Università di Sassari

Società Chimica Italiana
Sezione Sardegna

Università di Cagliari

La parola ai giovani 2014

Venerdi 5 Dicembre 2014,
Dipartimento di Chimica e Farmacia
Complesso Didattico, Aula Magna A, Via Vienna 2

Il comitato organizzatore:
Prof. Giuseppe Baldovino Suffritti,
Dr. Gabriele Mulas,
Dr.ssa Silvia Gaspa.

La XIII edizione del convegno “La Parola ai Giovani”, organizzato quest’anno dall’Università degli Studi di Sassari con il patrocinio della SCI, Società Chimica Italiana (Sezione Sardegna), dà la possibilità, come dice il titolo stesso del convegno, ai giovani ricercatori di esporre i risultati delle loro ricerche sia come presentazione orale sia sotto forma di poster.

Società Chimica Italiana

Sezione Sardegna

Si ringraziano la Assing S.p.A. per il supporto finanziario e il Dipartimento di Chimica e Farmacia per il sostegno alle attività di organizzazione del Convegno.

Il comitato organizzatore

Prof. Giuseppe Baldovino Suffritti

Dr. Gabriele Mulas

Dr.ssa Silvia Gaspa

PROGRAM

9.30-9.50	**REGISTRATION**		
9.50-10.00	**OPENING CEREMONY**		
10.00-10.40	Chairperson: Prof.re Stefano Enzo (UniSS)		
10.00-10.40	INV1: DOTT. LUTTEROTTI L.- The combined analysis approach for the characterization of materials		
10.40-11.30	**SESSION A** Chairperson: Marco Orecchioni (UniSS)		
	10.40	O1	GABRIELI A.- Optimization of Molecular Dynamics force fields for microporous materials
	10.50	O2	VALENTONI A.- Effects of metal halides on the desorption properties of the system $2LiNH_2+LiH+KBH_4$
	11.00	O3	REBIC M.- Coarse Grain simulations of non-canonical DNA structures
	11.10	O4	SESTU M.- Studying the structure of poorly crystalline materials using Debye Equation and Reverse Monte Carlo refinement
	11.20	O5	MANSOORI D.- Crystallographic characterisation and solution equilibrium study of 6,6'-(((2-(diethylamino)ethyl)azanediyl)bis(methylene))bis(5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one)
11.30-12.00	**COFFEE BREAK/ POSTER SESSION**		
12.00-13.20	**SESSION B** Chairperson: Donatella Farina (UniSS) + Matteo Sestu (UniCa)		
	12.00	O6	COCCO F.- XPS and XAES characterization of copper and zinc chemical states applied to brass alloys
	12.10	O7	CASTI M.- Salt crystallisation decay on monuments: the archaeological site of “Viale Trieste 105 in Cagliari”
	12.20	O8	MURRU A.- Cortical reinforcement for the conservation of Cultural Heritage: the Beata Vergine delle Grazie's church façade, Masullas (OR)
	12.30	O9	CABRAS V.- Mechanochemical Synthesis Study of a 2D Layered Compound
	12.40	O10	CARA C.- Dialkylamide-capped magnetite nanoparticles via a direct solvothermal synthesis
	12.50	O11	UGONE V.- Characterization of the coordination modes of flavonoids towards oxidovanadium(IV)
	13.00	O12	LAI R.- A brand new synthesis and characterization of 1,4-bis-(3-Pyridyl)butadiyne as spacer in the preparation of coordination polymers.
	13.10	O13	SANNA D.- Advances in the Frontal Ring Opening Metathesis Polymerization of Dicyclopentadiene
13.20-15.30	**LUNCH/ POSTER SESSION**		
15.30-16.10	Chairperson: Dr. Andrea Porcheddu (UniSS)		
15.30-16.10	INV2: DOTT. CARTA M.- Polymers of Intrinsic Microporosity (PIMs): organic multi-functional materials		
16.10-16.40	**SESSION C** Chairperson: Andrea Gabrieli (UniSS) + Federica Cocco (UniCA)		
	16.10	O14	CASULA A.- Asymmetric bis-ureidic receptors: synthesis, anion binding and sensing studies
	16.20	O15	CAPITTA F.- “Quick and click” assembly of functionalised indole rings via metal-promoted cyclative tandem reactions
	16.30	O16	GASPA S.- One-pot syntheses of hydroxamic acids from alcohols or aldehydes

16.40-17.00	**COFFEE BREAK/ POSTER SESSION**		
17.00-17.50	**SESSION D** Chairperson: Patrizia Monti (UniSS) + Claudio Cara (UniCA)		
	17.00	O17	MELIS N.- Synthesis of cyclobutanone α-amino acid derivatives through tandem condensation-asymmetric tautomerization sequence
	17.10	O18	DEMURTAS M.- Design, synthesis and pharmacological investigation of new FAAH inhibitors
	17.20	O19	SERRA I.- Dendrimeric peptides with membranolytic activity
	17.30	O20	ORECCHIONI M.- Carbon nanomaterial immunomodulators are able to fight immune function dysregulation in simulated spaceflight conditions
	17.40	O21	IDDA I.- Development and validation of a new GC-FID method for the determination of mono and disaccharides in milk and dairy foods
17.50-18.20	**CLOSING CERIMONY**		

Invited talks:

INV1) The combined analysis approach for the characterization of materials

Luca Lutterotti (luca.lutterotti@unitn.it)
Dipartimento Ingegneria Industriale, Università degli Studi di Trento, via Sommarive, 9, 38123-Trento, Italy

INV2) Polymers of Intrinsic Microporosity (PIMs):organic multi-functional materials

Mariolino Carta[a] (mariolino.carta@ed.ac.uk), C. Grazia Bezzu[a], Richard Malpass-Evans[a], Ian Rose[a], Neil B. McKeown[a], Johannes C. Jansen[b], Paola Bernardo[b], Gabriele Clarizia[b].
[a.] School of Chemistry, University of Edinburgh, David Brewster Road, EH9 3FJ Edinburgh, United Kingdom.
[b.]Institute on Membrane Technology, ITM-CNR,, c/o University of Calabria, Via P. Bucci 17/C, 87030 Rende (CS), Italy

Oral presentations:

O1) Optimization of Molecular Dynamics force fields for microporous materials.

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

O2) Effects of metal halides on the desorption properties of the system $2LiNH_2+LiH+KBH_4$

A.Valentoni (avalentoni@uniss.it)[a], G.Mulas[a], S.Garroni[a], and S.Enzo[a]
[a.] Department of Chemistry and Pharmacy and INSTM,, University of Sassari, Via Vienna 2, 07100 Sassari, Italy

O3) Coarse Grain simulations of non-canonical DNA structures

Matus Rebic[a],(rebicmatus@gmail.com) Francesca Mocci[b], Aatto Laaksonen[c] and Jozef Ulicny[a]
[a.] Department of Biophysics, UPJS, Jesenna 5, 04154, Kosice, Slovakia
[b.] Department of Chemical and Geological Sciences, UC, I-09042 Monserato, Italy
[c.] Arrhenius Laboratory, Stockholm University, 10691 Stockholm, Sweden

O4) Studying the structure of poorly crystalline materials using Debye Equation and Reverse Monte Carlo refinement

Matteo Sestu[a] (msestu@unica.it) and Gabriele Navarra[a]
[a.] Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Cittadella Universitaria SS 554 Bivio per Sestu, 09042, Monserrato (CA), Italy

O5) Crystallographic characterisation and solution equilibrium study of 6,6'-(((2-(diethylamino)ethyl)azanediyl)bis(methylene))bis(5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one)

Delara Mansoori (mansoori@unica.it)
Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Cittadella Universitaria, 09042 Monserrato-Cagliari

O6) XPS and XAES characterization of copper and zinc chemical states applied to brass alloys

Federica Cocco (fcocco@unica.it),[a] Bernhard Elsener,[a] Marzia Fantauzzi,[a] Antonella Rossi[a]
[a.] Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Complesso Universitario di Monserrato, SS 554 bivio per Sestu, 09042 Monserrato, Cagliari, Italy

O7) Salt crystallisation decay on monuments: the archaeological site of “Viale Trieste 105 in Cagliari”

Marta Casti[a,b](marta.casti@unica.it), Marta Cappai[a,b], Maura Carboni[a,b], Gianfranco Carcangiu[c,b], Giuseppe Desogus[a], Ombretta Cocco[a,b], Paola Meloni[b], Arianna Murru[a,,b,c] and Marcella Palomba[c], Roberto Ricciu[a]
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[c.] ISAC, CNR, UOS di Cagliari, 09042, Monserrato (CA), Italia

O8) Cortical reinforcement for the conservation of Cultural Heritage: the *Beata Vergine delle Grazie*'s church façade, Masullas (OR)

Arianna Murru[a,b,c] (ariannamurru@unica.it), Paola Meloni[b], Gianfranco Carcangiu [c,b], Francesco Secchi [d], Marta Casti[a,b], Marta Cappai [a,b], Ombretta Cocco[a,b], Marcella Palomba[c] and Maura Carboni[e]
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[e.] Dipartimento di Chimica e Farmacia, Università degli Studi di Sassari, Via Vienna 2, 07100, Sassari, Italy

O9) Mechanochemical Synthesis Study of a 2D Layered Compound

V. Cabras (valentina.cabras@unica.it), M. Pilloni, A. Scano, R. Lai, G. Ennas, M. C. Aragoni
Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Cittadella Universitaria di Monserrato,09042 Monserrato (Cagliari), Italia

O10) Dialkylamide-capped magnetite nanoparticles via a direct solvothermal synthesis

Claudio Cara (Cara.claudio16@gmail.com),[a,b] Anna Musinu,[a] Valentina Mameli,[a] Andrea Ardu,[a] Andrea M. Scorciapino,[c] Giorgia Manzo,[c] Carla Cannas[a,b]
[a.] Department of Chemical and Geological Sciences, Università di Cagliari, S.S. 554 bivio per Sestu, 09042, Monserrato (CA), Italy
[b.] Consorzio AUSI, Palazzo Bellavista Monteponi, 09016 Iglesias, Italy
[c.] Department of Biomedical Sciences, Biochemistry Unit, University of Cagliari, Italy

O11) Characterization of the coordination modes of flavonoids towards oxidovanadium(IV)

Valeria Ugone (vugone@uniss.it),[a] Daniele Sanna,[b] Giovanni Micera,[a] and Eugenio Garribba [a]
[a.] Dipartimento di Chimica e Farmacia, Università di Sassari, Via Vienna 2, I-07100 Sassari, Italy
[b.] Istituto CNR di Chimica Biomolecolare, Trav. La Crucca 3, I-07040 Sassari, Italy

O12) A brand new synthesis and characterization of 1,4-bis-(3-Pyridyl)butadiyne as spacer in the preparation of coordination polymers

R.Lai (rominide27@hotmail.it), M.C Aragoni, M.Arca, E.Podda, S.Coles, L.Mapp
Università degli Studi di Cagliari dipartimento di Scienze Chimiche e geologiche S.S 554 bivio per Sestu, Monserrato (CA)

O13) Advances in the Frontal Ring Opening Metathesis Polymerization of Dicyclopentadiene

Davide Sanna[a] *(dvdsnn13@hotmail.it), Andrea Ruiu*[a]*, Valeria Alzari*[a]*, Daniele Nuvoli*[a]*, Alberto Mariani*[a]
[a.] Dipartimento di Chimica e Farmacia, Università di Sassari, and local INSTM Unit, Via Vienna 2, 07100 Sassari, Italy

O14) Asymmetric bis-ureidic receptors: synthesis, anion binding and sensing studies
Arianna Casula (acasula@unica.it),[a] *Claudia Caltagirone,*[a] *and Martina Olivari*[a]
[a.] Università degli Studi di Cagliari, Dipartimento di Scienze Chimiche e Geologiche, S.S. 554 Bivio per Sestu, 09042 Monserrato (CA), Italy.

