessi di Pt(II) con 1,10-fenantrolina (phen) e due suoi derivati (Fig.1). I complessi Pt(II)-phen sono in grado di intercalare tra coppie di basi del DNA, attivando processi di apoptosi [3].



1,10-fenantrolina | *1,10-fenantrolin-5,6-dione* | *1,10-fenantrolin-5,6-diolo*

Fig.1 Leganti azotati utilizzati e nomi IUPAC.

Sono stati sintetizzati complessi misti contenenti un chelante azotato e un legante ausiliario imidazolidine-2-tione variamente sostituito. L'attività citotossica dei complessi sintetizzati è stata studiata in vitro su diverse linee tumorali (DU-145, HEP-G2, SK-MES-1, CCRF-CEM, CCRF-SB). L'attività citotossica delle famiglie di complessi di Pt(II) è stata correlata alla polarità della molecola. L'attività del farmaco dipende infatti dalla sua polarità rispetto all'idrofilicità/lipofilicità del comparto ambientale del tumore. La polarità dei diversi complessi, espressa come momento di dipolo, quando non misurabile sperimentalmente, è stata calcolata con metodi quantomeccanici.

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THE ROLE OF Y-PARK9 PROTEIN IN PREVENTING MANGANESE-INDUCED PARKINSON'S DISEASE

Massimiliano Peana,[a] MariaAntonietta Zoroddu,[a] Serenella Medici,[a] Maurizio Remelli [b]
(email: peana@uniss.it)

[a] University of Sassari, Department of Chemistry and Pharmacy, Via Vienna 2, I-07100 Sassari, Italy [b] University of Ferrara, Department of Chemical and Pharmaceutical Sciences, Via L. Borsari 16, I-44100 Ferrara, Italy;

A variety of metals are essential trace elements but can reach localized toxic concentrations through various disease processes or environmental exposures and have been implicated as having a role in neurodegeneration. In particular, chronic inorganic manganese exposure causes selective toxicity to the nigrostriatal dopaminergic system, resulting in a Parkinsonian-like neurological condition known as Manganism. YPK9 gene (Yeast PARK9; also known as YOR291W) encodes a transmembrane P-type transport ATPase presumably involved in metal coordination and transportation, though its substrate specificity still remains unknown. Mutations in the human homolog of YPK9, PARK9 (ATP13A2), have been linked to genetic forms of early onset parkinsonism. Recently a strong genetic interaction between YPK9 and another Parkinson's disease protein, α-synuclein, has been evidenced in multiple model systems, indicating a crucial role for YPK9 in manganese detoxification in yeast and a specific protecting effect against manganese poisoning [1,3].

With the purpose to shed light on the protective property of YPK9 in Manganese-induced Parkinsonism, we tested the binding ability of Mn(II) and other divalent cations (Cu(II), Zn(II)) towards several peptide sequences from YPK9, with a particular focus on highly conserved sequences from yeast to human. The work was carried out at different pH values and ligand/metal molar ratios by means of potentiometric and spectroscopic techniques (multidimensional and heteronuclear NMR and UV-visible), in order to evaluate and compare the coordination propensity of such fragments with Mn(II) and the other metal probes selected [4,5].

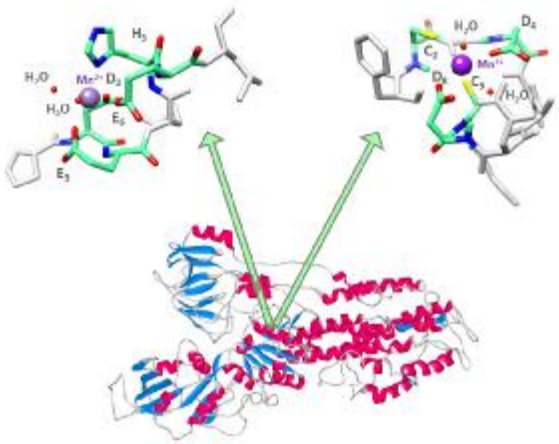

Figure 1. The model of the YPK9 protein built with ESyPred3D using the 3D crystal structure of the sodium-potassium pump (PDB 3B8E chain A) as the template, and the 3D structural models proposed for the Mn(II) ion complexed with selected fragments of YPK9 protein sequence.

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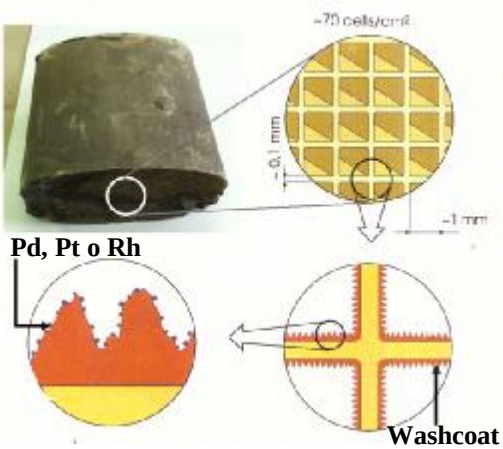
METODI DI RECUPERO ECO-COMPATIBILI DI METALLI NOBILI DA RIFIUTI HI-TECH: VALORIZZAZIONE E TRASFERIMENTO TECNOLOGICO

Americo Rigoldi, Paola Deplano, Maria Laura Mercuri, Angela Serpe
Dip. Scienze Chimiche e Geolog., Università di Cagliari, Citt.la Universitaria, 09042, Monserrato

La valorizzazione dei rifiuti rappresenta per la nostra società non solo una sfida ma un'esigenza dovuta anche dall'introduzione delle recenti normative europee ed extraeuropee in materia di gestione dei rifiuti [1]. Poiché il recupero dei metalli nobili quali Au, Pt, Pd e Rh, materiali strategici nell'elettronica e nella catalisi, è tradizionalmente basato su processi chimici a scarsa sostenibilità ambientale, è necessario lo studio e lo sviluppo di metodi di recupero eco-compatibili.



