Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase

Report 2013

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Summary

1A: Hard Matter (Nanomaterials and Solid Interfaces)

1B: Soft Matter (Nanomaterials and Liquid Interfaces)

1C: Theory and Modelling

2A: Art Restoration, Environmental Remediation and Textile Chemistry

2B: Metals and Ceramics

2C: Biotechnology

CSGI Research Activity

Outline

CSGI (Research Center for Colloids and Nanoscience) was established in Firenze, in December 1993. It has been officially recognized by the Italian Government in 1994, and is under the supervision and control of the Italian Ministry for University and Scientific Research (MIUR). Since 1995 CSGI began its scientific activity, devoted to basic research and to the development of high-tech new processes, and is supporting the activities of the small and medium size business industrial companies, that cannot afford the financial costs of an independent research activity.

In the last years, CSGI has sponsored several different research programs, mainly supported by European Union grants, and partly also by other international and national Institutions, such as the italian PRIN, PNR, FISR, FIRB, POR FESR and so forth.

CSGI has signed numerous contracts that involve about 75 national and international industrial companies, and some highly qualified research Centers, such as Procter & Gamble, Siemens, Tecnotessile SpA, Massachusetts Institute of Technology, Bayer-Schering, Solay, ENI, Giuliani SpA, CTG Italcementi, King Saud University, Rifinizione S. Stefano, AMSA, Pierre Fabre, Farmabios, University of Florida, È Così, Lachesis, MBN SpA, Novartis, W.A.D.A., Morphotec, Perkin Elmer, Grünenthal Gmbh, Lamberti SpA, Comune di Firenze, Teletron Euroricerche, VTT, etc.. Such lively activity has brought to several International Patents and research agreements.

CSGI has reached a very qualified standard, and its level has been acknowledged abroad, in several fields. For example, CSGI is a leader in a number of applications of Nanotechnology, in the conservation of cultural heritage, and in the production of nanophasic powders (with MBN) for the production of special materials for aeronautics, high resistance coatings, etc.. CSGI supports the local authorities for the safeguard and conservation of works or art ("Sovrintendenze Artistiche") in Tuscany and other Italian districts, with technologies that have been developed for this aim. Similar actions have been promoted in agreement with the Mexican Federal Government for the conservation of monuments (Puebla Cathedral, Maya and Aztec heritage, the archaeological site of Calakmul, Campeche), with museums and conservation institutions.

CSGI is active also in the training of specialized researchers, has granted several fellowships, PhD supporting programs, post-doc grants, and other education projects, and has organized several national and international Meetings. In particular, during the years 2011-2013, CSGI has issued 20 PhD scholarships, 90 fellowships, and 15 post-doc grants, and is actively participating in two European Master Programs: EMASCO-COSOM (European Master in Supramolecular and Colloidal Chemistry) and IMES (International Master on Bioenergy and Environment). CSGI has co-sponsored national and international congresses (International Workshop on Dynamic Crossover Phenomena in Water and Other Glass-forming Liquids and CSGI National Meeting).

The CSGI financial plan is solid, with a strong growth of its financial assets, mainly due to EU funding.

The main topics of CSGI research activity are:

- development of processes for the production of nanophasic systems (i) for the production of innovative textiles, (ii) for the synthesis of nanophasic alloys,

(iii) for ceramics and nanophasic or nanostructured composites (low temperature and low energy costs);
- setup of new additives for cement products. These projects are mainly carried out in collaboration with Italcementi and MIT, and are aimed at investigating and optimizing (i) the cement hydration process and the production of new, (ii) ceramics-like materials for the cement-related industry;
- formulation of dispersions in fluids, emulsions and inverted emulsions (paints, adhesives, sealing materials, detergents, etc.);
- development of systems for the confinement of proteins and for the controlled release of pharmaceutics;
- development of food-related industrial processes (for example the treatment of milk and milk derivatives in supercritical phase);
- development of innovative procedures for the conservation and restoration of works of art (paintings, frescoes and stone-based materials).

CSGI is a world leader in this research activity, and is involved in a significant campaign for the recover of archaeological treasures in Mexico (Calakmul), the largest Maya sites, and in several other countries (Cile, Argentina, Sweden, Spain, India, Egypt, Israel, Romania, etc.).

Fields of Interest

- Nanostructured and ultrafine materials.
- Structure and dynamics of supramolecular assemblies (monolayers, micelles, liposomes, microemulsions, Langmuir-Blodgett films, host-guest systems).
- Nanophasic ternary oxides.
- Structural analysis of biomolecules in solution, interaction processes, recognition of ligands with macromolecular surfaces, theoretical and experimental analysis of cellular metabolism, interactions between metals and ligands, characterization of the interaction sites.
- Formulation of nanophasic systems.
- Innovative processes for the conservation and restoration of cultural heritage (stone materials, wood materials, paintings, frescoes, paper, photographic material).

National Agency for the evaluation of Quality of Research (2004-2010): CSGI ranking

CSGI was one of the 26 Consortia that voluntary submitted their candidature to the Italian evaluation of universities and research centers: Valutazione della Qualità della Ricerca (VQR), an exercise to evaluate the quality of the research efforts in the period 2004-2010. The report was produced by Agenzia Nazionale di Valutazione del sistema Universitario e della Ricerca (ANVUR), an Italian national agency for the Italian research qualification. VQR2004-2010 resulted in the largest-scale evaluation of research in Italy's history.

The VQR examined research outcomes in 14 disciplinary areas of study published between 2004 and 2010 by 95 universities, 12 research centers and 26 other institutions to identify the significance of the nation's research output and how it compares globally. By reviewing a significant number of Italian research outcomes, ANVUR was able to gain a greater understanding of Italy's research strengths, impact and neglected fields of study.
CSGI ranked in the first positions among the other Italian Consortia for Chemical Sciences (Area 03) and for Biological Sciences (Area 05) for the period 2004-2010.
In particular, in the disciplines related to Chemical Sciences (the core of the CSGI research), CSGI resulted as excellent (74% of the submitted products were judged as excellent and the remaining 26% as good). The final indicators for the research and the third mission are well above the average values for Consortia in the same categories.