O15) "Quick and click" assembly of functionalised indole rings via metal-promoted cyclative tandem reactions
Francesca Capitta (francescacapitta@tiscali.it), Lidia De Luca and Andrea Porcheddu
Dipartimento di Chimica e Farmacia, Università degli Studi di Sassari, via Vienna 2, 07100 Sassari, Italy

O16) One-pot syntheses of hydroxamic acids from alcohols or aldehydes
Silvia Gaspa (sgaspa@uniss.it),[a] *Giovanna Dettori,*[a] *Andrea Porcheddu,*[a] *and Lidia De Luca*[a]
[a.] Department of Chemistry and Pharmacy, University of Sassari, Via Vienna 2, 07100 Sassari, Italy

O17) Synthesis of cyclobutanone α-amino acid derivatives through tandem condensation-asymmetric tautomerization sequence
Nicola Melis (nic.melis@unica.it),[a] *Francesco Secci*[a] *and Angelo Frongia*[a]
[a.] Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, S.S. 554, Bivio per Sestu, I-09042, Monserrato, Cagliari (Italy)

O18) Design, synthesis and pharmacological investigation of new FAAH inhibitors
Monica Demurtas (monicademurtas@tiscali.it),[a] *Valentina Onnis,*[a] *Cenzo Congiu,*[a] *Alessandro Deplano,*[a] *Mariateresa Cipriano,*[b] *Christopher Fowler,*[b] *Carmine Morgillo,*[c] *Bruno Catalanotti*[c]
[a.] Department of Life and Environmental Sciences, Unit of Pharmaceutical, Pharmacological and Nutraceutical Sciences, University of Cagliari, Via Ospedale 72, I-09124, Cagliari, Italy
[b.] Department of Pharmacology and Clinical Neuroscience, Umea University, SE901 87, Umea, Sweden
[c.] Department of Pharmacy, University of Naples, Via Montesano 49, I-80100, Napoli, Italy

O19) Dendrimeric peptides with membranolytic activity
I. Serra (ilaria.serra@unica.it),[a] *G. Manzo,*[b] *A.C. Rinaldi,*[b] *M.A. Scorciapino*[b] *e M. Casu*[c]
[a.] Dip. di Scienze Chimiche e Geologiche, Università di Cagliari
[b.] Dip. di Scienze Biomediche, Università di Cagliari
[c.] Dip. di Fisica, Università di Cagliari Complesso Universitario SP8 km 0.7, 09042 Monserrato (CA), Italia.

O20) Carbon nanomaterial immunomodulators are able to fight immune function dysregulation in simulated spaceflight conditions

Marco Orecchioni (lgdelogu@uniss.it)[a], Claudia Crescio[b], Cécilia Ménard-Moyon[c], Roberto Manetti[d], Proto Pippia[b], Francesco Sgarrella[a], Alberto Bianco[c], Lucia Gemma Delogu[a]

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[c.] CNRS, Institut de Biologie Moléculaire et Cellulaire, Laboratoire d'Immunologie et Chimie Thérapeutiques, 67000 Strasbourg, France.

[d.] Dipartimento di Medicina Clinica, Sperimentale e Oncologica, Università di Sassari, Sassari, Italy.

O21) Development and validation of a new GC-FID method for the determination of mono and disaccharides in milk and dairy foods

Ilenia Idda (ilenia.idda@gmail.com),[a] Nadia Spano,[a] Maria I. Pilo,[a] Gavino Sanna,[a]

[a.] Department of Chemistry and Pharmacy, University of Sassari, Via Vienna 2, 07100-Sassari, Italy

Poster presentations:

P1) Galactosyl prodrug of mefenamic acid: synthesis, stability and evaluations

Francesca Accioni (francesca.accioni@gmail.com), Antonio Carta, and Lucia Burrai

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P2) Switchable chiral heteroleptic d^8 metal dithiolenes

Salahuddin Attar[a] (attarsalah@unica.it); Davide Espa[a], Luciano Marchiò[b], M. Laura Mercuri[a], Angela Serpe[a], Flavia Artizzu[a], Elisa Sessini[a], Paola Deplano[a]

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[b.] Dipartimento di Chimica, Parco Area delle Scienze, 17/A, I-43100, Parma, Italy

P3) HPTLC fingerprint and quali-quantitative composition of anthocyanins in Myrtus communis L. berries growing in Sardinia

Antonio Porcu[a] (antonio.porcu.riqy@hotmail.com), Mariateresa Maldini[a], Mario Chessa[a], Giacomo Petretto[a], Marzia Foddai[a], Fabio Carboni[a] (carbonifab@gmail.com)and Giorgio Pintore[a]

[a.] Dept of Chemistry and Pharmacy, University of Sassari, via Muroni, 07100, Sassari, Italy

P4) Cultural Heritage and weathering test

Maura Carboni (carbonimaura@unica.it),[a,b] Marta Cappai,[c] Gianfranco Carcangiu,[d] Marta Casti,[c] P. Luca Mameli,[b,e] Paola Meloni,[b] Arianna Murru,[b,c,d] Marcella Palomba[d]

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[e.] DICAM, Alma Mater Studiorum Università di Bologna, Via Zamboni, 33 - 40126 Bologna, Italy

P5) Preparation and characterization of natural zeolite to be used against gastric infections caused by Helicobacter pylori

Farina M. [a] (maurofarina88@tiscali.it), Brundu A. [a], Cossu M. [b], Giunchedi P. [b], Rassu G. [b], Gavini E. [b], Juliano C. [b], Cerri G.

[a.] Department of Sciences for Nature and Environmental Resources, University of Sassari, 08100-Sassari, Italy

[b.] Department of Chemistry and Pharmacy, University of Sassari, 08100-Sassari, Italy

P6) A study about natural-like compounds with inhibitory activity on tyrosinase enzyme by means of a tyrosinase-based amperometric biosensor

Donatella Farina (dfarina@uniss.it),[a] Gaia Rocchitta,[a] Sara Cossu,[a] Rossana Migheli,[a] Giovanna Delogu,[b]Maria Antonietta Dettori,[b] Davide Fabbri,[b] and Pier Andrea Serra [a]

[a.] Department of Clinical and Experimental Medicine, Medical School, University of Sassari,07100 Sassari, Italy

[b.] Sassari Unit, Institute of Biomolecular Chemistry of CNR, 07100 Sassari, Italy.

P7) Electrochemical polythiophene-based biosensors for glucose detection in fruit juices

Roberta Farre (roberta.farre@tiscali.it)[a], Nina Senes[a], Elisabetta Masolo[a], Ana Sobral[a], Silvio Leoni[a], Gavino Sanna[a], Nadia Spano[a] and Maria Pilo[a]

[a.] Dipartimento di Chimica e Farmacia, Università di Sassari, Via Vienna 2, 07100 Sassari, Italy

P8) Imidazo[4,5-*g*]quinolones and pyrido[2,3-*g*]quinoxalines: design and synthesis of new possible antiviral agents

Simona Frau[a](simonafrau29@gmail.com), Irene Briguglio[a], Antonio Carta[a], Sandra Piras[a], Paola Corona[a]

[a.] Department of Chemistry and Pharmaci, University of Sassari, Via Muroni 23/A, 07100 Sassari, Italy

P9) $Mg(NH_2)_2$+2MH (M=Li-Na): Structural and desorption investigation

Antonio Valentoni (avalentoni@uniss.it),[a] Francesco Torre,[a] Giovanni Pireddu,[a] Christian Bonatto Minella,[b] Gabriele Mulas,[a] Stefano Enzo,[a] Chiara Milanese,[c] Claudio Pistidda,[d] Sebastiano Garroni[a]

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[b.] Karlsruhe Institute of Technology, Postfach 3640, 76021 Karlsruhe, Germany

[c.] Pavia Hydrogen Lab, C.S.G.I.-Department of Chemistry of Pavia, Pavia 27100, Italy

[d.] Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht, Germany

P10) The new and efficient method for synthesis of esters from aldehydes

Silvia Gaspa (sgaspa@uniss.it),[a] Andrea Porcheddu[a] and Lidia De Luca[a]

[a.] Department of Chemistry and Pharmacy, University of Sassari, Via Vienna 2, 07100 Sassari, Italy

P11) Study of antioxidants and antimicrobial properties in plant extracts elicriso

Stefano Mariani (marianistefano@email.it)

Department of Chemistry and Pharmacy, University of Sassari, Via Vienna 2, 07100 Sassari, Italy

P12) New Frontiers for Photo-Devices

Suvi Rajamäki[a] (suvi.rajamaki@saponina.com), Pier Carlo Ricci[b], Andrea Porcheddu[a]

[a.] Dipartimento di chimica e Technologie Farmaceutiche, Università degli Studi di Sassari

[b.] Dipartimento di Fisica, Università degli Studi di Cagliari

P13) The strange case of 6-methoxy-2,2'-bipyridine in rollover cyclometalation

Luca Maidich (luca.maidich@gmail.com),[a] Mondina Sedda,[a] Simona Galli,[b] Maria Agostina Cinellu,[a] Sergio Stoccoro[a] and Antonio Zucca[a] (zucca@uniss.it)

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[b.] Dipartimento di Scienza e Alta Tecnologia, Università dell'Insubria, Via Valleggio 11, 22100 Como, Italia

P14) Experiments explained by DFT calculations: N,C,N-pincer gold(III) complexes

Luca Maidich (luca.maidich@gmail.com), Sergio Stoccoro (stoccoro@uniss.it), Antonio Zucca, Maria Agostina Cinellu
Dipartimento di Chimica e Farmacia, Università di Sassari, Via Vienna, 2, 07100 Sassari, Italia

P15) Preparation of β-cyclodextrin-based components useful in biosensors of agricultural and food relevance

Patrizia Monti (pmonti@uniss.it),[a] Giammario Calia,[b] Davide Fabbri,[c] Maria Antonietta Dettori,[c] Quirico Migheli,[a] Pier Andrea Serra,[b] and Giovanna Delogu[c]
[a.] Dipartimento di Agraria, Università degli studi di Sassari, Viale Italia 39, I-07100, Sassari, Italy
[b.] Dipartimento di Medicina Clinica e Sperimentale, Università degli studi di Sassari, Viale San Pietro, I-07100, Sassari Italy
[c.] Istituto CNR di Chimica Biomolecolare - UOS Sassari - Traversa La Crucca 3, I-07100, Sassari, Italy

P16) Immobilization of Ampicillin on Ordered Mesoporous Silica

Valentina Nairi[a] (v.nairi@unica.it), Luca Medda[a], Federico Tocco[a], Andrea Salis[a], Maura Monduzzi[a]
[a.] Department of Chemical and Geological Science,University of Cagliari, SS 554 bivio per sestu,09042-Monserrato, Italy

P17) *Penicillum digitatum* activity in Citrus fruits treated with GRAS compounds

Valerio G. Nieddu (v.nieddu90@gmail.com),[a] Giacomo L. Petretto,[a] Tullio Venditti,[b] Gianfranca Ladu[b] and Giorgio Pintore[b]
[a.] Dipartimento di Chimica e Farmacia, Università di Sassari, Italia
[b.] Dipartimento di Scienze delle Produzioni Alimentari, CNR, Sassari, Italia

P18) Searching for the pharmacophore in β-diketo acid inhibitors of influenza virus PA endonuclease

Salvatore Nurra (snurra@uniss.it),[a] Nicolino Pala,[a] Mauro Carcelli,[b] Dominga Rogolino,[b] Annelies Stevaert,[c] Mario Sechi,[a] Lieve Naesens[c]
[a.] Dipartimento di Chimica e Farmacia, Università di Sassari, Via Vienna 2, 07100 - Sassari, Italia
[b.] Dipartimento di Chimica, Università di Parma, Parco Area delle Scienze 17/A, 43124 - Parma, Italia.
[c.] Departement Microbiologie en Immunologie Rega Institute, Katholieke Universiteit Leuven, Minderbroedersstraat 10, 3000 - Leuven, Belgium.

P19) A method based on VOCs composition to discriminate *Citrus mostruosa* from several *Citrus* spp

Alessandro Pibiri (ale.pib@tiscali.it),[a] Giacomo L. Petretto,[a] Mario Chessa,[a] Mariateresa Maldini[a] , Marzia Foddai[a] Fabio Carboni[a] and Giorgio Pintore[a]
[a.] Dipartimento di Chimica e Farmacia, Università di Sassari, Italia

P20) Chitosan nanoparticles for non-invasive tumor imaging

E.P. Porcu[a](elenapiera.porcu01@ateneopv.it), G. Rassu[b], E. Gavini[b], P. Dionigi[c], M. Maestri[d], P. Giunchedi[b]

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[c.] Department of Surgery, IRCCS Policlinico San Matteo Foundation , University of Pavia, Italy;
[d.] IRCCS Policlinico San Matteo Foundation, University of Pavia, Pavia, Italy

P21) Thermosensitive *in situ* gelling solutions for potential application in intraoperative fluorescence imaging and local therapy of hepatocellular carcinoma

Andrea Salis (asalis@uniss.it),[a] Giovanna Rassu,[a] Ilaria Benzoni[b] Marcello Maestri[b], Paolo Dionigi[c], Elena P. Porcu[d], Elisabetta Gavini[a], Paolo Giunchedi[a]
[a.] Department of Chemistry and Pharmacy, University of Sassari, 08100-Sassari, Italy
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[c.] Department of Clinical, Surgical, Diagnostic and Pediatric Sciences, University of Pavia, Pavia, Italy
[d.] PhD student in Experimental Medicine, University of Pavia, Pavia, Italy

INV1

The combined analysis approach for the characterization of materials

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Diffraction patterns contain a lot of information about our compounds and materials but the extraction is not always easy or sometimes it requires additional info from other techniques. The Rietveld method as incorporated in MAUD [1], can be regarded as a more generalized simulation technique to analyze not only the crystal structure or phase quantities but also microstructure, defects, texture or residual stresses. We have extended it to other techniques, to complement the analysis and take advantage of the synergies, like reflectivity, fluorescence (XRF) or energy minimization (DFT) and more are in the works. To take full advantage of the method, it is important to perform the experiment in a proper way. At the same time we can make use of some advances in the instrumentation like area, Si drift or curved detectors. Some examples of this combined analysis will be shown from crystal structure solution, to nanomaterials and thin films.