Questo lavoro si inquadra in un progetto che ha come obiettivo finale il recupero selettivo del Pd dai convertitori catalitici auto esausti del tipo TWC (Three-way catalyst) mediante l'utilizzo di un metodo, oggetto di brevetto, sviluppato negli ultimi anni dal gruppo di ricerca e messo a punto su catalizzatori modello ad invecchiamento controllato[2]. Il metodo si basa sull'uso di N,N'-dimethyl-perhydrodiazepine-2,3-dithione e consente di ottenere, sui campioni di sintesi, rese quantitative di recupero del palladio in condizioni blande (80°C) e con reagenti di facile impiego e a basso impatto ambientale.
Al fine di valutare l'efficacia del metodo sui catalizzatori reali, ancor prima di effettuare le prove di recupero del metallo d'interesse, è necessario affrontare due importanti problematiche: i) la caratterizzazione del catalizzatore in termini di contenuto dei metalli presenti; ii) l'eliminazione di eventuali interferenze metalliche e non metalliche derivanti dal ciclo di vita del catalizzatore stesso. Nella presente comunicazione si presenteranno i soddisfacenti risultati ottenuti nella disgregazione e caratterizzazione dei supporti catalitici selezionati ed opportunamente triturati. I convertitori catalitici studiati sono infatti costituiti da un supporto ceramico refrattario di cordierite ($2MgO\text{-}2Al_2O_3\text{-}5SiO_2$), distribuito a formare una struttura "a nido d'ape" caratterizzata da circa 70 celle/cm^2, rivestita da una soluzione solida chiamata "washcoat" ($Al_2O_3/CeO_2/ZrO_2$) sulla quale vengono depositati i metalli attivi (Pt, Pd e Rh), cosi come rappresentato in Figura. Il monolita ceramico è estremamente friabile, può quindi essere ridotto in polvere con relativa facilità, ma è difficilmente attaccabile chimicamente per portarlo in soluzione al fine di una completa caratterizzazione. Grazie alle tecniche di mineralizzazione a microonde e selezionando opportunamente le condizioni sperimentali è stato possibile ottenere la completa dissoluzione dei campioni ed effettuare l'analisi quantitativa del materiale mediante spettroscopia di emissione atomica a plasma ad Accoppiamento induttivo (ICP-AES) ottenendo risultati estremamente riproducibili sul tenore dei metalli nobili contenuti. Verranno inoltre riportati i risultati preliminari relativi ai protocolli di lavaggio del materiale ceramico polverizzato, utilizzando soluzioni acide diluite al fine di eliminare le interferenze metalliche e non metalliche presenti nel catalizzatore ed evidenziate dalla caratterizzazione chimica. L'ottimizzazione del processo di lavaggio consentirà di procedere al recupero del Pd per reazione con i lisci vianti selezionati e verificare l'efficienza del metodo sui catalizzatori reali.

Si ringrazia la Regione Autonoma della Sardegna e la Fondazione Banco di Sardegna per il sostegno finanziario e le aziende West Recycling e 3R Metals partners del progetto.

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DERIVATI DELL'IBUPROFENE QUALI INIBITORI DUALI DI FAAH E COX

Alessandro Deplano[a], **Cenzo Congiu**[a], **Valentina Onnis**[a], **Christopher Fowler**[b]
(deplano.a@gmail.it)

[a]Dipartimento di Scienze della Vita e dell'Ambiente, Università di Cagliari, Via Ospedale 72 – Cagliari Italy

[b] Department of Pharmacology and Clinical Neuroscience, Umea University, Sweden

La modulazione del tono del sistema cannabinoide può essere sfruttata per la terapia di diverse patologie tra cui il dolore e l'infiammazione, risultano infatti fondamentali per questa attività i recettori dei cannabinoidi. Inibendo la FAAH, idrolasi delle amidi degli acidi grassi, enzima deputato principalmente alla degradazione dell'anandamide, il più importante ligando endogeno dei recettori dei cannabinoidi si provoca un aumento localizzato dei livelli dell'endocannabinoide nei siti in cui fisiologicamente è attivata la loro produzione, evitando così gli effetti collaterali causati dall'attivazione globale del sistema cannabinoide. Inoltre composti che agiscano contemporaneamente sia sulle ciclossigenasi (COX) sia sul sistema cannabinoide consentono di ottenere un effetto sinergico, infatti è stato dimostrato che la somministrazione congiunta di un inibitore FAAH insieme ad un FANS, produce un effetto analgesico a concentrazioni decisamente più basse rispetto alla somministrazione del solo FANS, inoltre anche l'effetto ulcerogeno tipico di questa classe di composti risulta notevolmente ridotto [1].

In questa comunicazione verrà descritta la sintesi e l'attività biologia di derivati amidici dell'ibuprofene che presentano attività inibitoria duplice sia sulle COX sia sulla FAAH. L'ibuprofene [2] infatti presenta un scarsa attività nei confronti della FAAH quindi si è cercato di modificarlo al fine di ottenere un bilanciamento ottimale dell'attività inibitoria nei confronti dei due enzimi attraverso la formazione di derivati amidici ottenendo così un effetto additivo dovuto all'inibizione contemporanea dei due enzimi.