Structure and Organization of CSGI

Management Offices
President, Council, Director, Audit Council, Technical-Scientific Board.

Director of CSGI
Prof. Piero Baglioni, Department of Chemistry, University of Florence.

President of CSGI
Prof. Giovanni Marletta, Department of Chemical Sciences, University of Catania.

Website
http://www.csgi.unifi.it/

Foundation
December 21st, 1993

Official recognition by the Italian Government
November 15th, 1994 (G.U. Nr. 267)

Academic Units and Associated Centers

University of Florence (headquarter)
Scuola Normale Superiore in Pisa
University of Bari
University of Bergamo
University of Catania
University of Cagliari
University of Molise (Campobasso)
University of Naples “Federico II”
University of Pavia
University of Siena
Laboratory CSGI of Treviso

Polytechnic Institute of Milan
University of Bologna
University of Milan, Bicocca
University of Perugia
University of Rome, La Sapienza
University of Venice

Personnel

CSGI gathers about 300 researchers including Full Professors, Associate Professors, University Researchers, that belong to the academic members.
Moreover, CSGI employs 75 researchers and 3 administration employees on its own. Several PhD and post-doc students are financially supported through CSGI fellowships. CSGI hosts researchers hired by industrial companies for training and specific research activities, in the framework of particular projects.
CSGI owes two research Laboratories, located in Vascon di Carbonera (Nanophases Laboratory) and in Prato (Laboratory for the refinement and surface modification of textiles). These plants collaborate closely with the local industrial activities.

Previous and Current Academic Collaborations

ANU - Australian National University
Argonne National Laboratory
Aston University (Birmingham)
Brookhaven National Laboratory
California Institute of Technology – CalTech
Centro di Istochimica del CNR di Pavia
Chalmers University of Technology
CNIC - Centro Nacional de Ivestigaciones Cientificas (Cuba)
CNR - Consiglio Nazionale delle Ricerche
CNRS - Centre National de la Recherche Scientifique
Collège de France
Columbia University
CPMCRI - California Pacific Medical Center Research Institute-, San Francisco
CSIC (Sevilla)
East China Normal University (Shangai)
École Normale Supérieure (Lion)
Escuela Superior Politecnica del Chimborazo
ETH Zürich - Eidgenössische Technische Hochschule Zürich
Hahn-Meitner Institut (Berlin)
Hull University
Inst. Nat. Polytechnique de Lorraine (Nancy)
Inst. Science des Matériaux
Inst. Scientific Instruments (Czech Rep.)
Institut Laser Technology
ITER - International Thermonuclear Experimental Reactor
Laboratoire Leon Brillouin (Saclay)
Lehstul Fertigungstechnologie
Massachusetts Institute of Technology
Max Planck Institut (Berlin)
Max Plank Institut Biofisica (Francoforte)
Museum of Fine Arts (Boston)
Nuclear Research Institute (Prague)
Oak Ridge National Laboratory
Oklahoma State University
Risø National Laboratory
Technical University di Budapest
Technische Universität Darmstadt
Tekniska Hogskolan I Luleå
The Getty Conservation Institute
UCLA - University of California Los Angeles
Università degli Studi della Calabria
Università degli Studi di Bari
Università degli Studi di Camerino
Università degli Studi di Chieti
Università degli Studi di Ferrara
Università degli Studi di Genova
Università degli Studi di Milano
Università degli Studi di Padova
Università degli Studi di Palermo
Università degli Studi di Parma
Università degli Studi di Pisa
Università degli Studi di Salerno
Università degli Studi di Siena
Università degli Studi di Torino
Università degli Studi di Trento
Università degli Studi di Urbino
Universitad de Santiago de Compostela
Universitad del Salvador
Universitad Estadual de Campinas
Universität Gesamthoschule Kassel
Universität Heidelberg
Universität Konstanz
Université “Louis Pasteur” (Strasbourg)
Université de Bourgogne
Université de Grenoble
Université de Montpellier II
University College (London)
University of Berkeley
University of Bristol
University of Cambridge
University of Detroit
University of East Anglia
University of Houston
University of Leiden
University of Lund
University of South Florida
University of Sydney
University of York
Weizmann Institute (Israel)

Previous and Current Industrial Partners

3M
Alcea
Alfa Test
Alfa Wasserman
Angelini
Ansaldo
Aprilia
Ascor chimici
Ausimont
Bigagli
Biokimica S.p.A
Bioscreen Technology srl
Bitossi
BTG-Holland
Chemia
Chiesi Farmaceutici S.p.A
Chimet S.p.A.
Comune di Firenze
Consorzio delle Buone Idee
Cover
D'Appolonia
Dynamotive
Elf-Atochem
ENEA (Energy Department – Casaccia)
Eniricerche
Enitecnologie
EUBIA (Bruxelles)
Firenze-Prato-Pistoia
Flory's
Getty Conservation Institute
Glaxo-Wellcome
Icmese
INASCO-Hellas (Int. Aerosp. Sci. Corp.)
Industrial Materials Technology GmbH
Industrie Casearie Podda
Ineti
Institute for the Care of Hystorical Monuments (Prague)
Instituto Nacional de Antropologìa e Historia - INAH
International Broker
Inver
IRBM
Italcementi S.p.A.
Italfarmaco
JRC (Joint Research Centre of the European Commission)
Lamberti S.p.A.
Lilly
Lima
Lombardia
Mapei
Mariplast
Martelli S.p.A.
MBN Nanomaterialia
Merk
Microtec (Germany)
National Museum of Denmark
Nicox
Novuspharma Omrod Diesel (UK)
Orion Pharma
Pharmacia-Upjon (USA and Sweden)
Pharmaness
Philips
Procter & Gamble
Reggio Calabria
Rifiniture BP
Roma
S.I.F.I.
Sem
Siemens AG
Sigma-tau
Sintech
SIR Industriale
Sirio Panel
Solvay
Soprintendenze ai Beni Ambientali ed Architettonici di:
Soprintendenze ai Beni Artistici e Storici di: FI-PO-PT, SI-GR, PI-LU-MS
Tecnotessile SpA
TIL (Tooling International Ltd UK)
TNO (Netherlands)
Transfergomma (Padova)
Veneto Orientale
VTT (Finland).
WIP (Germany)

CSGI Patents

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2) Matteazzi Paolo, Baglioni Piero, Basset Diego – "Process for Recycling, by Milling, Solid Industrial Waste and Materials at the end of their Service Life". European Patent Application 97203735.2, Priority IT96 FI96A000280.