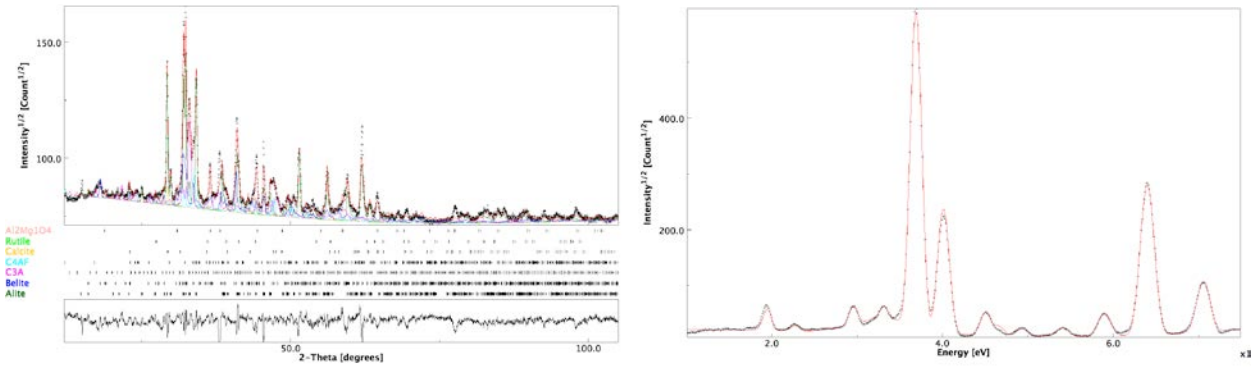

Figure 1: XRD (left) and XRF (right) fitting by the combined analysis on a cement sample using the software MAUD.

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INV2

Polymers of Intrinsic Microporosity (PIMs): organic multi-functional materials

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Polymers of Intrinsic Microporosity (PIMs) are a class of materials which combine the processability of polymers with a high degree of microporosity. This microporosity is generated solely from the inefficient packing of their rigid and contorted macromolecular structures. They are attracting attention for a number of applications including as membrane materials for gas separations [1]. This talk will describe our latest work on synthesis of novel PIMs using both the previously used dibenzodioxin-based polymerisations or a novel reaction based on Tröger's base formation (Fig. 1). In particular, we will focus on the design, synthesis and gas permeability of PIMs with exceptionally rigid polymeric structures. In addition to very high permeability, some of these polymers demonstrate improved gas selectivity which produces performances that lie well above the benchmark 2008 Robeson upper bounds for the important O_2/N_2 and H_2/N_2 gas pairs. Along with their use as gas separation membranes, we demonstrated the versatility of these materials by successfully using them for applications such as heterogeneous catalysis [2] and electrochemistry [3].

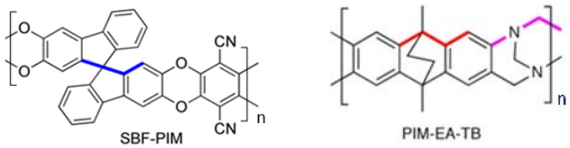

Figure 1: Dibenzodioxin and Tröger's base polymers

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O1

Optimization of Molecular Dynamics force fields for microporous materials

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Microporous materials[1] have always received great attention from the scientific community as they are employed in many fields, including economically relevant industrial processes. In recent years there was an increase of interest in such materials due to the discover of Metal Organic Frameworks, a new class of materials which has astounding physico-chemical properties and can be easily tuned during synthesis. Due to the large number of possible structures, a fast, economical, and effective method to perform a screening is required. Molecular Dynamics simulations are one of the best tool for this purpose. To perform such simulations, thought, one must provide a force field[2,3] to describe the system interactions. Various database of generic force fields are available, but these are not so accurate when applied to systems other than those on which they were developed.

In this work a method to obtain reliable force fields, based on the *force matching* technique[4], is presented[5]. Such method enables the automated generation of classical force fields tailored to each specific structure in less than ten minutes on a common desktop pc. The procedure has been applied to the ZIF-8 crystal and validated against *ab-initio* reference data.

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O2

Effects of metal halides on the desorption properties of the system $2LiNH_2+LiH+KBH_4$.

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The ternary system $2LiNH_2+LiH+KBH_4$, according to thermodynamic calculations has been indicated as an interesting candidate for solid state hydrogen storage for on-board applications.[1] Unfortunately, experimental studies have shown that strong kinetic barriers limit their applicability.[2,3] To date, we decided to study the effect of ball milling and the addition of metal halides, such as $AlCl_3$, $ZnCl_2$ and NbF_5 with the aim of reducing the desorption temperatures and improving the kinetics performance. The analysis was performed using TPD measurements, before evaluating the effect of increasing times of mechanical treatment on the mixture. Later, the effect of the addition of $AlCl_3$, $ZnCl_2$ and NbF_5, introduced in catalytic amount, was tested. In all cases it was observed a decrease on the desorption temperature followed by a faster release of gas, index that all additives can contribute efficiently to destabilize the system.

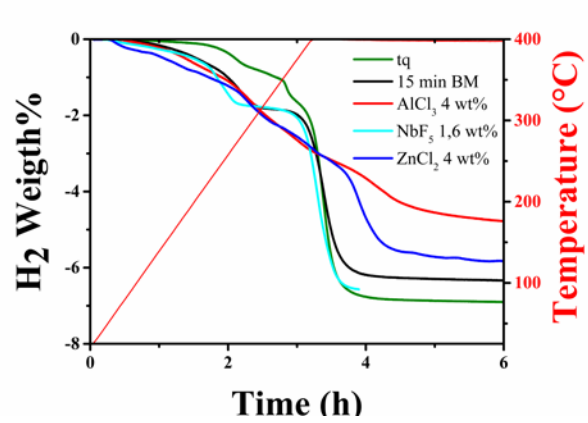

Figure 1: Effect of the addictives on the sorbitive properties of the system.

References:

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O3

Coarse Grain simulations of non-canonical DNA structures

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We present a Coarse Grain (CG) model of human telomeric G-quadruplex, obtained using Inverse Monte Carlo [1] and Iterative Boltzmann Inversion [2] techniques implemented within the software package called MagiC [3]. As a starting point the 2HY9 [4] human telomeric quadruplex topology was modeled performing a one microsecond long atomistic Molecular Dynamics (MD) simulation. The chosen quadruplex includes two kinds of loops and all possible combinations of relative orientations of guanine strands that can be found in quadruplexes. The effective CG potential for a one bead per nucleotide model has been developed from the radial distribution functions of this reference system. The obtained potentials take into account explicitly the interaction with counter ions, while the effect of the solvent is included implicitly. The structural properties of obtained CG model of the quadruplex provided a perfect match to those resulting from the reference atomistic MD simulation. The same set of interaction potentials was then used to simulate at the CG level another quadruplex topology (PDB id 1KF1 [5]). The results of the CG MD simulations of 1KF1 are very encouraging and suggest that the CG model based on the 2HY9 can be used to simulate quadruplexes with different topologies. Our CG model was further applied to a higher order human telomeric quadruplex [6] formed by the repetition, twenty times, of the 1KF1 quadruplex structure. The CG simulation predicts interesting dynamical properties of higher order structure (not achievable by classical all-atom approach). We expect that the general structure of the model is transferable and allows to extend the computational explorations to the much wider range of topologies involving G-tetrad building motifs with a wide range of potential applications in cell regulation as well as in the construction of nano structures and nano materials.

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O4

Studying the structure of poorly crystalline materials using Debye Equation and Reverse Monte Carlo refinement

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Debye scattering equation is known since 1915 [1]. Although this formula can, in principle, describe scattering from any multiple particle systems, its application is normally limited to small domains as clusters or low-sized nanoparticles. This is mostly due to the very high computing time needed, that strongly depends on the number of atoms.

In recent years, the availability of highly performant graphics processing units (GPU) allowed their use for general purposes including strongly demanding scientific applications. This feature was exploited in the Debye Function Analysis to study more complex systems with several thousand of atoms [2].

We present a refinement code using both the Debye scattering equation implemented on a commercial GPU and the Reverse Monte Carlo algorithm [3], to study the structure of poorly crystalline nano-sized iron oxy-hydroxides. Debate about the exact nature of their structure is under way: different interpretations of their X-ray diffraction pattern have been put forward by several authors who proposed different structural models. To evaluate their validity, some of these models are used as starting atom sets in the Reverse Monte Carlo refinement procedure; to speed up calculation time, a parallelized version of the equation is optimized to run on Nvidia GeForce 690 GPU.

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O5

Crystallographic characterisation and solution equilibrium study of 6,6'-(((2-(diethylamino)ethyl)azanediyl)bis(methylene))bis(5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one)

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In the frame of the research on new iron chelating agents going on since several years in our laboratories, attention was paid to the tetradentate kojic acid derivatives [1].

The ligand 6,6'-(((2-(diethylamino)ethyl)azanediyl)bis(methylene))bis(5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one), (L9), was synthesized and characterised during my work of thesis. Complex formation equilibria with the trivalent metal ions Fe^{III} ed Al^{III}, target of the chelating therapy, have been studied, and with the essential bivalent metal ions Cu^{II} and Zn^{II}. The variety of used techniques (potentiometry, spectrophotometry UV-Vis, 1D and 2D NMR spectroscopy, ESI-MS and X-ray diffraction) have provided an exhaustive picture of the protonation and complex formation solution equilibria, and of the structural characteristics of the ligand and of its complexes with zinc and iron (Figure 1) [2].

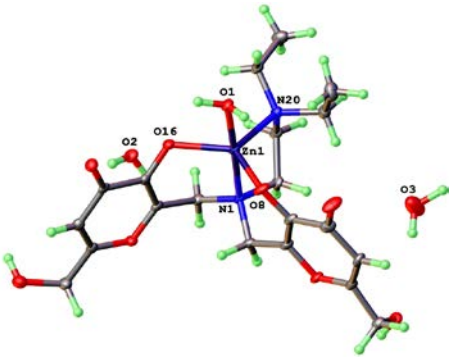

Figure 1. Asymmetric unit in the crystal of ZnL9 complex of stoichiometry $[Zn(L9)(H_2O)]2H_2O$.

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O6

XPS and XAES characterization of copper and zinc chemical states applied to brass alloys

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X-ray photoelectron spectroscopy (XPS) is a powerful surface analytical technique that allows the identification of the elements present, the determination of their chemical state and the quantitative analysis of thin-layered systems in the nanometre range. Different chemical states of an element result in a binding energy difference ΔBE, e.g. between iron in the metallic state Fe(0) and iron Fe(III) in iron oxide a difference ΔBE of ca. 5.5 eV is found. This change in the binding energy of a photoelectron signal due to a variation of the chemical state of an atom in a compound with respect to the same signal in the elemental state is known as "**chemical shift**" ΔBE [ISO 18115-1:2010].

For copper and zinc compounds however the chemical state identification based on the binding energy is challenging as the chemical shifts between Zn(II) and Zn(0) in the Zn2p signal and between Cu(I) and Cu(0) in the Cu2p signal are very small [1]. In this investigation it is proposed to rely on the x-ray induced Auger signals for chemical state identification of copper and zinc, respectively, using the two-dimensional chemical state plot. It is shown that the different copper and zinc compounds can clearly be distinguished.

For a quantitative analysis the x-ray induced Auger signals of pure copper and zinc in the metallic state and of copper and zinc oxide were measured as internal standards and the envelope of the peaks could be curve-fitted in agreement with theory. This allowed the analysis of oxide films on zinc and copper, respectively. In the case of brass alloys where both, copper and zinc, are present a superposition of x-ray induced Auger signals of zinc with those of copper have to be taken into account. The analytical approach developed in this work will be discussed for a CuZn37 model brass alloy after various surface pre-treatments where the surface oxide film thickness and composition had to be determined.