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NUOVI COMPLESSI DI RAME(II) CON DERIVATI DELL'1,10-FENANTROLINA: SINTESI, EQUILIBRI IN SOLUZIONE, ATTIVITÀ CITOTOSSICA E DNA-BINDING

Elisa Valletta[a], Federica Trudu[a], Francesco Isaia[a], Daniela Perra[b], Elisabetta Pinna[b], Alessandra Pani[b], Carlo Castellano[c], Francesco Demartini[c], Tiziana Pivetta[a]
(*elisa.valletta@unica.it*)
[a]Dipartimento di Scienze Chimiche e Geologiche, [b]Dipartimento di Scienze Biomediche, Università degli Studi di Cagliari, Cittadella Universitaria – 09042 Monserrato – Cagliari; [c]Dipartimento di Chimica,Università degli Studi di Milano, 20133 Milano;

La scoperta del cisplatino come farmaco anticancro ha aperto una nuova era nella cura contro i tumori. Il cisplatino viene utilizzato per la cura di diversi tumori, ma il trattamento è limitato da vari effetti collaterali, come neuro e nefrotossicità. Complessi con ioni metallici essenziali possono essere meno tossici di quelli con ioni non essenziali [1]. Il rame è presente in tutti gli organismi viventi ed è importante per la funzione di diversi enzimi e proteine coinvolti nel metabolismo energetico, nella respirazione e nella sintesi del DNA. Alcuni complessi di rame(II) e 1,10-fenantrolina (phen) sono in grado di scindere la molecola del DNA [2] e $[Cu(phen)_2(OH_2)](ClO_4)_2$ è stato efficacemente testato su cellule di neuroblastoma murino e su diverse linee cellulari tumorali umane [3-5].
In questo lavoro vengono presentati i risultati preliminari sulla reattività chimica e biologica tra rame(II) e phen, 1,10-fenatrolina-5,6-dione (phendione) e 1,10-fenantrolina-5,6-diolo (phendiolo) (Fig.1).

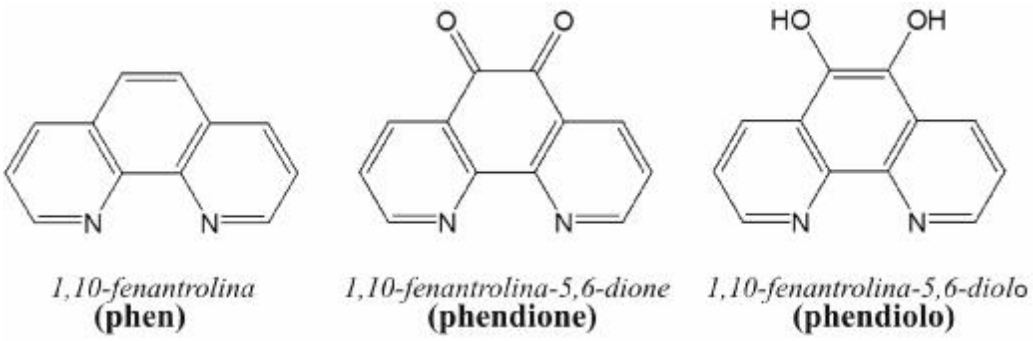

Figura 1. Struttura, nome IUPAC e acronimi dei leganti studiati.

Sono stati studiati gli equilibri in soluzione attraverso titolazioni potenziometriche in NaCl 0,1 M a 25 e 37 °C. E' stata testata l'attività antiproliferativa dei complessi sintetizzati e dei leganti da soli su linee cellulari tumorali umane (DU-145, carcinoma prostatico; HEP-G2, carcinoma epatocellulare; SK-MES-1, carcinoma del polmone; CCRF-CEM, leucemia T-linfoblastica acuta; CCRF-SB, leucemia B-linfoblastica acuta) e sulla linea umana normale (CRL-7065, fibroblasti cutanei). Sono state determinate le costanti di binding tra i complessi di rame(II) e DNA (calf thymus DNA) attraverso titolazioni spettrofotometriche a 25 °C in PIPES 0,01 M a pH 7.0.

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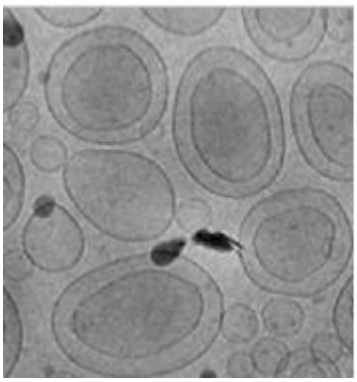
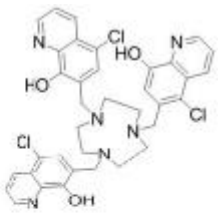
NAAOT/C_{12}MIMBR CATANIONIC VESCICLES AS NANOCARRIER FOR FLUORESCENT CHEMOSENSORS

Valeria Meli,[a] Francesco Caddeo,[a] Claudia Caltagirone,[a] Sandrina Lampis,[a] Vito Lippolis,[a] Maura Monduzzi, Sergio Murgia [a]

[a]Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, S.S. 554 bivio per Sestu, I 09042 Monserrato (CA).