3) Grassi Giuliano, Chiaramonti David, Baglioni Piero – "Apparato a combustione di etanolo o miscele etanolo per cucine, stufe e illuminazione a uso domestico". Italian Patent FI/98/A42, deposit date 24/ 02/ 1998.

4) Ambrosone Luigi, Ceglie Andrea – "Software per l'analisi grafica e numerica di dati di Risonanza Magnetica Nucleare per la determinazione della polidispersità di emulsioni". Italian Patent FI99A000044, deposit date 09/03/1999.

5) Baglioni Piero, Carretti Emiliano, Dei Luigi – "Microemulsioni ed emulsioni di olio in acqua, loro uso per la solubilizzazione di resine polimeriche e impacchi contenenti detti microemulsioni o emulsioni". Italian Patent FI99A000071, deposit date 02/ 04/1999.

6) Baglioni Piero, Fratini Emiliano, Ricceri Riccardo, Sarti Giuseppe, Chiaramonti David – "Engine fuels consisting of an emulsion comprising mineral and/or natural oils, their preparation and use in internal combustion engine". PCT International Application WO n. 99936473.0 del 02/07/1999.

7) Baglioni Piero, Bardi Ugo, Bonini Massimo – New method for the production of solid powder and films by compartimentalised solution thermal spraying (CSTS). European Patent Application EP 00-105673.8, deposit date 17/03/2000.

8) Angelico Ruggero, Ceglie Andrea, Hochoeppler Alejandro, Palazzo Gerardo, Stefan Alessandra – "Macroemulsioni acqua-in olio a lunga stabilità, loro preparazione ed uso". Patent Query N. FI2001A000016, deposit date 29/01/2001.

9) Baglioni Piero, Dei Luigi, Fratoni Laura, Lo Nostro Pierandrea, Moroni Michelangelo – "Processo per la preparazione di nano e microparticelle di ossidi e idrossidi di metalli del secondo gruppo e di transizione, nano e microparticelle così ottenute e loro impiego in campo ceramico, tessile e cartario". Patent Query N. FI2002A000052, deposit date 28/03/2002 – EP 03745367.7.

10) Baglioni Piero, Dei Luigi, Giorgi Rodorigo, Claudio Vinicius Schettino – "Basic Suspensions their Preparation and Use in Processes for Paper Deacidification". European Patent Application EP 02714088.8, deposit date 15/01/2002.

11) Ambrosone Luigi, Ceglie Andrea – "Materiale assorbente e suoi usi nei processi di bonifica di falde acquifere inquinate da prodotti chimici". Patent Query FI2003A000236, deposit date 11/09/2003.

12) Ambrosone Luigi, Ceglie Andrea – "Gel stabili contenenti gelatina". Patent Query N. FI2003A000237, deposit date 11/09/2003.

13) Baglioni Piero, Dei Luigi, Fratoni Laura, Lo Nostro Pierandrea, Moroni Michelangelo – "Preparation of nano and micro-particles of group II and transition metals oxides and hydroxides and their use in the ceramic, textile and paper industries". PCT Int. Appl. (2003), 10 pp. CODEN: PIXXD2 WO 2003082742 A2 20031009 CAN 139:278604 AN 2003:796605.

14) Fratoni Laura, Lo Nostro Pierandrea – "Composizione detergente a base di un estere dell'acido L-ascorbico". Patent Query N. TO2003A001032, deposit date 22/12/2003.

15) Baglioni Piero, Dei Luigi, Giorgi Rodorico, Ninham Barry W. – "Process for preparing nano- and micro-sized particles of inorganic compounds". European Patent Application EP 04101822.7, deposit date 29/04/2004.

16) Ambrosi Moira, Baglioni Piero, Bonini Massimo, Fratini Emiliano – "Nanoparticelle monodisperse di ossidi ed idrossidi metallici e loro applicazione nei settori tessile, cartario e ceramico". Patent Query FI 2006A000313 – RIF. 7845 PTIT, deposit date 11/12/2006.

17) Baglioni Piero, Ambrosi Moira, Dei Luigi, Faneschi Mauro, Mancioli Luciano, Santoni Sergio – "Ceramic products comprising nanoparticles of zirconium hydroxide and/or glass frits". Patent Query 7303 PTEP/2006 EP06112439.2, deposit date 10/04/2006.

18) Ceglie Andrea, Venditti Francesco, Lopez Francesco, Palazzo Gerardo, Colafemmina Giuseppe, Angelico Ruggero, Ambrosone Luigi – "Materiale adsorbente contenente tensioattivo cationico, sua preparazione ed uso per la rimozione di metalli da soluzioni acquose". Patent Query N. FI 2006 A000113 – RIF. 7490 PTIT, deposit date 10/05/2006.

19) Ballistreri Alberto, Cambria Maria Grazia, Carnemolla Giovanni Marco, Guglielmino Salvatore Pietro Paolo, Impallomeni Giuseppe, Nicolo Marco Sebastiano – "Production of biodegradable plastics from Brassica carinata oil with high content of erucic acid and from very long chain fatty acids". Italian Patent IT 1392236, deposit date 13/10/2008.