Reference:

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O7

Salt crystallisation decay on monuments: the archaeological site of "Viale Trieste 105 in Cagliari"

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Salt crystallisation decay is one of the most dangerous problems for the conservation of Cultural Heritage built in porous stone materials. The extreme spread of this form of decay derives from the copious amounts of soluble salts sources available near the monuments (soil, marine aerosols, use of cement or particular restoration products, air pollution). Salt crystallisation strongly depends on the hygrothermal parameters of the environment becoming more insidious where they have frequent variations; in these conditions repeated cycles of crystal growth and dissolution occur, involving high crystallization pressures within porous network, resulting in a breakage of materials.

The "archaeological site of Viale Trieste 105" in Cagliari is an exemplary case of salt crystallization in porous stone materials. Large amounts of sodium sulphate contaminate the archaeological structures, built in "pietra cantone", producing detachments and pulverization of materials. The decay study was carried out by microclimatic monitoring inside the site and laboratory analysis (mineralogical and petrographic characterization of sample from the site and quantitative analysis by ion chromatography).

Similar materials to those that constitute archaeological structures were selected in order to investigate the salt crystallisation phenomenon and to suggest some possible conservation strategies. These materials were characterized by MIP, XRD, MO, SEM and TG-DTA techniques; physical-mechanical properties and resistance to salt crystallisation were also investigated.

O8

Cortical reinforcement for the conservation of Cultural Heritage: the *Beata Vergine delle Grazie*'s church façade, Masullas (OR)

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Cortical consolidation of historical and artistic assets is still one of the most fragile and uncertain aspect within the protocol for restoration.

Cultural artifacts introduces themselves through the surface, therefore is important to reduce the continuous loss of materials resulting from decay processes.

The aim of cortical consolidation is the recovery as well as the enhancement of original cohesion condition. Consolidation is responsible for the improvement of physical properties that affect the durability of surfaces (such as mechanical strength, abrasion resistance, reduction of the porosity) and consequently the entire structure.

In this work the effects induced by four commercial products on specimens stone (widely used in the cultural heritage conservation field) were investigated, referring to the case study of *Beata Vergine delle Grazie*'s church restoration project.

Here, the majestic of the façade decorations is completely compromised by several conservation problems related to the building material decay.

In order to verify the effectiveness of consolidation treatments, stone materials similar to those in situ have been collected in different local outcrops and submitted to physical and mechanical characterization (such as US, mechanical strength and MIP).

The mineralogical and chemical characterization of the building stones and the sample materials have been carried out through XRD, MO, TG-DTA, SEM-EDS techniques.

O9

Mechanochemical Synthesis Study of a 2D Layered Compound

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Metal Organic Frameworks (MOFs), named also porous coordination networks, porous coordination polymers, etc., are coordination polymers formed by connecting metal ions with polytopic organic linkers resulting in 1D, 2D or 3D ordered structures that possess high surface areas. MOFs are very useful in gas storage, gas/vapor separation, catalysis and drug delivery. Design strategies for the prediction and preparation of MOF have been receiving considerable attention during the last few years. One of the most rational methods is the "pillaring" strategy which consists in connecting well-defined 2D layers with appropriate pillars [1]. Nowadays, this is a strategy used only under solvothermal conditions. We present here how pillaring can be achieved by a mechanochemical approach and we report on the reactivity study under grinding conditions between Ni(II) complexes and N-donor aromatic ligands such as pyridinyl and bipyridine derivates to obtain 2D layered compounds. In particular we present here the synthesis and characterization of the coordination polymer [Ni((EtO)$_2$PS$_2$)$_2$·bipy] (fig.1), obtained by grinding *bis*-(*O*,*O*'diethyldithiophosphato)nickel(II) [Ni((EtO)$_2$PS$_2$)$_2$] (**1**) and 4,4'-bipyridine (bipy) (**2**) in a ball mill with and without added solvent, giving rise to LAG and Solvent Free methods respectively. Several grinding variables (milling time, balls size, impact frequency) were investigated in order to promote reaction between (**1**) and (**2**), keeping constant the powder/balls mass ratio. The synthesized ball milling sample has been compared to the corresponding sample prepared by solvothermal approach [2]. Samples were characterizated by X-ray Powder Diffraction (XRPD), Infrared Spectroscopy (IR), Termogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC). The obtained results indicate that solvothermal and ball milling samples were isostructural with very similar thermal behavior.

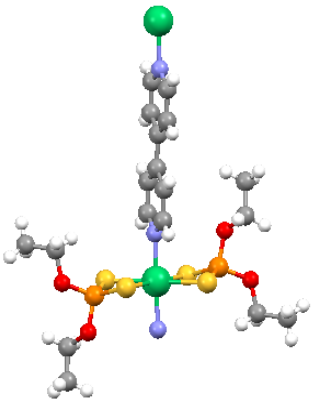

Fig.1:([Ni((EtO)$_2$PS$_2$)$_2$(bipy)) coordination polymer.

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O10

Dialkylamide-capped magnetite nanoparticles via a direct solvothermal synthesis

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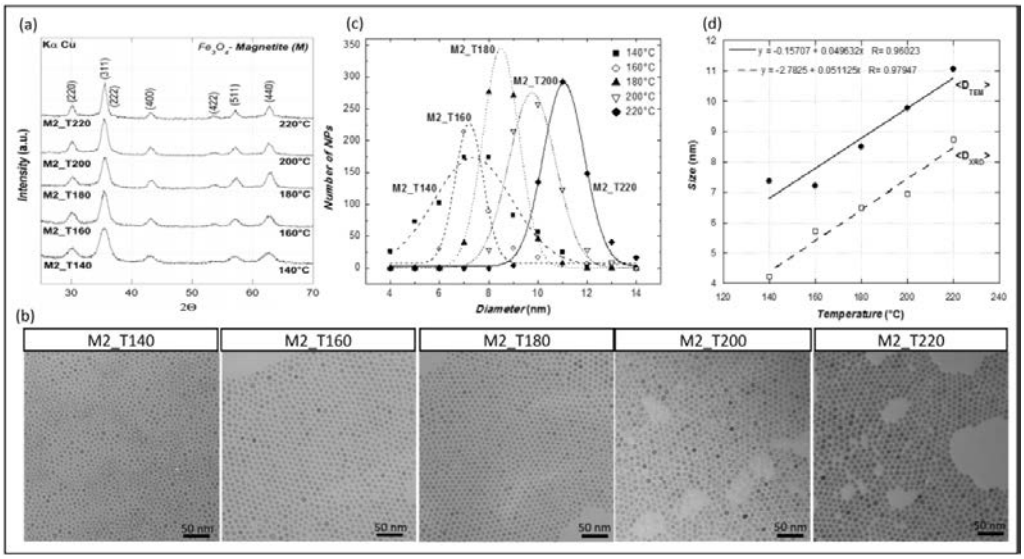
An eco-friendly, low-cost one-pot solvothermal approach can be developed to prepare magnetite nanoparticles capped with a dialkylamide. Iron isopropoxide, water vapour and absolute ethanol were used as iron oxide precursor, hydrolysis agent and solvent, respectively. The role of each surfactant was investigated and an accurate correlation between the synthetic parameters, the crystallographic phases and both crystallite and particle size was found. The size and the polydispersity can be finely tailored by choosing the appropriate amounts of oleylamine and oleic acid, used as surfactants, and by varying the synthesis temperature. The amine functional group results to be fundamental as reduction promoter and to obtain magnetite, as demonstrated using different amines. A dual ^{1}H-NMR / FTIR approach was used to investigate the actual nature of the capping agent. To this end, different experiments were set up also in the presence of a diamagnetic anatase phase. The amide is the new co-surfactant for the size and shape regulation and represents the biocompatible molecular coating of magnetite nanoparticles.



XRD patterns (a), TEM bright images (b), Particle Size Distributions (c) and D_{XRD} and D_{TEM} size versus temperature (d) of the samples obtained in the same synthetic conditions of M2_OAc_OAm = M2_T180 (see Table 1) at different reaction temperatures.

O11

Characterization of the coordination modes of flavonoids towards oxidovanadium(IV)

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Vanadium compounds formed by flavonoid ligands show promising antitumor effects [1]. In particular, they are effective against osteosarcoma cell lines [2]. In this work the coordination mode and geometry assumed in solution by VO^{2+} complexes formed by different flavonoids were studied by spectroscopic (EPR) and computational (DFT) methods [3]. Flavonoid ligands can bind VO^{2+} ion using different donor sets (shown in Figure 1) and the formation of different geometries are possible (square pyramidal or octahedral). The comparison with simple model ligands (like acetylacetone, maltol and cathecol), allowed us to identify the species formed in solution. The determination of the coordination mode and the geometry of the species formed at the physiological conditions is important to hypothesize the biotransformation of these pharmacologically active vanadium complexes in biological fluids and their active form in the organism.

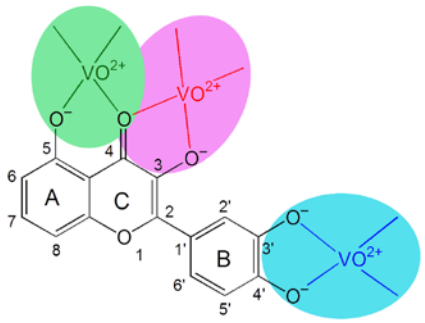

Figure 1: Possible coordination modes of a flavonoid ligand.

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O12

A brand new synthesis and characterization of 1,4-bis-(3-Pyridyl)butadiyne as spacer in the preparation of coordination polymers.

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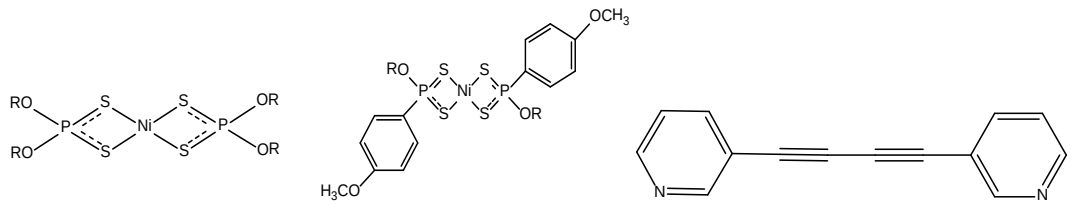
Crystal engineering is an important field of supramolecular chemistry, which utilises the understanding of intermolecular interactions in the design of new solids with desired physical and chemical properties.[1] Self-assembly processes involving metal ions and well-designed organic ligands are almost certainly the most employed approach to coordination polymers with predetermined molecular architecture.The synthesis of polymeric complexes by using neutral coordination complexes held together by additional donor molecules or secondary bonding interactions is acquiring increasing importance in the field of crystal engineering.[1] In this context, we have started a synthetic program based on the ability of neutral dithiophosphato complexes [Ni(RO$dtf)_2$] and dithiophosphonato complexes [Ni(RO$dtp)_2$] [ROdtf = $(RO)_2PS_2^-$; ROdtp = $(4\text{-}MeOC_6H_4)(RO)PS_2^-$; R = alkyl substituent] to act as building blocks for the predictable assembly of inorganic coordination polymers [2]. In fact, due to their coordinative unsaturation, these square-planar complexes tend to complete the Ni^{II} coordination sphere, being axially bound by monodentate donor molecules, such as pyridine, to yield octahedral complexes.[3,4]· We report here the reactions of the dithiophosphato complexes [Ni(RO$dtf)_2$] [R = Me (**1**), Et (**2**)] and dithiophosphonato complexes [Ni(RO$dtp)_2$] [R = Me (**3**), Et(**4**)] with the ligand 1,4-di-3-pyridyl-1,3-butadiyne (**L**),[5] and the corresponding 1:1 coordination polymers $(\mathbf{1}\cdot\mathbf{L})_\infty$, $(\mathbf{2}\cdot\mathbf{L})_\infty$, $(\mathbf{3}\cdot\mathbf{L})_\infty$, and $(\mathbf{4}\cdot\mathbf{L})_\infty$ (Figure).



R = Me (**1**), Et (**2**)R = Me (**3**), Et (**4**) (**L**)

Figure: (top) formula structures of dithiophosphato (**1**, **2**) and dithiophosphonato (**3**, **4**) nickel complexes and 1,4-di-3-pyridyl-1,3-butadiyne (**L**); (bottom) 1D polymeric chain of $(\mathbf{2}\cdot\mathbf{L})_\infty$ (hydrogen atoms are omitted for clarity reasons)

The syntheses and characterisation of the ligand and the coordination polymers along with the results obtained by X-ray diffraction on single crystal are discussed and the differences in the crystal structures deriving from the different nature of the substituents at the phosphorous atoms in the starting complexes are commented. Moreover, the stability constants of the adduct formations determined by UV-vis titrations of complexes **1**-**4** with increasing amounts of **L** are presented.