A new OFF-ON fluorescent chemosensor for Cd^{2+} recognition based on 1,4,7,10-triazacyclododecane and three 5-chloro-8-hydroxyquinoline moieties is synthesized and its photochemical properties in solution both in MeCN/H_2O 1:1 and in pure water are studied. We found out that in the latter case the enhancement of the fluorescence emission due to the selectivity of the ligand towards Cd^{2+} was damped. With the aim to overcome this quenching effect by the water and make the ligand suitable for environmental analysis, a new vesicular formulation based on sodium bis(2-ethylhexyl) sulfosuccinate (NaAOT) and 1-dodecyl-3-methylimidazolium bromide (C_{12}mimBr an ionic liquid) aqueous mixture is presented. Samples of the vesicular system with different NaAOT/C_{12}mimBr ratio were prepared and their physicochemical properties investigated through DLS, SAXS and Cryo-TEM techniques.





Enclosing the chemosensor within the bilayer of the catanionic vesicles its fluorescence emission upon addition of Cd^{2+} is actually regained, making possible the detection of Cd^{2+} in aqueous media.

A COARSE-GRAINED MODEL FOR DIFFUSION IN ZEOLITES BASED ON CLUSTERING OF SHORT MD TRAJECTORIES

Alberto M. Pintus, Andrea Gabrieli, Federico G. Pazzona, Pierfranco Demontis, Giuseppe B. Suffritti (spintus@uniss.it)

Dipartimento di Chimica e Farmacia, Università degli Studi di Sassari, Via Vienna 2 , 07100 Sassari

Zeolites form a class of microporous aluminosilicates of great interest due to their multifarious applications in industry and everyday life. Their porous structure allows small molecules to be adsorbed and to diffuse inside crystals, and depending on the zeolite type and on the diffusant species a variety of behaviours is possible. Molecular Dynamics is now widely used in order to understand the microscopic mechanisms of adsorption and diffusion occurring within these materials as well as in MOFs and ZIFs [1]. A major drawback of MD for this kind of systems is its high computational cost, so that coarse-grained methods, speeding up simulations without losing the essential features of dynamics, are valuable tools for exploring the behaviour of guest molecules on time and space scales hardly, if at all, reachable with ordinary MD.

The first step in our proposed method is the clustering of MD trajectories to obtain a discretized version of the motion of adsorbed molecules within the zeolite. Each pore in the aluminosilicate is partitioned in a number of regions and each point in the original trajectory is mapped to the proper region based on a distance criterion. The regions correspond roughly to the main basins in the potential energy surface (PES).

This discrete trajectories in space are then mapped to moves-space trajectories: given a certain lag-time we replace the two discrete positions at the start and end of each interval with the corrisponding discrete displacements. Using the free software EMMA [2] we then perform a statistical analysis of the trajectories and obtain the transition probabilities from each discrete move to each other as a transition matrix. This matrix is at the basis of the evolution rule of the model.

Considering the transitions between moves allows one to circumvent the inherent non-markovity of the space partition, at least to a reasonable degree of approximation. Simulating the motion of guest molecules as a simple random walk on the lattice of regions obtained in the first step of coarse-graining would be inaccurate due to the low barriers in the PES, expecially at low loadings. By considering the transitions between moves, short time memory effects are naturally taken into account and this allows us to treat the dynamics of interest as a simple random walk in the moves-space, ruled by the transition matrix. The trajectory on this space then naturally implies a trajectory in the real discretized space.

Our method gives self-diffusivity, moves frequency and occupation probabilities of regions and pores in good agreement with the MD results for spherical, or roughly spherical, guest molecules, such as Ar, Kr, Xe and CH4 in zeolite ZK4. The application to other molecular geometries and zeolite types is currently under study.

This suggests the algorithm can be succefully used for the simulation of massive zeolite-like systems, with various sorbates, for time scales substantially longer than previously possible on ordinary machines.

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DEVELOPMENT OF RELIABLE CLASSICAL FORCE FIELDS FOR SIMULATIONS IN MICROPOROUS MATERIALS

Andrea Gabrieli, Marco Sant, Pierfranco Demontis, Giuseppe B. Suffritti
(agabrieli@uniss.it)
Dipartimento di Chimica e Farmacia, Università degli Studi di Sassari, via Vienna 2, 07100, Sassari

Microporous materials, such as zeolites [1], receive continuously strong attention from the scientific community, thanks to their widespread application in industrial processes (e.g., heterogeneous catalysis and gas separation, among many others).
In recent years, the increase of the computational power has made possible to study with *ab-initio* methods a wide number of systems. Despite that, as today, it is possible to perform a Born Oppenheimer Molecular Dynamics (BOMD) simulation only (without a supercomputer) for small systems (hundreds of atoms) and for short trajectory length (several ps).
For this reason the most common tool to investigate the diffusion of sorbed molecules inside these materials is the classical Molecular Dynamics technique, but, in order to perform reliable simulations one has to provide a full force field [2,3] to describe the system interactions.
The aim of this work is to obtain such force field starting from data obtained via DFT computations by means of a technique called force matching [4] which allows the automated search of the best parameters. The force matching procedure allows reproducing high quality results (DFT), by means of less expensive computations (classical MD).
The data are collected by performing short BOMD runs. The accuracy of the whole procedure is verified computing the Infra-Red (IR) spectra via both BOMD and classical MD, and comparing them with the experimental ones taken from the literature.