20) Ballistreri Alberto, Cambria Maria Grazia, Carnemolla Giovanni Marco, Guglielmino Salvatore Pietro Paolo, Impallomeni Giuseppe, Nicolo Marco Sebastiano – "Production of biodegradable plastics from Brassica carinata oil with high content of erucic acid and from very long chain fatty acids". World Organization Patent WO 2010044118 Priority IT 2008-RM545.

21) Hochkoeppler Alejandro, Baglioni Piero, Stefan Alessandra – "Espressione batterica di un gene artificiale per la produzione di CRM 197 e derivati". Patent Query FI 2009A000137 – RIF. 9741 PTIT, deposit date 25/06/2009.

22) Primiceri Giuseppe, Roda Elena, Stefan Alessandra, Panizza Lucio, Hochkoeppler Alejandro – "Enzyme composition for reducing the release of pharmaceutical active ingredients into the environment". WO/2009/138455A1.

23) Hochkoeppler Alejandro, Roda Elena, Panizza Lucio, Stefan Alessandra – "Method for preventing and controlling biofouling on marine objects". WO/2010/145905A.

24) Panizza Lucio, Roda Elena, Stefan Alessandra, Hochkoeppler Alejandro – "Method for preventing and controlling organisms that infest aqueous systems." WO/2010/145988A1.

25) Smets Johan, Pintens An, Keijzer Olav Pieter Dora Tony, Bodet Jean-Francois, Lebron Ariel, Fratini Emiliano, Vannucci Chiara, Ambrosi Moira, Baglioni Piero, Guinebretiere Sandra Jaqueline, Yan Nianxi, Liu Hongwei – "Encapsulates". Attorney's Docket No. 11547P – 21/04/2010.

26) Fernandez Prieto Susana, Smets Johan, Aouad Yousef Georges, Wevers Jean, Baglioni Piero, Ambrosi Moira, Vannucci Chiara – "Particles". Attorney's Docket No. 11812P2, 15/04/2011.

27) Angelico Ruggero, Lampis Sandrina, Monduzzi Maura, Ceglie Andrea – "Metodo innovativo per la "plastificazione" di grassi vegetali". Italian Patent FI2012A000186, deposit date 19/09/2012.

28) Paduano Luigi, D'Errico Gerardino, Montesarchio Daniela, Vitiello Giuseppe, Mangiapia Gaetano, Luchini Alessandra, Irace Carlo, Colonna Alfredo, Santamaria Rita – "Nanoparticelle ibride magnetite-oro funzionalizzate con struttura nucleo-guscio". Italian patent, deposit date 19/10/2012.

29) Piero Baglioni, Stefano del Buffa, Francesca Ridi, Massimo Bonini – "Materiale per la rigenerazione dei tessuti ossei contenente minerali argillosi aventi morfologia nanotubolare e stronzio". Italian Patent FI2013A000240, deposit date 15/10/2013.

CSGI Registered Trade Marks

1) Nanorestore® International Class 01,37,40 FI2008C00067527508 RIF. 19558

2) Nanorestore Paper® International Class 01, 16, 40 FI2011C0009935263 RIF. 27175

Prospective CSGI Activity in 2014-2015

CSGI is involved in 7 European programs, in several international and national projects, and in collaborations with industries and SME (small and medium enterprises.
CSGI is developing its own research activity in order to optimize the application of research projects inspired by the urging demands of small and medium size companies.

CSGI is actively working in order to offer a valid support to the Italian industrial system to set and develop of projects and pre-industrial processes.