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O13

Advances in the Frontal Ring Opening Metathesis Polymerization of Dicyclopentadiene

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The frontal ring opening metathesis polymerization (FROMP) of dicyclopentadiene using first and second generation Grubbs' catalysts is reported. To have sufficiently long pot lives, dimethylaminopyridine is added as an inhibitor. By choosing the proper compositions, it is possible to determine the ranges in which pure frontal polymerization occurs. A thorough study on the effect of the above components on the maximum temperatures reached by the front and on its velocities is performed. Namely, temperatures range from 164 to 205 ºC (**Figure 1a**) depending on the type of catalyst and the above component ratios. Besides, front velocities range from 1.0 to 15.0 cm/min (**Figure 1b**), which are one of the lowest and one of the highest values reported so far in any frontal polymerization experiment reported in literature. This finding allows the complete control of the frontal ring opening polymerization of dicyclopentadiene also in practical applications.

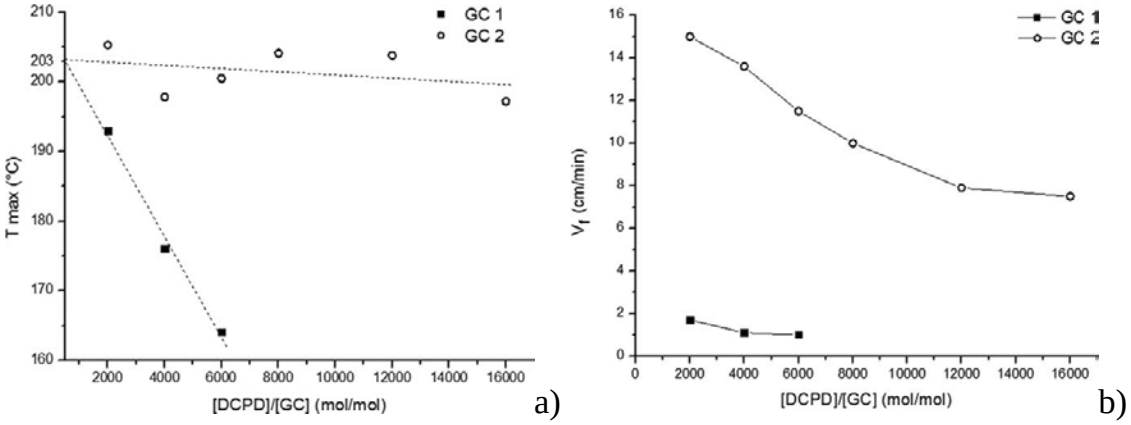

Figure 1: a) T_{max} as a function of the DCPD/GC molar ratio (DMAP/GC = 1 mol/mol). The two interpolation lines cross the T_{max} axis almost at the same value (T = 203 °C), very close to the adiabatic temperature of 206 °C; b) V_f as a function of the DCPD/GC molar ratio (DMAP/ GC = 1 mol/mol).

O14

Asymmetric bis-ureidic receptors: synthesis, anion binding and sensing studies

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Anion recognition and sensing has recently received considerable attention because of the central role played by anions in biological, industrial, and environmental processes [1].

Among anions, pyrophosphate (Ppi) is a biologically important target because it is the product of ATP hydrolysis and its detection has become important in cancer research and for some rheumatologic disorder as CPDD. We have recently reported the synthesis, the anion binding properties and the application as fluorescent chemosensors of two new bis ureidic receptors **L^1** and **L^2** bearing two naphtyl ureidic moieties (Figure 1) [2]. Both **L^1** and **L^2** showed a selective fluorescent response for $HPpi^{3-}$ in DMSO. For these reasons two new asymmetric bis ureidic receptors **L^3** and **L^4** (Figure 1) containing a naphtyl and an indole moieties have been synthesised. The binding properties of L^3 and L^4 towards different anions have been studied by means of ^{1}H-NMR, UV-Vis and fluorescence spectroscopies and, also in this case, a remarkable affinity for $HPpi^{3-}$ has been observed for both receptors in DMSO. The results relative to the synthesis, anion binding studies and fluorescence will be presented.

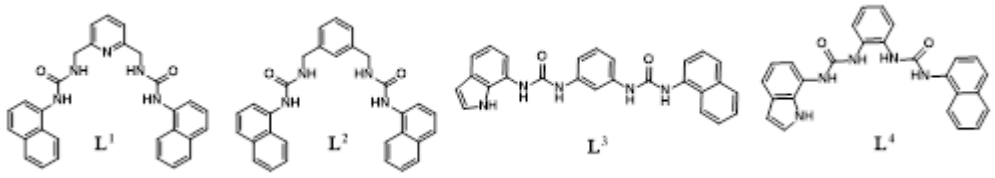

Figure 1: Scheme of the receptors.

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O15

"Quick and click" assembly of functionalised indole rings via metal-promoted cyclative tandem reactions

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An efficient and convenient synthesis of a variety of decorated indoles [1] using a three-component tandem [2] metal-catalysed process is described. We propose here a new "synthetic kit" that allows for the "quick and click" assembly of indole rings using readily available, and inexpensive starting materials under environmentally friendly reaction conditions. The optimised reactions allow the aldehydes to be used as a source of terminal alkynes, leading to the construction of a wide range of diversely functionalized indoles in good yields and with a broad scope. [3]

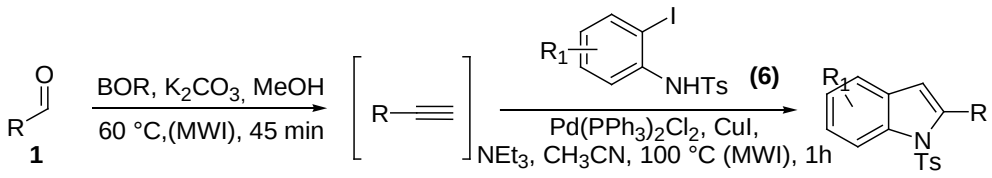

Figure 1: Tandem heteronnulation reaction with in-situ generated internal alkynes.

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O16

One-pot syntheses of hydroxamic acids from alcohols or aldehydes

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Hydroxamic acids are an important class of compounds with a broad array of biological activities including antibacterial, antifungal, anti-inflammatory and anti-asthmatic properties. They are commonly prepared from activated carboxylic acids and *O*-protected or *N*,*O*-protected hydroxylamines. This classical synthesis is highly dependent on the structure of the target molecules, requires additional deprotection steps, and isolation of the product can be extremely difficult. A one-pot oxidative transformation of aldehydes or alcohols into hydroxamic acids by the use of an aqueous solution of hydroxylamine provides an elegant and eco-friendly alternative to the classical approach. We have developed two new metal- and base-free protocols for the synthesis of hydroxamic acids starting from either aldehydes [1] or alcohols [2], forming an activated ester as an intermediate and its subsequent reaction with aqueous hydroxylamine.

The developed methodologies give high yields and uses cheap, abundant and easily available reagents.

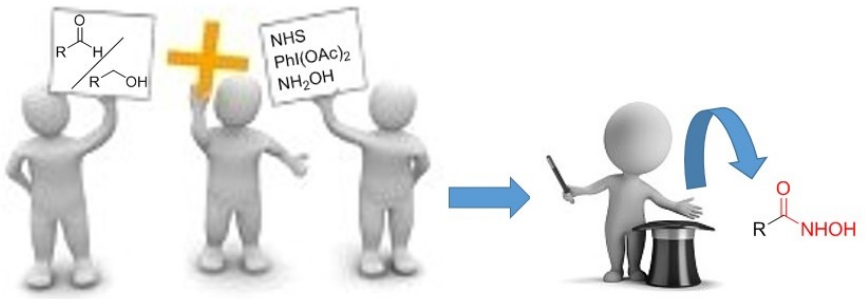

Figure 1: One-pot syntheses of hydroxamic acids from alcohols or aldehydes

References:

[1] G. Dettori, S. Gaspa, A. Porcheddu and L. De Luca, *Adv. Synth. Catal.*, **2014**, *356*, 2709.
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O17

Synthesis of cyclobutanone α-amino acid derivatives through tandem condensation-asymmetric tautomerization sequence

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The widespread use of α-aminocarbonyl compounds [1] as building block in the synthesis of nitrogen-containing compounds makes the development of new synthetic methodologies for this class of optically active compounds, extremely important. In fact, in this context, in our laboratory it has been developed an organocatalyzed methodology that involve a tandem condensation-enantioselective tautomerization sequence between a racemic α-hydroxyketone and amine derivative. This reaction was successfully applied in the synthesis of α-arylaminoketones [2] and α-alkylarylaminocyclobutanones [3].

This presentation reports the preliminary application of this methodology for the stereocontrolled synthesis of optically active cyclobutanone α-amino acid containing derivatives [4].

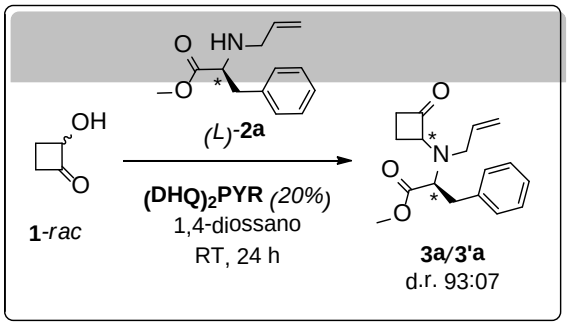

Figura 1

Reference:

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O18

Design, synthesis and pharmacological investigation of new FAAH inhibitors

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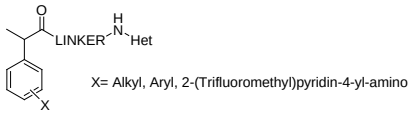
Fatty acid amide hydrolase (FAAH) is a serine hydrolase that catalyzes the deactivating hydrolysis of the fatty acid ethanolamide family of signaling lipids, which includes anandamide (AEA), an endogenous ligand for cannabinoid receptors. Endogenous FAAH substrates such as AEA serve key regulatory functions in the body and have been implicated in a variety of pathological conditions including pain, inflammation, sleep disorders, anxiety, depression, and vascular hypertension, and there has been an increasing interest in the development of inhibitors of this enzyme. Different structural classes of FAAH inhibitors have been reported including α-ketoheterocycles, (thio)hydantoins, piperidine/piperazine ureas, and carbamate derivatives. These compounds have been shown to be efficacious in models of inflammatory, visceral, and in some cases neuropathic pain without producing the central effects seen with directly acting cannabinoid receptor agonists [1-3]. An intriguing aspect of FAAH inhibition is that some currently marketed nonsteroidal anti-inflammatory drugs (NSAIDs) have also been shown to be weak inhibitors of FAAH [4], but can be used as a template for the design of more potent compounds. The findings led us to design new series of FAAH inhibitors based on profen templates.



In this communication, we report synthetic pathways, binding mode and FAAH inhibition profile studies on the new inhibitor series.

References

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O19

Dendrimeric peptides with membranolytic activity

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During the last two decades, the interesting towards lipid membrane active peptides has increased because of the potential uses of this novel class of compounds as antimicrobial agents or as adjuvants [1,2]. In particular, dendrimeric peptides show several advantages when compared to a linear peptide with the same amino acid sequence. These are branched molecules where different copies of the functional peptide unit are linked on a central core. The branched structure ensures an improved resistance to proteases, whereas the increased activity is due to the higher number of bioactive units per molecule. SB056 is a novel dendrimeric peptide, found to be active against both Gram-negative and -positive bacteria [3]. Its peculiar amino acid sequence [WKKIRVRLSA] suggests a beta-strand/-sheet like folding. The alternation of charged/polar and hydrophobic residues along the sequence, promoting such an overall amphipathic structure, has been improved by exchanging the first two residues, β-SB056 [KWKIRVRLSA]. The peptide to membrane binding constant has been determined for both the two dendrimeric peptides and their linear analogues, through steady-state tryptophan fluorescence measurements. The experiments were performed both in the absence and presence of electrolytes at physiological concentration. The optimization of the peptide amphiphilic profile resulted in a significant membrane binding enhancement. The dendrimeric scaffold seems able to preserve an effective interaction also in the presence of the electrolytes. Liposomes calcein-leakage assay showed that these peptides affect lipid bilayer permeability. This effect was found to be strongly dependent upon anionic lipid concentration. Clustering of the latter is proposed as peptides mechanism of action.