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Complessi di oro con leganti imidazolici di interesse farmacologico

Maria Serratrice, Maria Agostina Cinellu, Sergio Stoccoro, Antonio Zucca
Dipartimento di Chimica e Farmacia, Via Vienna 2 - 07100 Sassari

L'imidazolo gioca un ruolo importante nella chimica biologica, difatti costituisce un componente laterale dell'istidina, amminoacido essenziale, e si trova anche in molte proteine.
Molti farmaci attualmente in uso come antifungini sono caratterizzati dalla presenza di anelli imidazolici, per esempio l'econazolo e il miconazolo.
Essendo questo eterociclo un composto importante sia all'interno dell'organismo che nell'industria farmaceutica, l'interesse verso la sintesi di nuovi farmaci contenenti anelli imidazolici cresce nel campo della ricerca, anche in quello degli antitumorali.
Sono già noti complessi con il Rutenio con proprietà antitumorali ed antimetastatiche che si trovano in fase clinica avanzata come per esempio il NAMI-A[1].
Nel nostro gruppo di ricerca da anni ci si occupa della sintesi di complessi con leganti eterociclici azotati, con metalli di transizione come oro, platino e palladio, sia con scopi catalitici che con scopi farmaceutici.
Nello specifico il mio lavoro si è basato sulla sintesi di complessi di oro(I) e oro(III) con leganti contenenti anelli imidazolici.
Una serie di complessi di Au(I/III) sia mono che dinucleari e anche misti eterodinucleari Au(I)/ Pt(II) sono stati ottenuti con il legante 2-(2'-piridil)benzoimidazolo, quasi tutti sono stati testati sulla linea cellulare del tumore ovarico umano A2780, sia R che S e si è studiato il loro comportamento mediante spettroscopia UV-Vis simulando l'ambiente fisiologico, a 37°C, per 72h sia in assenza che in presenza di ascorbato di sodio[2].
Con i leganti 2-(2'-piridilimidazolo), 2-fenilimidazolo e 2,6-bis(benzoimidazo-2-yl)piridina si son sintetizzati dei complessi di Au(I/III) che son stati testati sulle linee cellulari A2780 R ed S, MCF7 e son stati condotti degli studi sull'interazione con la proteina PARP-1[3].
Infine con i leganti 1,3 bis(benzoimidazolil)benzene e 1,3-bis (2-metibenzoimidazolil)benzene si sono ottenuti una serie di complessi dinucleari di oro(I) sui quali al momento sono in corso studi di citotossicità.

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AL-SBA-15 FOR THE PRODUCTION OF METHYL LACTATE FROM C_3-SUGARS

Danio Perra, Daniela Meloni, M. Giorgia Cutrufello (perra.d@unica.it)
Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, Complesso Universitario di Monserrato

Lactic acid is an interesting platform chemical with many promising applications. These include the use as a building block for the production of biodegradable plastics and environmentally friendly solvents. [1] The most common commercial processes for the production of lactic acid are based on carbohydrate fermentation; lactic acid is then generally converted to his methyl ester to facilitate separation from the reaction mixture. Drawbacks of such processes include low productivities and the need for expensive and energy inefficient separation and purification steps. In this context, the development of an alternative, sustainable method for producing lactic acid and lactates from renewable sources would be of great relevance. [2] Lactic acid and its esters can be obtained by catalytic conversion of trioses (dihydroxiacetone and/or glyceraldehydes), that can be produced from biomass feedstock.
Production of methyl lactate from trioses monosaccharides using Al-SBA-15 catalysts has been studied. Five samples of Al-SBA-15 mesostructrured material were prepared by the "pH adjustment" method, with different Si/Al ratio to vary their acidity. Each catalyst was characterized by ICP-AES for elemental analysis, XRD for structural properties and N_2 adsorption-desorption for textural properties. Catalytic tests were performed in 15 cm^3 pressure tubes with magnetic stirring. In each run, 80 mg catalyst, 1.25 mmol dihydroxyacetone, and 4 g methanol were added and mixed. The pressure tube was then dipped into an oil bath 115 °C and the reaction was followed for 24 hours. The main reaction products, methyl-lactate and pyruvaldehyde dimethyl-acetale, were analyzed by gas-chromatography using n-eptane as an internal standard.
The Al-SBA-15 samples were synthetized with Si/Al ratios between 6 and 61 as confirmed by ICP-AES analysis. From low angle XRD analysis an ordered mesopore structure was observed. N_2 adsorption-desorption experiments showed large BET surface area (between 350 and 650 m^2/g) and regular pore diameter (6.5 nm). Decreasing the Si/Al ratio of the catalyst the 24 hour yields in methyl lactate increased from 4 to 70 %. It is likely that lowering the Si/Al ratio increases the number of Lewis acid sites with respect to the Brønsted acid sites. Lewis acid sites are probably the active catalytic sites for the formation of methyl-lactate.

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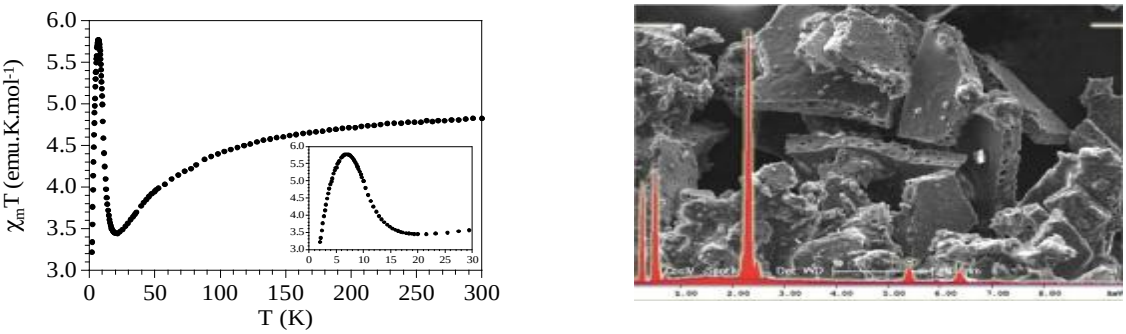
Processing of multifunctional materials: conducting PEDOT thin films doped with magnetic complexes