List of Publications 2011-2013

1. 1-Substituted-(1,2,3-triazol-4-yl)thiophene-2-sulfonamides strongly inhibit human carbonic anhydrases I, II, IX and XII: solution and X-ray crystallographic studies. Leitans, J.; Sprudza, A.; Tanc, M.; Vozny, I.; Zalubovskis, R.; Tars, K.; Supuran, C.T. Bioorg. Med. Chem., 21, 5130-5138 (2013).
2. 7-Substituted-sulfocoumarins are isoform-selective, potent carbonic anhydrase II inhibitors. Tanc, M.; Carta, F.; Bozdag, M.; Scozzafava, A.; Supuran, C.T. Bioorg. Med. Chem., 21, 4502-4510 (2013).
3. A class of sulfonamides with strong inhibitory action against the α-carbonic anhydrase from Trypanosoma cruzi. Güzel-Akdemir, Ö.; Akdemir, A.; Pan, P.; Vermelho, A.B.; Parkkila, S.; Scozzafava, A.; Capasso, C.; Supuran, C.T. J. Med. Chem., 56, 5773-5781 (2013).
4. A highly catalytically active γ-carbonic anhydrase from the pathogenic anaerobe Porphyromonas gingivalis and its inhibition profile with anions and small molecules. Del Prete, S.; Vullo, D.; De Luca, V.; Carginale, V.; Scozzafava, A.; Supuran, C.T.; Capasso, C. Bioorg. Med. Chem. Lett., 23, 4067-4071 (2013).
5. A method to measure hydrolytic activity of adenosinetriphosphatases (ATPases). Bartolommei, G.; Moncelli, M.R.; Tadini-Buoninsegni, F. PLoS ONE, 8, e58615 (2013).
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7. A new family of bis-ureidic receptors for pyrophosphate optical sensing. Caltagirone, C.; Bazzicalupi, C.; Isaia, F.; Light, M.E.; Lippolis, V.; Montis, R.; Murgia, S.; Olivari, M.; Picci, G. Organic & Biomolecular Chemistry, 11, 2445-2451 (2013).
8. A novel preservation technique applied to fiordilatte cheese. Conte, A.; Longano, D.; Costa, C.; Ditaranto, N.; Ancona, A.; Cioffi, N.; Scrocco, C.; Sabbatini, L.; Contò, F.; Del Nobile, M.A. Innovative Food Science and Emerging Technologies, 19, 158-165 (2013).
9. A spectroscopic characterization of a phenolic natural mediator in the laccase biocatalytic reaction. Martorana, A.; Sorace, L.; Boer H.; Vazquez-Duhalt, R.; Basosi, R.; Baratto, M.C. Journal of Molecular Catalysis B: Enzymatic, 97, 203-208 (2013).
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11. Adult-Onset Cyclic Esotropia: A Case Report. Di Meo, A.; Costagliola, C.; Della Corte, M.; Romano, A.; Foria, C.; Di Costanzo, A. Optometry and Vision Science, 90 (3), E95-E98 (2013).
12. Advances in lipid-based platforms for RNAi therapeutics. Falsini, S.; Ciani, L.; Ristori, S.; Fortunato, A.; Arcangeli A. Journal of Medicinal Chemistry. In press (2013).
13. Alkylation of complementary ribonucleotides in nanoreactors. Angelico, R.; Losito, I.; Cuomo, F.; Ceglie, A.; Palmisano, F. Physical Chemistry Chemical Physics, 15 (2), 586-595 (2013).
14. An ab initio investigation of Li2M0.5N0.5SiO4 (M, N = Mn, Fe, Co Ni) as Li-ion battery cathode materials. Kalantarian, M.M.; Asgari, S.; Capsoni, D.; Mustarelli, P. Phys. Chem. Chem. Phys., 15, 8035-8041 (2013).
15. An Experimental and Theoretical Investigation of Loperamide Hydrochloride-Glutaric Acid Co-Crystals. Bruni, G.; Maietta, M.; Maggi, L.; Mustarelli, P.; Ferrara, C.; Berbenni, V.; Freccero, M.; Scotti, F.; Milanese, C.; Girella, A.; Marini A. J. Phys. Chem. B, 117, 27, 8113-8121 doi 10.1021/jp404273x (2013).
16. An extra-mitochondrial domain rich in carbonic anhydrase activity improves myocardial energetics. Schroeder, M.A.; Ali, M.; Supuran, C.T.; Clarke, K.; Vaughan-Jones, R.D.; Tyler, D.J.; Swietach, P. Proc. Natl. Acad. Sci. USA, 110, E958-E967 (2013).
17. An unusual thiazolo[5,4-d]thiazole sensitizer for dye-sensitized solar cells. Zani, L.; Reginato, G.; Mordini, A.; Calamante, M.; Peruzzini, M.; Taddei, M.; Sinicropi, A.; Parisi, M.L.; Fabrizi de Biani, F.; Basosi, R.; Cavallaro, A.; Bruzzi, M. Tetrahedron Letters, 54, 30, 3944-3948 (2013).
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Koz, O.; Ekinci, D.; Perrone, A.; Piacente, S.; Alankus-Caliskan, O.; Bedir, E.; Supuran, C.T. J. Enzyme Inhib. Med. Chem., 28, 412-417 (2013).