Reference:

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O20

Carbon nanomaterial immunomodulators are able to fight immune function dysregulation in simulated spaceflight conditions

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Experiments conducted by scientists in dedicated space missions and in simulations studies on Earth have shown that mammalian cells are sensitive to gravitational changes. Hashemi et al. reported a down regulation of CD25 and CD69 cell membrane activation markers in T cells after 24 hours under microgravity conditions [1]. In previous study our group reported that functionalized multi-walled carbon nanotubes (f-MWCNTs) by 1,3 dipolar cycloaddiction reaction lead to an up-regulation of CD25 and CD69 marker expression in human primary immune cells, in particular in monocytes without significant toxicity [2, 3]. In this study we wanted to evaluate the possibility of taking advantage of f-CNT immunostimulatory properties against microgravity of immune functions. We find the non-impact of microgravity on the functionalization of CNTs analyzed by TEM and the Kaiser test (**Figure 1)**. We then focused on CD25 and CD69 expression immune cells, we found that samples treated with f-CNTs together with ConA did not show the down-regulation of both CD25 and CD69. Cytokines analysis also confirms these data. In summary we confirm that f-CNTs are able to stimulate immune cells having very interesting broad future applications in immunotherapy and as possible fighters to contrast spaceflight immune dysregulation.

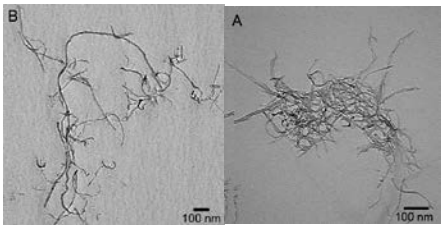

Figure 1: TEM images of OX-MWCNT-NH_3^+ before (A) and after microgravity treatment (B).

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O21

Development and validation of a new GC-FID method for the determination of mono and disaccharides in milk and dairy foods

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A new GC method for the determination of simple carbohydrates profile (lactose, glucose, galactose, *myo*-inositol and tagatose) in milk of different origins and in ripened sheep cheese samples has been developed and validated.

Whereas the first four carbohydrates are ubiquitous for milk of different origins, tagatose has been previously described as a marker of possible high-temperature thermal treatments underwent by milk.

The key steps of the analytical procedure are the assessment of i) a procedure of sample pretreatment, aimed to remove fats and proteins from the whey and ii) the derivatization step, needed to transform the polar analytes in compounds suitable for the GC analysis.

The entire procedure has been validated for each analyte in terms of detection (LOD) and quantification (LOQ) limits, linearity ranges, precision and bias. The very low LOD and LOQ values achieved for lactose make the proposed method suitable to verify a possible lactose-free condition for a number of dairy foods. Hence, the method was firstly tested on different cow milk samples (i.e. partially skimmed and lactose-free milk samples). Furthermore, the method has been extended, just modifying the pretreatment step of sample, to measure the concentration of lactose in a statistically significant number of PDO Sardinian sheep cheese samples (i.e. the PDO Pecorino Romano Cheese) collected at different ripening levels and produced in different zones of Sardinia island. Analytical data showed the substantial absence of lactose in all cheese samples (the concentration of this analyte is always below its LOQ value).

P1

Galactosyl prodrug of mefenamic acid: synthesis, stability and evaluations.

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Mefenamic acid is a widely diffused non-steroidal anti-inflammatory drug with remarkable analgesic properties; unfortunately its use has been strongly limited owning the high incidence of gastric side effects [1]. In this work we describe the synthesis and the stability profile of "Mefegal", a mefenamic acid prodrug, The prodrug approach allowed to obtain an orally administrable derivative, characterized by a significant reduction of the parent drug toxicological properties, without altering its pharmacological activity.

Mefenamic acid was conjugated to D-galactose through esterification, since metabolizable carbohydrates, especially hexoses, are gastroprotective agents, being components of the gastric mucus [2].

Drug stability experiments were carried out to verify the handling of this new prodrug and its ability to release the parent drug both enzymatically and non-enzymatically in plasma, and under physiological (pH 7.4) and gastric conditions (pH 1.0), respectively.

For the stability study a fast and easy LC-UV method has been developed.

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P1

Galactosyl prodrug of mefenamic acid: synthesis, stability and evaluations.

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For the stability study a fast and easy LC-UV method has been developed.

References:

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P2

Switchable chiral heteroleptic d^8 metal dithiolenes

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d^8 mixed-ligand dithiolenes (Ni, Pd, Pt) based on different ligands with significantly different electron-withdrawing capability, have been prepared by using different Ligands (L) and a chiral dithioxammide. These systems are suitable to work as second-order non linear chromophores, whose activity is redox and proton switchable. Complexes with suitable luminescent ligands show proton dependent dual luminescence. These complexes are also found to be switchable in solid state.[a,b]

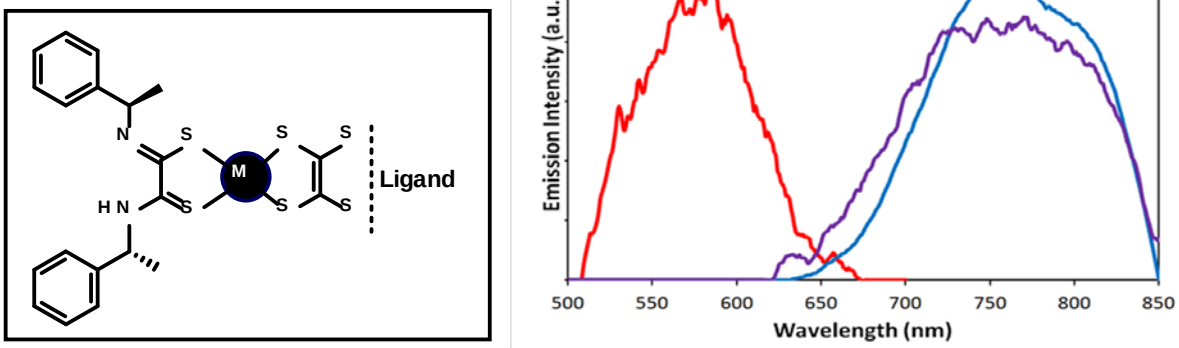

Figure 1: general structure, proton dependent dual luminescence

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P3

HPTLC fingerprint and quali-quantitative composition of anthocyanins in Myrtus communis L. berries growing in Sardinia

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Myrtus communis L. (Myrtaceae) is a spontaneous shrub, characteristic of Sardinia. The plant is employed, in popular medicine, for its anti-inflammatory, antiseptic, antimicrobic, hypoglycemic and balsamic properties [1]. Furthermore, berries and leaves are employed for the production of characteristic sweet myrtle liqueur. The berries are characterized by an high content of polyphenols, mainly anthocyanins, and volatiles that are strongly associated with the red-purple color and peculiar fruit flavor of the liqueur. Anthocyanins composition is quite specific for each vegetable and fruit and can be used as a fingerprint by which it's possible to determine the authenticity, the geographical origin and the quality of raw materials, products and extracts [2]. Thus, the aim of this study is a qualitative and quantitative evaluation of anthocyanins occurring in myrtle berries collected in different areas of Sardinia. The study is carried out using different methods of analysis: for a rapid fingerprint of extracts, HPTLC (High Performance Thin Layer Chromatography) technique is employed, whilst different Liquid Chromatography Tandem Mass Spectrometry (LC-MS, LC-MS/MS) methods are developed to obtain quali-quantitative anthocyanins profiles. In addition, we use PCA approach (Principal Component Analysis) to evaluate differences/similarities between the extracts analyzed. Thus, 16 anthocyanins belonging to the class of cyanidins, delphinidins, malvidins, petunidins, pelargonidins and peonidins are identified in the berries extracts. The results allowed us to identify qualitative and quantitative differences among myrtle samples collected in 17 different areas of Sardinia.

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P4

Cultural Heritage and weathering test.

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Outdoor architectural heritage is constantly exposed to weathering processes and to irreversible damages caused by pollutants and biological agents. Efforts have focused on the strong critical issues related to the synthesis of new products, their wanted effects and their delivery within the porous framework. Unfortunately, nowdays most of commercial consolidating agents are not specifically produced for conservation use on carbonate substrates. This study illustrates different stone materials and their degradation products characterized by mean of different diagnostic techniques such as Scanning Electron Microscopy (SEM), Mercury Intrusion Porosimetry (MIP), X-ray diffraction (XRD) and infra-red spectroscopy (FT-IR).

Consolidation effects of calcium oxalate on some stone materials, such as carrara marble and "*Santa Caterina*" limestone, are also shown. The same types of stone underwent treatments with some commercial formulations usually employed in conservation field. Treatment with ammonium oxalate appeared more effective the more deteriorated the stone material was. In particular, marble specimens showed 500 μm thickness of calcium oxalate coating on the outer pore walls, resulting in reinforcement of intergranular cohesion. Even though restoration set up on transformation of the former material cannot be acceptable *a priori*, it is a good argument when organic materials used as consolidating agents can lead to undesired and irreversible effects on inorganic substrates such as carbonate porous materials.

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P5

Preparation and characterization of natural zeolite to be used against gastric infections caused by Helicobacter pylori

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Helicobacter pylori is a gram-negative flagellated bacterium that has been recognized to be responsible for up to 70% of gastric ulcers. To survive in gastric environment the bacterium hydrolyses the urea present in the gastric juices generating ammonia which increases the pH in the stomach as, due to H^+ presence, ammonia is converted to NH_4^+. Ammonia is toxic to cells by itself and after endosomal accumulation of the ion form (NH_4^+), it leads to swelling of vacuoles generated VacA. This process helps to cause damaging of gastric cells. Some zeolites are highly selective toward ammonium ion. A research has been started (PRIN 2010MKHT9B_008 granted to G. Cerri) to investigate if some zeolites, particularly clinoptilolite, are able to develop a synergic action with some antibiotic in the treatment against *H. pylori*.

A clinoptilolite-rich Sardinian epiclastite has been used to prepare a micronized powder with a higher grade of zeolite (obtained by beneficiation process). Later, the material has been modified to in Na-form by ion-exchange. Chemical and mineralogical composition, technological properties and microbiological quality of materials have been determined. Tests have been also performed to evaluate the resistance of Na-clinoptilolite, its ability to uptake $NH4^+$ and release of contaminants in simulated gastrointestinal fluids.

The powder prepared has a zeolite grade of about 90 wt. %. The volume-surface diameter, dvs, is 4.96 ± 0.51μm. The true density is 2.18 ± 0.00 g/cm3. The material shows a scarce flow capacity but good compactability. The material is resistant in the gastric environment and able to uptake $NH4^+$ releasing Na^+ in simulated gastric juice. Heavy metals release tested in the same conditions is extremely low, comparable or lower than some clays already traded in pharmaceutical field. Microbiological tests reveal that the material is compatible with oral administration.

P6

A study about natural-like compounds with inhibitory activity on tyrosinase enzyme by means of a tyrosinase-based amperometric biosensor.

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Tyrosinase catalyses the hydroxylation of tyrosine to L-DOPA and the oxidation of the L-DOPA to dopaquinone [1]. Futhermore, in humans, dopaquinone is converted by a series of complex reactions which finally result in the formation of melanin in melanocytes [2]. However, this beneficial trait comes in hand with some human diseases because of the overproduction of melanin [3]. Therefore, Tyrosinase inhibition has thus been explored as an avenue for therapies to these diseases (such as melanoma and Parkinson's disease, PD) [4]. The aim of the present study is the development of new pharmacological tools for preliminary studies on the Tyrosinase enzyme inhibition role. In this study, it was designed, synthesized and characterized a new class of low molecular weight phenols that are reminiscent of natural structures, having inhibitory activity against tyrosinase. Firstly the inhibitory activity of each molecule by means of an amperometric biosensor has been determined. This device exploits the ability of the Tyrosinase to catalytically transform catechols to quinones. The interaction between inhibitor and enzyme could be revealed from the variations in the Michaelis-Menten kinetic parameters, extrapolated both in the presence and absence of the molecule inhibitor. Moreover, the effects of same molecules were preliminary tested on the viability of PC12 cells, a cell line derived by murine pheochromocytoma, in order to test their eventual biological properties.

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P7

Electrochemical polythiophene-based biosensors for glucose detection in fruit juices

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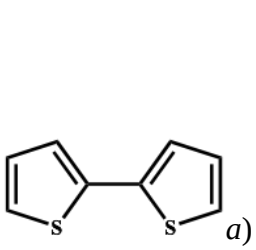
Abstract. In this study, two thiophene-based conducting polymers are used as a matrix for the entrapment of glucose oxidase (GOx) and served as the working electrode for glucose detection. Polymer films were obtained by electrochemical polymerization of: *a*) 2,2'-bithiophene and *b*) a new 4,4'-disubstituted-2,2'-bithiophene obtained by our research group, that is 4,4'-bis(2-methyl-3-butin-2-ol)-2,2'-bithiophene. GOx was covalently immobilized on the polythiophene film using 1-Cyclohexyl-3-(2-morpholinoethyl)-carbodiimide metho-p-toluenesulfonate (CMC) as condensing agent [1]. Amperometric response of biosensor at varying the concentration of glucose was recorded in a three-electrode cell containing phosphate buffer (pH 7) and p-benzoquinone as a redox mediator. The biosensor performance has been checked in standard samples, then it has been applied to the glucose determination in fruit juices. The preliminary results obtained for the same juices using both the films were compared and show statistically acceptable results.