E. Sessini,[a] M. Atzori[a], F. Artizzu[a], P. Deplano[a], A. Serpe[a], G. Concas[c], C. J. Gomez-Garcia[b] and M. L. Mercuri[a] (e.sessini@unica.it)

a) Dip. di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari-S.S. 554 - Bivio per Sestu-09042 Monserrato (CA) – Italy; b) Dip. di Fisica, Università degli Studi di Cagliari-S.S. 554 - Bivio per Sestu-09042 Monserrato (CA) – Italy; c) Institute for Molecular Science, University of Valencia, Valencia-Spain

In the field of magnetic molecular conductors, mono- and hetero bi-metallic oxalato complexes have been chosen as carriers of magnetism in a large number of these materials and peculiar examples are $[(BEDT\text{-}TTF)_3][MnCr(ox)_3]$, a molecular ferromagnetic metal [1] and $[(BEDT\text{-}TTF)_4][(H_2O)Fe(ox)_3]\cdot C_6H_5CN$, a paramagnetic superconductor [2].

Recently, much research efforts have been addressed to the development of processing methodologies for the incorporation of magnetic systems into polymeric conducting matrices as thin films. Among the conducting organic polymers, poly(3,4-ethylenedioxythiophene) (PEDOT) have been selected for several advantageous properties: low oxidation potential, high conductivity, high transparency in thin, oxidized films. [3,4] The aim of this work is to integrate in PEDOT films different magnetic complexes following different methods (chemical or electrochemical polymerization) tailored on the chemical nature of metal complexes. Therefore mono- and hetero bi-metallic complexes based on oxalato, croconato and anilato ligands with Fe^{III} and Cr^{III} metals have been synthesized. They have been embedded into the PEDOT matrices. Particularly, the thin film, doped with $[Fe^{II}Cr^{III}(ox)_3]^-$ anion (**1**), show ferromagnetic coupling due to Fe^{II} - Cr^{III} ions and a superparamagnetic behavior in the doped polymer (Figure1, a). Also SEM images and mapping, EDX analyses (Figure 1, b) and conducting measurements have been performed.



(a) (b)

Figure 1: (a) Thermal variation of the $\chi_m T$ product for (**1**); inset shows the low temperature region; (b) SEM micrography and EDX analysis for (**1**) thin film.

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RESVERATROL-LOADED NANOPARTICLES BASED ON POLYMERIC BLEND FOR PROSTATE CANCER TREATMENT

Vanna Sanna,[1,2] **Imtiaz A. Siddiqui**,[2] **Mario Sechi**,[1,2] **Hasan Mukhtar**[2]

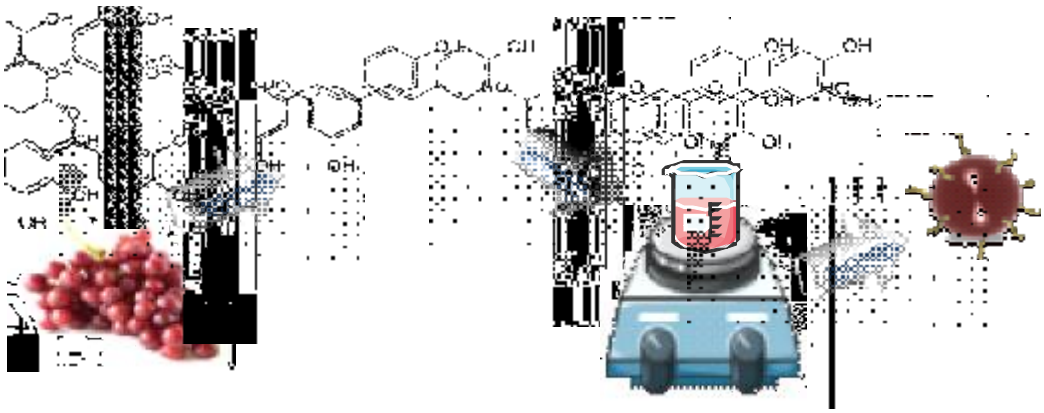
[1]Department of Chemistry and Pharmacy, Laboratory of Nanomedicine, University of Sassari, Sassari, Italy

[2]University of Wisconsin-Madison, Madison, WI

The trans-resveratrol (RSV) has been reported to act as an antiproliferative and chemopreventive agent against a wide variety of tumors, including prostate cancer (PCa)[1,2]. Nanoencapsulation of RSV represents a powerful strategy to provide protection of degradation, enhancement of bioavailability, improvement of intracellular penetration and control delivery[3,4].

We developed novel polymeric nanoparticles (NPs) encapsulating RSV (nano-RSV), based on a polymeric blend, as effective prototypes for PCa treatment. NPs were characterized in terms of morphology, encapsulation efficiency, and in vitro release studies. Moreover, cellular uptake and antiproliferative efficacy of nano-RSV in PC-3, DU-145, and LNCaP cell lines, were evaluated.