22. Anion inhibition studies of the α-carbonic anhydrase from the pathogenic bacterium Vibrio cholerae. Vullo, D.; Isik, S.; Del Prete, S.; De Luca, V.; Carginale, V.; Scozzafava, A.; Supuran, C.T.; Capasso, C. Bioorg. Med. Chem. Lett., 23, 1636-1638 (2013).
23. Anion inhibition studies of the α-carbonic anhydrase from the protozoan pathogen Trypanosoma cruzi, the causative agent of Chagas disease. Pan, P.; Vermelho, A.B.; Scozzafava, A.; Parkkila, S.; Capasso, C.; Supuran, C.T. Bioorg. Med. Chem., 21, 4472-4476 (2013).
24. Anticancer carbonic anhydrase inhibitors: A patent review (2008-2013). Monti, S.M.; Supuran, C.T.; De Simone, G. Expert Opin. Ther. Pat., 23, 737-749 (2013).
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1. Angelico, R.; Ripoli, M.; Piazzolla, V.; Santoro, R.; Mottola, L.; Petruzzellis, D.; Mangia, A. Digestive Disease Week, Orlando (USA), 18-21/05/2013. "Liposome-encapsulated silybin and hepatitis C virus infection". Poster presentation.
2. Baglioni, P. Ancient Mexican Codices: Scientific and Historical Perspectives, Roma, Accademia Nazionale dei Lincei, 04/06/2013. "Maya mural paintings technique". Invited lecture.
3. Baglion, P. 245th ACS National Meeting & Exposition, New Orleans, LA (USA), 07-11/04/2013. "Self assembled systems for the conservation of cultural heritage". Invited lecture.
4. Baglioni, P. 27th Conference of European Colloid and Interface Society, Sofia (Bulgaria), 01-06/09/2013. "Monitoring the interaction of nucleolipoplexes with model membranes". Invited lecture.
5. Baglioni, P. Training School "Colloids and Medical Applications", Sofia (Bulgaria), 31/08-01/09/2013. "Magneto-responsive nanocomposites: preparation and integration of magnetic nanoparticles into films, capsules and gels". Invited lecture.
6. Baglioni, P. Training School "Colloids and Medical Applications", Sofia (Bulgaria), 31/08-01/09/2013. "Nanostructures for magnetically triggered release of drugs and biomolecules". Invited lecture.
7. Baglioni, P. 1st International Conference on Innovation in Art Research and Technology, Evora (Portogallo), 10-13/07/2013. "Nanoscience for the conservation of cultural heritage". Invited lecture.
8. Baglioni, P. Gordon Research Conferences-Adhesion, Science of-Interfacial Chemistry and Mechanics in Hard and Soft Material Systems, Mount Holyoke College, MA (USA), 14-19/07/2013. "Self assembled systems and gels for the conservation of cultural heritage". Invited lecture.
9. Baglioni, P. Workshop: El Conocimiento de las nanopartículas en la conservación de bienes culturales, Madrid (Spagna), 30/09/2013. "Nanotechnology applied to Heritage: NanoForArt EU Project". Invited lecture.
10. Baglioni, P. Nanotecnología para la limpieza de bienes culturales, Escuela de Conservación y Restauración de Occidente y El Instituto Nacional de Antropología e Historia a través del Museo Nacional de Antropología, Guadalajara , Jalisco (Messico), 08/02/2013. "La nanotecnología aplicada a la Conservación de Pintura Mural y Monumentos". Invited lecture.
11. Baglioni, P. Nanotecnología aplicada a bienes culturales, El Instituto Nacional de Antropología e Historia a través de la Escuela Nacional de Conservación, Restauración y Museografia y Museo Nacional de Antropología, Mexico City (Messico), 07/02/2013. "Pintura mural". Invited lecture.
12. Baglioni, P. NIST Center for Neutron Research, Gaithersburg, MD (USA), 21/02/2013. "Self assembled systems and gels for the conservation of cultural heritage". Invited lecture.
13. Baglioni, P. Joint Seminar on Atomic and Colloidal Sciences, Oak Ridge National Laboratory (USA), 25-26/02/2013. "Cement hydration and nanostructure". Invited lecture.
14. Baglioni, P. Workshop, Supranano: Self-Assemblies, Paris (Francia), 06-07/06/2013. "Micelles, microemulsions and gels for conservation and maintenance of cultural heritage". Invited lecture.
15. Baglioni, P. Protection of cultural heritage objects with multifunctional advanced materials, Perugia, 08-09/05/2013. "Nano structured materials for the consolidation of artworks". Plenary lecture.
16. Baglioni, P. Design and industrial development of advanced drug delivery systems, University of Pavia, 21-23/11/2013. "Smart lipids assemblies for programmable nanomaterials: structure at the nanoscale and interaction with membrane models". Invited lecture.
17. Baglioni, P. 17th Swedish Neutron Scattering Society Meeting, Uppsala University (Svezia), 13-14/05/2013. "Curating cultural heritage". Open lecture.
18. Baglioni, P. Science and Innovation for the Study and Conservation of Works of Art, Auditorium of US National Academy of Sciences, Washington, DC (USA) with Accademia Nazionale dei Lincei, 07-10/10/2013. "Nanosciences for cultural heritage conservation". Invited lecture.
19. Banchelli, M.; Guardiani, C.; Tenori, E.; Menichetti, S.; Caminati, G.; Procacci, P. 5th International Conference on Drug Discovery & Therapy, Dubai (UAE), 18-21/02/2013. "Characterization and optimization of tartrate-based Tumor Necrosis Factor-alpha Converting Enzyme inhibitors". Oral presentation.
20. Baratto, M.C. Emory-Unisi Summer School, Chemistry for Life&Environment Education, Collaboration, Innovation, VIII Edition, Siena, 27/05-03/07/2013. "EPR spectroscopy for radical detection". Oral presentation.
21. Baratto, M.C.; Martorana, A.; Sorace, L.; Boer, H.; Vazquez-Duhalt, R.; Basosi, R. TUMA 2013, Sesto Fiorentino (FI), 01-02/07/2013. "Identification and spectroscopic characterization of dimethoxyphenol radicals in the Coriolopsis gallica laccase catalytic reaction". Oral presentation.
22. Baratto, M.C.; Martorana, A.; Vazquez-Duhalt, R.; Basosi, R. Emory@Unisi Summer School, Chemistry for Life&Environment Education, Collaboration, Innovation, VIII Edition, Siena, 27/05-03/07/2013. "EPR spectroscopy for the characterization of 2,6-dimethoxyphenol radicals formed in

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the Coriolopsis gallica laccase-mediator system". Poster presentation.