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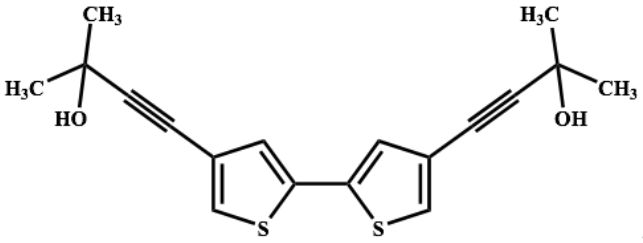

b)

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P8

IMIDAZO[4,5-*g*]QUINOLINES AND PYRIDO[2,3-*g*]QUINOXALINES: DESIGN AND SYNTHESIS OF NEW POSSIBLE ANTIVIRAL AGENTS

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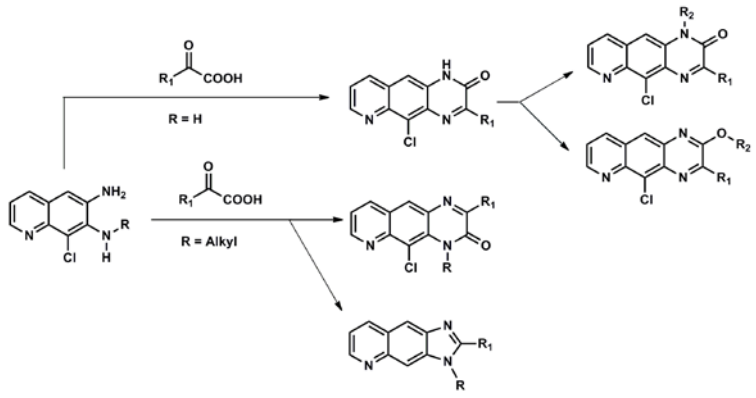
Linear aromatic *N*-tricyclic compounds with a promising antiviral activity associated with little or no cytotoxicity, were prepared and analyzed in the last years [1]. The pyrido[2,3-*g*]quinoxaline nucleus turned out to be principally active against several pathogenic RNA viruses interesting for veterinary and human therapies. Compound (**1**), selected as lead compound, was modified with the aim to enhance the antiviral activity and reduce or cancel the cytotoxicity. Therefore, several substituents were inserted on the nitrogen in position 7 of diaminoquinoline intermediates and, at the same time, on the nitrogen in position 1 or on the oxygen in position 2 of (**1**). Title compounds were tested in cell-based assays for cytotoxicity and antiviral activity against single-stranded RNA viruses negative or (ssRNA-) positive (ssRNA+) sense, double-stranded genomes (dsRNA), as well as against representatives of two DNA virus families. Some derivatives represent attractive leads for the development of antiviral agents against some viruses of public health significance, such as RSV, Reo, BVDV and HCV.



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P9

$Mg(NH_2)_2$+2MH (M=Li-Na): Structural and desorption investigation

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The $Mg(NH_2)_2$+2MH (M=Li-Na) systems are considered promising candidates as solid state hydrogen storage materials for on-board applications [1,2]. The $Mg(NH_2)_2$+2MH (M=Li-Na) mixtures were prepared via metathesis reaction induced by mechanical input starting from $LiNH_2/MgH_2$ and $NaNH_2/MgH_2$, respectively. The milling products were fully characterized by XRD and FT-IR. The TPD measurements showed that the increasing time of mechanical treatment improved the kinetics and decreased the desorption temperature. Ex-situ PD-XRD measurements performed at various stages of the desorption showed the formation of two new phases, not yet resolved, presumably ascribed to a mixed Na-Mg tetra-amide and Na-Mg imide phases.

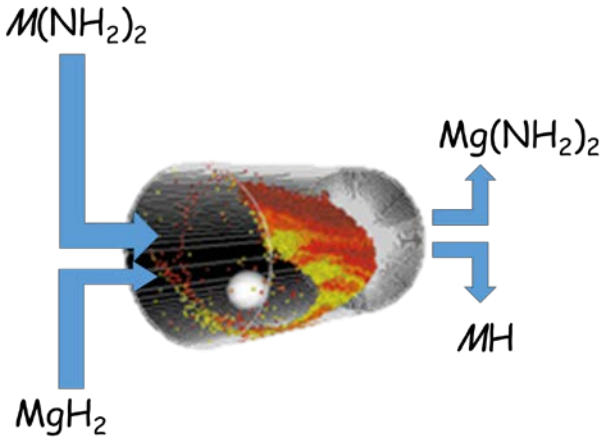

Figure: Preparation of the mixture by mechanical activation.

References:

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P10

The new and efficient method for synthesis of esters from aldehydes

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Esters are one of the most important functional groups in organic chemistry and are present in many biologically active compounds with significant pharmacological and industrial properties. The classical synthetic routes to esters either couple an activated carboxylic acid derivative with the appropriate alcohol or employ an equilibrium mediated esterification/transesterification protocol [1]. The most important limitation of these techniques is the use of toxic coupling reagents in stoichiometric concentrations [2]. To overcome these problems many alternative strategies have been studied. An elegant, eco-friendly alternative is the transformation of aldehydes into acyl chlorides that subsequently react with alcohols.

We have developed a synthetic protocol for the direct synthesis of esters from alcohols and acyl chlorides, prepared in situ, using trichloroisocyanuric acid and aldehydes.

The method is simple, convenient and uses inexpensive and commercially available reagents.

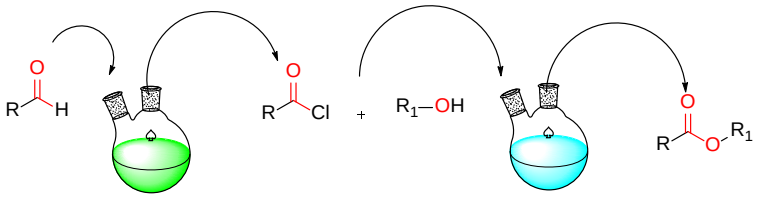

Figure 1: Reaction scheme for the synthesis of esters starting from aldehydes.

References:

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P11

STUDY OF ANTIOXIDANTS AND ANTIMICROBIAL PROPERTIES IN PLANT EXTRACTS ELICRISO.

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The aim of this work is to study the antimicrobial and antioxidant activity of extracts of Helichrysum (Helychrisum italicum (Roth G. Don fil. Subsp. Microphyllum). For the selection of plant species have been used to traditional medicine starting from studies ethnobotany based on the use of plants as remedies healthful.

The plant has among its active ingredients an essential oil and a rich polyphenolic component justifying the well-known antimicrobial properties and antioxidants. The drug has been divided into flowers, green parts of the stems and woody parts. The extracts were prepared by ASE (accelerated solvent extraction), a very versatile tool that allows you to extract active ingredients from complex matrices. It was decided to use four solvents, of which three organic, with different polarity, and an inorganic, such as water. The extracts obtained were then evaluated using the following tests:

• As for the antimicrobial activity was determined by MIC (minimum inhibitory concentration) and MCB (minimum bactericidal concentration) against the following strains of bacteria: Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa, Candida albicans (mycobacteria). The extracts obtained using the green parts of the stems and flowers have shown inhibitory activity that is bactericidal against the bacterial strain Staphylococcus aureus. No activity was observed against other microorganisms.

• As for the antioxidant activity was used the rate of DPPH, a very stable radical which absorbs in the UV-visible and is therefore monitored by spectrophotometry. After the collection of data was calculated the percent inhibition (I%). Aqueous extracts of green stems have reached values of I% 66.4%; while those obtained with organic solvents are inferior results with values of I% of 61.3%. The extracts obtained from the flowers have values of I% very similar, at around 63%.

P12

NEW FRONTIERS FOR PHOTO-DEVICES

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Light-emitting diodes (LEDs) are of particular interest due to their energy-saving properties. However, at the moment most LEDs rely on Rare Earth Elements (REEs) to function. Substitution of REEs is one of the most critical issues of modern research. In particular the use of REE in white light emitting diodes (WLEDs) is problematic from a strategic point of view due to REE availability, costs, and supply disruption. The development of a new class of photo-devices that totally eliminate REE in WLED using hybrid organic/inorganic luminescence alternatives would solve this problem.

We have designed and synthesized a small library of metal organic compounds and tested their luminescence properties. We have identified a class of triazine-based compounds that show promising luminescence properties and could be adapted to use in LEDs.

P13

The strange case of 6-methoxy-2,2'-bipyridine in rollover cyclometalation

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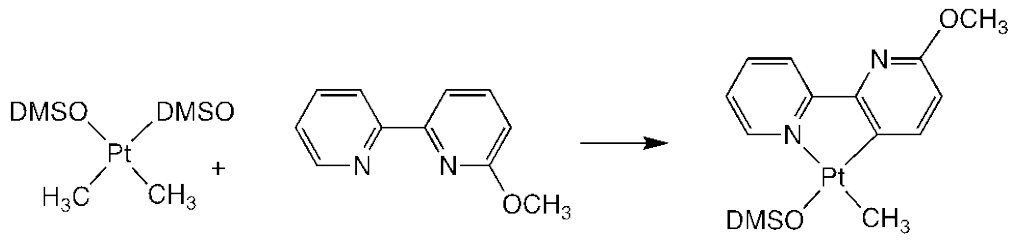
Rollover cyclometalated complexes arise from a special type of intramolecular C-H activation which may occur with bidentate heterocyclic ligands.[1] Following our long-standing interest in this field we recently started to investigate how steric and electronic parameters affect the C-H activation process and the reactivity of the corresponding cyclometalated complexes.[2]

Here we present our most recent results regarding the newly synthesized 6-methoxy-2,2'-bipyridine (bpy^{6OMe}) where the substituent has a double nature being both electron-releasing (positive mesomeric effect, +M) and electron-withdrawing (negative inductive effect, -I).

Bpy^{6OMe} reactivity with different Pt(II) common precursors was explored and the reactivity of the cyclometalated complexes obtained was investigated. With electron-rich Pt(II) precursors rollover cyclometalation occurs even at room temperature.



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P14

Experiments explained by DFT calculations: N,C,N-pincer gold(III) complexes

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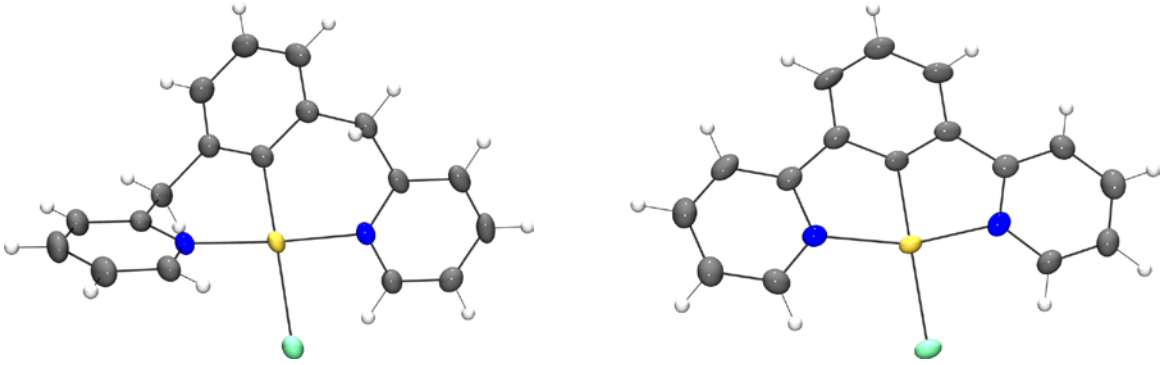
In our previous studies we managed to synthesize a series of N,C,N-cyclometalated pincer[1] complexes with gold(III) and we completely characterized them both in solution and in solid phase.[2] In the series $[Au(N,C,N)Cl]^+$, where N,C,N is a meta-disubstituted benzene containing pyridyl groups, the reactivity of the Au-Cl bond was found to be dependent on the delocalization of the metallacycle, *i.e.* when the complex has two six membered rings, such as in **1**, the chloride readily reacts while in the case of the extensively delocalized **2** the chloride is not reactive even in harsh conditions.

We investigated the reasons behind this different behaviour using Density Functional Theory calculations and found that metalloaromaticity[3] is a good explanation.



1 **2**

Figure 1: Crystal structures of two cyclometalated N,C,N-pincer complexes studied.