RSV was successfully loaded in NPs with an average diameter of 150 nm and encapsulation efficiencies ranging from 74% to 98%. NPs are able to control the RSV release at pH 6.5 and 7.4, with only 55% of RSV released within 7 h. On the other hand, in gastrointestinal simulated fluids, NPs released about 55% of RSV in the first 2 h in acidic medium, and their total RSV content within the subsequent 5 h at pH 7.4. Confocal fluorescence microscopy revealed that NPs were efficiently taken up by PCa cell lines. Furthermore, nano-RSV significantly improved the cytotoxicity than that of free RSV in all tested cell lines, both at 10 µM and 20 µM concentrations. Our results support the potential use of these prototypes for the controlled delivery of RSV for PCa treatment.



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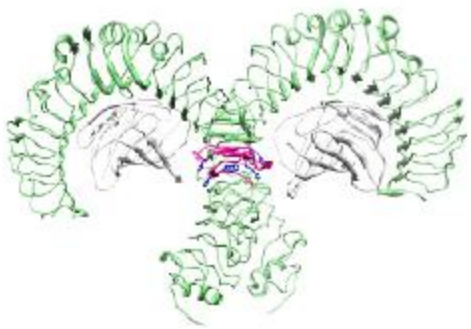
Ni(II) BINDING TO THE HUMAN TOOL LIKE RECEPTOR (HTLR4)

Massimiliano Peana,[a] MariaAntonietta Zoroddu,[a] Serenella Medici,[a] Slawomir Potocki,[b] Henryk Kozlowski[b] (email: peana@uniss.it)

[a] University of Sassari, Department of Chemistry and Pharmacy, Via Vienna 2, I-07100 Sassari, Italy [b] Department of Chemistry, University of Wroclaw, F. Joliot-Curie 14, 50-383 Wroclaw, Poland.;

Nickel allergy is the most frequent cause of contact hypersensitivity (burning, redness, itching, swelling and even blisters) in industrialized countries, with 30% of population being affected. Contact allergy is commonly induced by nickel ions present in nickel-containing jewelry such as rings and earrings, as well as in nickel-containing cellular telephones. Ni(II) seems to trigger an inflammatory response by activating human Toll-like-Receptor 4 (hTLR4) [1-4]. Species-specific activation, as in this case, requires distinct sequence motifs that are present in humans but not in mouse, a species not sensitive to nickel-induced allergies. A sequence containing three histidine residues, H_{431}, and the non-conserved H_{456} and H_{458}, localized in the C-terminus, could be identified as the specific region of human TLR4 responsible for nickel responses. It has been proposed that the imidazole side chain of the histidine residues H_{456} and H_{458} may provide a potential binding site for this metal because they are located at an optimal distance to interact with Ni(II) ions, whereas H_{431} is located further apart. The aim of our research was to verify the possibility of metal binding to the sequence containing the three histidines supposedly involved in nickel response. The chosen segment was the 32aa peptide FQH_{431}SNLKQMSEFSVFLSLRNLIYLDISH_{456}TH_{458}TR, which was studied in order to understand both its binding properties and the thermodynamic stability of its metal complexes. Formation equilibria of Ni(II) complexes have been investigated in aqueous solution and in a wide pH range. Protonation and complex-formation constants have been potentiometrically determined; complex-formation models and species stoichiometry have been checked by means of UV-Vis absorption and CD spectroscopy and investigation through multidimensional and eteronuclear NMR spectroscopy. The predominant species for a 1:1 peptide/Ni(II) molar ratio was obtained at physiological pH and showed an effective binding of the metal to the target sequence.



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ROLE OF STRUCURAL AND TEXTURAL PROPERTIES OF FeBTC- MOF IN ADSORPTIVE DESULPHURIZATION OF DIESEL FUEL

M. Pilloni[a], M. Bellusci[b], C. Delitala[c], G. Ennas[a], I. Ferino[a] S.Lai[a] , M. Pentimalli[b], E. Rombi[a], A. Scano[d], F. Sini[a] and F. Padella[b] (martina.pilloni@unica.it)

[a]Università degli Studi di Cagliari, Dipartimento di Scienze Chimiche e Geologiche, s.p. Monserrato-Sestu Km 0.700, 09042 Monserrato (Ca), Italia

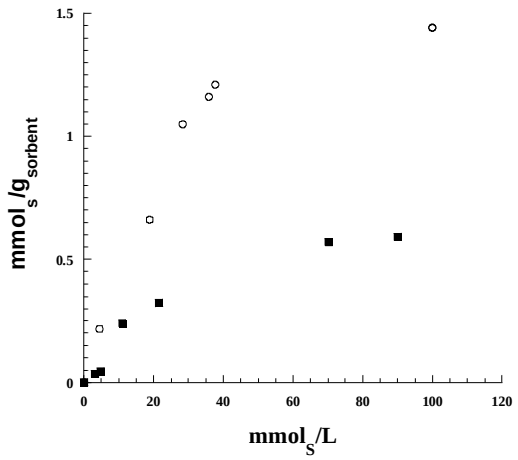
[b]ENEA - Agenzia Nazionale per le Nuove Tecnologie, l'Energia e lo Sviluppo Economico Sostenibile , via Anguillarese 301, 00123 Roma, Italia

[c]Saras Ricerche e Tecnologie SpA, V strada, trav. C, Z.I. Macchiareddu, 09032 Assemini, Italia

[d]Centro de Ingenieria Avanzada de Superficies, AIN, Carretera Pamplona,1 31191 Cordovilla (Navarra) Spain

Metal Organic Frameworks (MOFs) are inorganic–organic hybrid materials assembled by coordination bonds between metal ions or polynuclear metal cluster and multidentate organic linker. The coordination bonds give arise a strong crystalline structures with exceptionally high porosity and high specific surface area. Regarding the synthesis of MOFs, different methods has been proposed in literature [1]. The main objective in MOF synthesis is to create the conditions that lead to defined inorganic building blocks without decomposition of the organic linker. Moreover the kinetics of crystallization must be appropriate to allow the nucleation and growth of the desired phase. Different synthetic methods can lead to compounds with different particle sizes, size distributions and morphologies features that have an important influence on the material's properties.