23. Baratto, M.C.; Martorana, A.; Vazquez-Duhalt, R.; Basosi, R. XLI Congresso Nazionale di Chimica Fisica, Alessandria, 23-27/06/2013. "Spectroscopic characterization of 2,6-dimethoxyphenol mediator radicals formed in the laccase biocatalytic mechanism". Oral presentation.
24. Bartolommei, G.; Moncelli, M.R.; Tadini-Buoninsegni, F. 38th FEBS Congress, St. Petersburg, Russia, 6-11/07/2013. "Hydrolytic activity of adenosinetriphosphatases (ATPases) measured by a new experimental method". Poster presentation.
25. Benvenuti, E.; Barile, G.; Caminati, G. XLI Congresso Nazionale di Chimica Fisica Alessandria (Italy), 23-27/06/2013 "Core-shell polymer nanoparticles as emitting layer in white-pholed". Poster presentation.
26. Bergemann, N.; Pistidda, C.; Milanese, C.; Girella, A.; Bellosta von Colbe, J.; Marini, A.; Klassen, T.; Dornheim, M. Gordon Research Conference on "Hydrogen-Metal systems. Hydrogen Interactions in Energy Storage", Il Ciocco Resort (Barga, Italy), 14-19/07/2013. "NaAlH4 production from waste aluminum by reactive ball milling". Poster presentation.
27. Bernini, C.; Arezzini, E; Pogni, R.; Basosi, R.; Sinicropi, A. Emory@Unisi Chemistry for Life & Environment, Education, Collaboration, Innovation, X Edition, Siena (SI) 27/05-03/06/2013. "Cytochrome c Peroxidase: In Silico Characterization of the Active Site". Poster presentation.
28. Bernini, C.; Arezzini, E., Pogni, R.; Olivucci, M.; Basosi, R.; Sinicropi, A. 1st International workshop on protein electron transfer: from fundamentals to applications for health, Modena, 29-30/10/2013. "Triptophan and Tyrosine radicals mediating ET processes in peroxidases and blue copper proteins". Poster presentation.
29. Bernini, C.; Pogni, R.; Olivucci, M; Basosi, R.; Sinicropi, A. Emory@Unisi Chemistry for Life & Environment, Education, Collaboration, Innovation, X Edition, Siena (SI) 27/05-03/06/2013. "In Silico Studies on Redox-Active Amino Acids involved in Long-Range Electron Transfer Pathways in Proteins". Poster presentation.
30. Bonechi, C.; Rossi, C.; Butini, S.; Campiani, G.; Donati, A. XLI Congresso Nazionale di Chimica Fisica Alessandria, 23-27/06/2013. "NMR study of linear and cyclic oligopeptides mimicking NUR77 binding site". Poster presentation.
31. Bruni, G.; Maietta, M.; Maggi, L.; Mustarelli, P.; Ferrara, C.; Berbenni, V.; Scotti, F.; Milanese, C.; Girella, A.; Marini, A. The 7th Workshop on Crystal form, Bologna (Italy), 09-11/06/2013. "Preparation, physico-chemical characterization and dissolution rate of loperamide hydrochloride-glutaric acid co-crystals". Poster presentation.
32. Capsoni, D.; Bini, M.; Ferrari, S.; Spreafico, C.; Tealdi, C.; Mustarelli, P. XLI Congresso Nazionale di Chimica Fisica, Alessandria 23-27/06/2013. "A Combined experimental and computational study of cation disorder in Li2Fe0.5Mn0.5SiO4". Poster presentation.
33. Carretti, E. Workshop hold at the Croatian Conservation Institute, Restoration centre, Ludbreg, 27-29/05/2013. "Inorganic materials in wall painting conservation". Oral presentation.
34. Carretti, E.; Ghelardi, E.; Matarrese, C.; Natali, I.; Bonini, M.; Fratini, E.; Dei, L.; Baglioni, P. XIV Congresso Nazionale di Chimica dell'Ambiente e dei Beni Culturali, "La Chimica nella Società Sostenibile", Rimini 02-05/06/2013. "Sistemi supramolecolari costituiti da polivinilalcol, tensioattivi e microemulsioni: proprietà e applicazioni nel campo della pulitura di beni artistico/architettonici". Poster presentation.
35. Cuomo, F.; Lopez, F.; Ceglie, A. Workshop "Dalla Nanomedicina al Brain Imaging", Pula (CA) Italy, 17-19/04/2013. "Fabrication of stimuli-responsive polymeric nanocapsules onto liposome template". Poster presentation.
36. Falsini, S.; In, M.; Ciani, L.; Di Cola, E.; Arcangeli, A; Ristori S. "Complexing a small interfering RNA with divalent cationic surfactants" 11th International Conference on Biology and Synchrotron Radiation. Hamburg (Germany). 08-11/09/2013. Poster presentation.
37. Ferrari, S.; Bini, M.; Capsoni, D.; Mozzati, M.C.; Ferrara, C.; Mustarelli, P. 19th International Conference on Solid State Ionics, Kyoto (Japan) 02-07/06/2013. "Magnetic and spectroscopic properties of Li2MSiO4 (M= Fe, Mn)". Poster presentation.
38. Ferrari, S.; Quinzeni, I.; Quartarone, E.; Bini, M.; Capsoni, D.; Mustarelli, P. 19th International Conference on Solid State Ionics, Kyoto (Japan) 02-07/06/2013. "Structural, morphological and electrochemical properties of Li2MSiO4 (M = Fe, Mn) thin films deposited by means of radiofrequency magnetron sputtering". Poster presentation.
39. Fratini, E. 3th Cement Workshop: "Nuove metodologie analitiche per il controllo di qualità, di processo e nella ricerca sui cementi", Bergamo (BG) 16 /10/2013. "Water as a Probe for Hydration Kinetics and Microstructure Evolution in Cement Pastes". Oral presentation.
40. Fratini, E. ESS Science Symposium on New Generation Green Construction Materials. Stockholm (Sweden) 03-04/04/2013. "Cement hydration and nanostructure". Oral presentation.
41. Fratini, E. Third Annual Niels Bohr International Academy Workshop on ESS Science: "Crossing space and time domains with SAS and QENS", Copenaghen (Denmark) 24-28/03/2013. "Structure and Dynamics in Concentrated Protein Solutions". Oral presentation.