References:

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P15

Preparation of β-cyclodextrin-based components useful in biosensors of agricultural and food relevance

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β-cyclodextrin (βCD), a natural, non-toxic cycloeptaamilose macrocycle, is a useful stabilizer and immobilizing agent for enzymes because of the affinity of its cavity for hydrophobic guest molecules (e.g., aminoacids) [1]. βCD is currently esterified preferentially at C6 primary OH with polycarboxylic acid (PCA) *via* anhydride formation [2]. In quite similar conditions [2,3] we have found that βCD with 1,2,3,4-butanetetracarboxylic acid (BTCA) or its more reactive anhydride (BTCAa) have formed preferentially different complexes rather than the esterification product.

βCD formed a complex with a sulphonated polyphenol by means of rotavapor, sonication and microwave irradiation in a more straightforward way than under classical conditions. Complex stability and guest position into the macrocycle cavity are influenced by the complexation conditions.

βCD in the presence of dimethylcarbonate under basic conditions or monochlorotriazine βCD in the presence of diols were assayed in order to obtain a modified linked βCD. The water-soluble βCD based complexes and linked βCDs are characterized by ^{1}H and ^{13}C NMR and could be tested in a biosensor design to investigate their effect on the polymer/modifier composite selectivity [4].

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Immobilization of Ampicillin on Ordered Mesoporous Silica

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Ordered Mesoporous Silicas are highly reproducible materials synthesized using the self-assembly properties of ionic and non ionic surfactants (Fig. 1a). The obtained mesoporous materials have high values of surface area (up to 1000 m^2/g) and narrow distributions of the pore size (2-30 nm). These features make them perfect carriers for the sustained release of therapeutic molecules [1-3]. In this work the hexagonal MCM-41 and SBA-15 mesoporous materials were synthesized and characterized through small-angle X-ray scattering, N_2 adsorption–desorption isotherms, Fourier transform infrared spectroscopy, transmission electron microscopy and dynamic light scattering. The two materials differ for the pore size, being 27 Å and 64 Å for MCM-41 and SBA-15 respectively (Fig. 1b). These materials were then used as carriers for the immobilization of ampicillin, a β-lactamic antibiotic used as a model drug (Fig. 1c). The adsorption kinetics and the adsorption isotherm of ampicillin on both SBA-15 and MCM-41 were studied. It was found that, besides pore size, the adsorption pH has a strong influence on ampicillin loading .

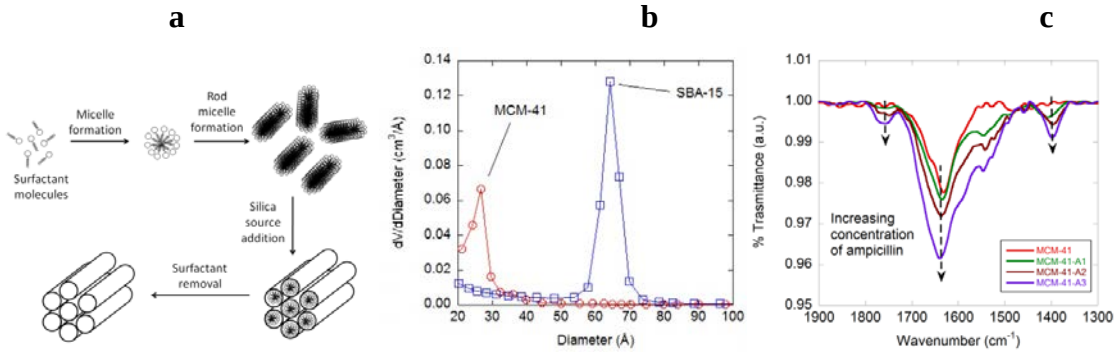

Figure 1: (a) Synthesis mechanism of ordered mesoporous silica. (b) Pore size distribution of MCM-41 and SBA-15. (c) FTIR spectra of MCM-41 loaded with different amounts of ampicillin.

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P17

Penicillum digitatum activity in Citrus fruits treated with GRAS compounds

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The main pathogen which leads the alteration of *citrus* structure giving rise to the food losses are: *Penicillium digitatum (green mold Pd)* and *Penicillium italicum (blue mold)*.

During ripening time three main enzymes are produce by the fruit, namely: *polygalacturonase, pectinesterase* and *pectin lyase*, whose are produced with the aim to degrade the cell walls and then to give a controlled softening of the fruit. The same enzymes are as well produced by the *penicillium* spp. which, takes advantages of their action on the cell walls to obtain simple sugars as nutrients. Several chemical and physical methods have been employed in the technology for pest control.

Recently, on the basis of food processors and consumers preferences, safe natural products are replacing synthetic chemical additives, since many of them are suspected to be harmful for health. Compounds classified by the Food and Drug Administration as generally recognized as safe are now largely used as preservative for preventing microbial spoilage. Among them the most deeply studied are sodium carbonate (SC) and sodium bicarbonate (SBC). The main effect of SC/SBC is to increase the pH indeed has been observed that there is not a direct interaction between SC/SBC and the pathogen; Pd usually produce *polygalacturonase, pectinesterase, pectin lyase* at low values of pH consequently in presence of SC/SBC it seem to be inhibited in the production of enzymes.

Herein we report a study of the behavior of Pd; the experiment were carried out after 0, 24 h, 48h e 72 h from the inoculation. The cell wall sugar components were fractionated and analyzed by GC-MS technique and by spectrophotometric methods. The determined quali-quantitative sugar composition is related to the activity of the inoculated pathogen.

All analyses were carried out in duplicate on a control, SBC-treated *Citrus paradisi* albedo and on an SBC-treated *Citrus paradisi* albedo at pH=5.

P18

Searching for the pharmacophore in β-diketo acid inhibitors of influenza virus PA endonuclease

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Vaccination and antiviral therapy are the primary measures to combat human influenza viruses. However, due to the increasing resistance against current medications (e.g. oseltamivir) there is an urgent need for entirely novel inhibitors with an original mode of action. In this context, the influenza virus RNA polymerase complex is recognized as a novel and attractive target for antiviral drug development, due to its essential role in virus replication [1]. A particularly promising concept is inhibition of the PA endonuclease subunit, which cleaves capped host pre-mRNAs to generate the primer for initiation of viral mRNA synthesis [1,2]. In the course of an extensive drug discovery program, researchers at Merck discovered a series of 2,4-dioxobutanoic acids (i.e. β-diketo acids; DKAs) that selectively target this endonuclease activity. Among them, compound L-742,001 was identified as one of the most potent small molecule inhibitors of the influenza virus endonuclease reaction, both in enzyme- and cell-based assays [3-5]. This compound interferes with the catalytic activity of PA by causing functional sequestration of one or both divalent metal ions present in the active site. Recently, to elucidate the binding mode of L-742,001 within the PA endonuclease, we performed a comprehensive mutational analysis on amino acids within or around the catalytic center of PA, and evaluated their impact on antiviral sensitivity to L-742,001 [6].

Herein, to formulate possible structure–activity relationships and identify the unique pharmacophore within the chemical class of DKAs, we report on the investigation of a series of substituted β-diketo acids. Compound design and synthesis, pharmacophore refinement and inhibitory activities in a PA-Nter enzymatic assay, as well antiviral activities in a cell-based virus-yield assay, will be presented.

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P19

A method based on VOCs composition to discriminate *Citrus mostruosa* from several *Citrus* spp.

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Citrus mostruosa is a tree of *Rutaceae* family, similar to the grapefruit. It is cultivated in a narrow area in the south-est of Sardinia. Its origin is unknown, but some author believe it is a spontaneous cross between *Citrus limon* and *C. medica*. The fruit of *C. mostruosa* is yellow when ripe and it becomes rather large in size, up to a weight of 700 grams. Although the flesh is not edible, the fruit albedo is traditionally used as raw material in the making of a typical dish called "Sa Pompia", whereas a liqueur is obtained by hydroalcoholic infusion of the flavedo.

In this work we address the study of the chemical composition of the Volatile Organic Compounds (VOCs) of eight *Citrus* spp., including *C. mostruosa*. The aim of the work is to achieve detection and classification based on variability of VOCs composition.

To study the VOCs chemical composition of the eight *Citrus* spp. by Solid Phase Micro Extraction (HS-SPME) coupled with a GC-MS analysis, has been applied successfully on *C. mostruosa*, *C. aurantium*, *C. limon*, *C. reticulata*, *C. sinensis*, *C. medica*, *C. paradisi* and *C. myrtifolia*.

With this analysis forty-four compounds have been identified, among them Limonene resulted the main component in all studied species. Others compounds resulted specific in only one of the eight analyzed *Citrus* spp. Principal Component Analysis of VOCs have allowed to discriminate the *C. mostruosa* samples among the studied *Citrus* samples.

Finally the quali-quantitative determination of the chemical composition of the essential oil of *C. mostruosa,* obtained by steam distillation has been determined by GC-FID analysis, with internal standard method, coupled with GC-MS technique.

P20

CHITOSAN NANOPARTICLES FOR NON-INVASIVE TUMOR IMAGING

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The aim of the present work was to prepare near-infrared fluorescence chitosan (CS) nanoparticles (NPs) as possible diagnostic platforms for the identification of hepatic cancer. Indocyanine green (ICG) has been used as non-invasive imaging agent. Efficient accumulation of ICG to the tumor site and its retention is required for application of ICG in cancer diagnosis. One of the approaches in order to allow ICG accumulation to the tumor site can be its loading into a polymeric nanoparticulate system [1]. In this work, CS NPs were prepared by ionic gelation method, using sodium tripolyphosphate (TPP) or sodium hexametaphosphate (SHMP) as cross-linker (CL) agents. Previously, CS (MW 35 kDa) was subjected to a rigorous purification process. The following formulative parameters have been considered: CS form (base or chloride), CS concentration, type of CL (TPP or SHMP) and CL concentration. CS/CL mass ratio was kept constant (4:1). CS/TPP and CS/SHMP NPs were formed by dropwise addition of CL solution into CS solution under magnetic stirring. ICG-loaded NPs were prepared using the same conditions as for the blank systems, dissolving the dye in the dispersing medium of CS. After the ionic gelation, the aqueous suspensions obtained were characterized in terms of particle size and size distribution by Photonic Correlation Spectroscopy. Furthermore, NPs suspensions were analysed after 1 day and 1, 2, 3 and 4 weeks, at 20 °C and 4°C.

NPs obtained showed mean diameter comprised between 90 nm and 390 nm, depending on the composition. Nanosystems prepared with SHMP were always bigger than those formed with TPP, because of the molecular weight of CL. NPs size decreases depending on CL concentrations decrease, with both cross-linkers. The same behaviour was observed when CS concentration was reduced and the other parameters were fixed. The formulations prepared with CS chloride showed that, in certain conditions, the use of TPP carried out at phase separation. On the basis of these first results, two samples with different CL agents were chosen as leader formulations for ICG loading. The loading of the dye determined size NPs increase in both batches. *In vitro* stability tests were carried out on blank formulations. The results demonstrated that NPs size is dependent on temperature storage. Mean diameter increased in every batch at room temperature, especially in the fourth week, while at 4°C no significant effect on size was detected, regardless of the variation of different formulative parameters. In conclusion, CS NPs are good systems to loading ICG through ionic interactions and could be employed as diagnostic platforms in hepatocellular carcinoma, after appropriate functionalization.

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P21

Thermosensitive *in situ* gelling solutions for potential application in intraoperative fluorescence imaging and local therapy of hepatocellular carcinoma

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Hepatocellular carcinoma (HCC) is classified as a highly chemoresistant disease and conventional systemic chemotherapy plays almost no role in the treatment of advanced HCCs. For these reasons, localized anticancer therapies must be taken into account [1]. Embolization without chemotherapy (transarterial embolization, TAE) can be classified as one of the forms of local treatment of HCC. TAE consists of embolization of the artery feeding the tumor, which results in ischemia and subsequent tumor necrosis. Thermosensitive chitosan/glycerophosphate (C/GP) solutions exhibiting sol-gel transition around body temperature, were prepared with the aim to develop a class of injectable hydrogel platforms that can be used for the imaging and loco-regional treatment of hepatocellular carcinoma (HCC). Indocyanine green (ICG), an usefull amphiphilic tricarbocyanine dye for intraoperative imaging, was loaded in the thermosensitive solutions in order to assess their potential for the detection of tumor nodules by fluorescence. The gelling time of these ICG loaded formulations as well as *in vitro* dye release behaviour were investigated. *Ex vivo* embolization studies were carried out for a preliminary evaluation by using an isolated bovine liver. It was observed that ICG was not released from the hydrogels because of a strong electrostatic interaction between C and ICG. *Ex vivo* studies revealed that these injectable formulations remain in correspondence of the injected site. In conclusion, the developed ICG-loaded hydrogels have the potential for intraoperative fluorescence imaging and local therapy of HCC as embolic agents.

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