This work report an experimental comparison of two different sample: Fe_3BTC_2-MOF(BTC: 1,3,5-benzenetricarboxylate) obtained in our laboratory and the corresponding commercial product Basolite F300 (BAFS).The Fe_3BTC_2-MOF, synthesized with a mechanochemical route, was a no fluorinate crystalline porous material which display two types of mesoporous cages (25 and 29 Å) accessible through microporous windows (5.5 and 8.6 Å) [2]. The samples characterization by different techniques, XRPD, TGA , FT-IR, SEM and microcalorimetry was reported and discussed.



The samples were tested on 4,6-dimethyl-dibenzothiophene (4,6DMDBT) adsorption from diesel fuel in a typical batch experiment[3]. The results of 4,6DMDBT adsorption were reported (Fig.1) and the different performances on adsorptive desulphurization of diesel fuel has been discussed in the light of the structural and textural differences between the two materials.

Fig.1 Adsorption isotherms of 4,6DMDBT in diesel fuel on FeBTC-MOF (o) and F300(■) samples at 298K and atmospheric pressure

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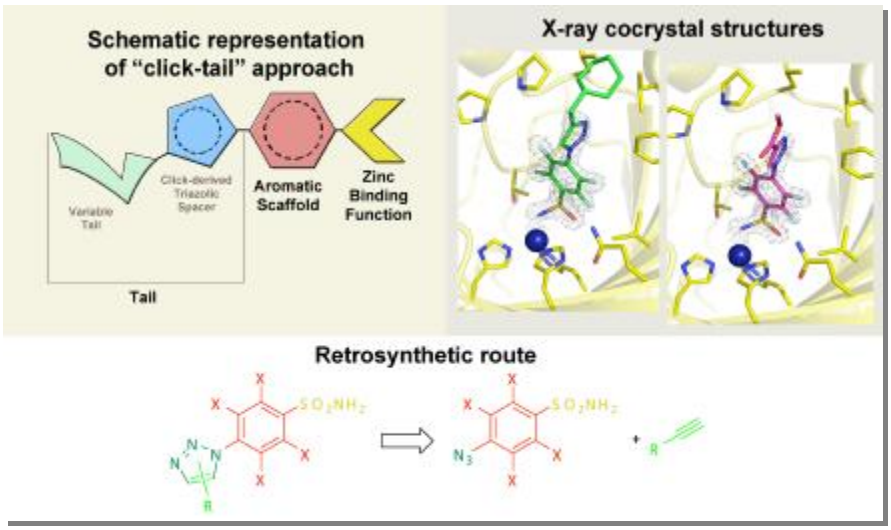
THE "CLICK-TAIL APPROACH" FOR THE DESIGN AND SYNTHESIS OF NOVEL CARBONIC ANHYDRASE INHIBITORS

Nicolino Pala[a], Laura Micheletto[a], Simone Ihm[a], Fabrizio Carta[b], Robert McKenna,[c] Claudiu T. Supuran[b], Mario Sechi[a] (nikpal@uniss.it)

a) Dipartimento di Chimica e Farmacia, Università di Sassari, via Vienna 2, 07100 Sassari, Italy; b) Università degli Studi di Firenze, Polo Scientifico, Laboratorio di Chimica Bioinorganica, Via della Lastruccia 3, 50019 Sesto Fiorentino (Firenze), Italy; c) Department of Biochemistry and Molecular Biology, College of Medicine, University of Florida, Box 100245, Gainesville, FL 32610, USA; d) Università degli Studi di Firenze, NEUROFARBA Dept., Sezione di Scienze Farmaceutiche, 50019 Sesto Fiorentino (Firenze), Italy.

The Carbonic Anhydrases (CAs) are a family of zinc enzymes deputed to the interconversion of carbonic dioxide to hydrogen carbonate. Factors such as primary sequence, localization, activity and tissue distribution concur to differentiate XVI mammalian isoforms. In human, CAs are involved in several physiopathological processes including respiration, acid/base homeostasis, calcification, gluconeogenesis, lipogenesis, glaucoma, high blood pressure, oedema, epilepsy, obesity, and cancer. In this context, CAs are emerged as important biological targets for several therapeutic applications.[1,2] To date, a plethora of compounds have been tested for their inhibitory activity against CAs[1-3] and, among them, the compounds bearing a substituted arylsulfonamide chemotype constitute the most important chemical class. Such chemical scaffold presents a well know pharmacophoric pattern constituted by an aromatic moiety bearing a Zinc Binding Function (ZBF) and a variable tail.[4] Herein, we report on a sustainable modular strategy, also called "click-tail approach",[5] used to obtain two series of 4-(4-substituted-1*H*-1,2,3-triazol-1-yl)benzenesulfonamides. Design and synthesis strategies, x-ray derived CA-ligand binding mode and enzyme-based inhibition results will be presented.



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