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42. Garroni, S.; Masolo, E.; Tolu, E.; Senes, N.; Pellicer, E.; Sort, J.; Milanese, C.; Baró, M.D.; Enzo, S.; Pilo, M.; Mulas, G. Third International Conference on Multifunctional, Hybrid and Nanomaterials (Hybrid Materials 2013), Sorrento (Italy), 03-07/03/2013. "Mesoporous Materials for Energy Storage and Production". Poster presentation.
43. Garroni, S.; Peru, F.; Soru, S.; Campesi, R.; Napolitano, E.; Milanese, C.; Barò, M.D.; Enzo, S.; Mulas, G. NIS Colloquium "Materials for hydrogen storage", Torino (Italy), 15/02/2013. "Sorption properties of nanosized hydrides confined into highly ordered mesoporous matrixes". Invited Oral presentation.
44. Giamblanco, N.; Langhammer, E.M., Marletta, G. E-MRS 2013 SPRING MEETING, Strasburgo 28-30/05/2013. "Localized surface plasmon resonance study of protein adsorption: long- and short-range force effect at solid-liquid interfaces". Oral presentation.
45. Giamblanco, N.; Langhammer, E.M., Marletta, G. XLI Congresso Nazionale di Chimica Fisica, Alessandria (TO) 23-27/06/2013. "Localized surface plasmon resonance study of protein adsorption: long- and short-range force effect at solid-liquid interfaces". Oral presentation.
46. Giamblanco, N.; Marletta, G. Euro BioMAT 2013, Weimar, Germany, 23-24/04/2013. "Competitive protein adsorption from complex blood serum". Oral presentation.
47. Giorgi, R. Nanotecnología para la limpieza de bienes culturales, Escuela de Conservación y Restauración de Occidente y El Instituto Nacional de Antropología e Historia a través del Museo Nacional de Antropología, Guadalajara , Jalisco (Messico), 08/02/2013. "Nanomaterials y geles empleados para la limpieza y desacidificación de objectos constituidos por celulosa". Invited lecture.
48. Giorgi, R. Nanotecnología aplicada a bienes culturales, El Instituto Nacional de Antropología e Historia a través de la Escuela Nacional de Conservación, Restauración y Museografia y Museo Nacional de Antropología, Mexico City (Messico), 07/02/2013. "Celulosa". Invited lecture.
49. Jepsen, J.; Milanese, C.; Bellosta von Colbe, J.; Metz, O.; Lozano, G.A.; Klassen, T.; Dornheim, M. Gordon Research Conference on "Hydrogen-Metal systems. Hydrogen Interactions in Energy Storage", Il Ciocco Resort (Barga, Italy), 14-19/07/2013. "Design and evaluation of a LiBH4 □ MgH2 storage system". Poster presentation.
50. Lampis, S.; Murgia, S.; Falchi, A.M.; Schmidt, J.; Talmon, Y.; Monduzzi, M. Nanomed Workshop - Dalla Nanomedicina al brain imaging, Pula (CA) 17-19/04/2013. "Nanoparticles from Lipid-Based Liquid Crystals: Emulsifier Influence on Morphology and Cytotoxicity". Poster presentation.
51. Liu, Y.; Falus, P.; Porcar, L.; Fratini, E.; Chen, W.R.; Faraone, A.; Hong, K.; Baglioni, P. American Physical Society Meeting Baltimore, (MD) 18-22/03/2013. "Transition from monomeric phase to dynamic cluster phase in lysozyme protein solutions". Oral presentation.
52. Luchini, A.; Mangiapia, G.; Vitiello, G.; D'Errico, G.; Montesarchio, D.; Paduano, L. XL Congresso Nazionale di Chimica Fisica, Alessandria 23-27/06/2013. "Preparation and structural characterization of functionalized theranostic nanoparticles". Oral presentation.
53. Maranghi, S.; Parisi, M.L.; Basosi, R. VII Convegno della Rete Italiana LCA, Milano (MI) 27-28/06/2013. "LCA come strumento di previsione per l'ottimizzazione di tecnologie fotovoltaiche innovative". Oral presentation.
54. Marletta, G. Spring Meeting E-MRS 2013, SymposiumW on "Ion Beams Applications: New and Innovative approaches", Strasbourg (France), 27-31/05/2013. "Ion Beam for Smart Biointerfaces". Invited lecture.
55. Martina, M.R.; Baglioni, P.; Caminati, G. 27th European Colloid and Interface Society Conference, Sofia (Bulgaria) 01-06/09/2013. "Raft-like domains in phospholipid monolayers promote lysozyme aggregation and misfolding". Poster presentation.
56. Martina, M.R.; Baglioni, P.; Caminati, G. XLI Congresso Nazionale di Chimica Fisica Alessandria (Italy), 23-27/06/2013, "Amiloyd-like aggregates of lysozyme induced by lipid rafts domains in phospholipid monolayers". Poster presentation.
57. Martina, M.R.; Matteini, P.; Pini, R.; Dei, L.; Caminati, G. 27th European Colloid and Interface Society Conference, Sofia (Bulgaria) 01-06/09/2013. "Thermoresponsive polymeric micelles as efficient tool for controlled drug delivery". Poster presentation.
58. Matteini, P.; Martina, M.R.; Giambastiani, G.; Tatini, F.; Cascella, R.; Ratto, F.; Cecchi, C.; Caminati, G.; Dei, L.; Pini, R. E-MRS 2013 Spring Meeting, Strasbourg (France), 27-31/05/2013. "Light-responsive hybrid sponges for on demand chemical release". Oral presentation.
59. Medda, L.; Barse, B.; Cugia, F.; Parsons, D.F.; Ninham, B.W.; Monduzzi, M.; Salis, A. Nanomed Workshop - Dalla Nanomedicina al brain imaging, Pula (CA) 17-19/04/2013. "Interfacial properties of proteins: Hofmeister effects on surface charge of BSA". Poster presentation.
60. Medda, L.; Barse, B.; Cugia, F.; Parsons, D.F.; Ninham, B.W.; Monduzzi, M.; Salis, A. XLI Congresso Nazionale di Chimica-Fisica, Alessandria 23-27/06/2013. "Hofmeister challenges: ion binding and charge of the BSA protein as explicit examples" Oral presentation.
61. Messina, G.M.L.; Lettieri, R.; Venanzi, M.; Marletta, G. ESF-EMBO Symposium Biological Surfaces and Interfaces, Sant Feliu de Guixols (Spain) 26/06-01/07/2013. "Peptide trapping in nanopores for antibacterial surfaces". Poster presentation.

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62. Messina, G.M.L.; Marletta, G. European Materials Research Society, Strasbourg (France) 14-18/05/2012. "Selective protein confinement in nanostructured surfaces". Oral presentation.
63. Messina, G.M.L.; Sciacca, M.F.M.; La Rosa, C.; Marletta, G. European Materials Research Society, Strasbourg (France) 27-31/05/2013. "Self-Assembly peptides: a mechanism of cell membrane disruption". Oral presentation.
64. Messina, G.M.L.; Sciacca, M.F.M.; La Rosa, C.; Marletta, G. XLI Congresso Nazionale di Chimica Fisica, Alessandria 23-27/06/2013. "A mechanism of cell membrane disruption by self-assembly peptides". Poster presentation.
65. Milanese, C. Department of Chemistry and Pharmacy, University of Sassari, Sassari (Italy), 14/03/2013. "Thermodynamic and kinetic investigation on hydrogen storage materials". Invited Oral Seminar.
66. Milanese, C.; Girella, A.; Berbenni, V.; Bruni, G.; Garroni, S.; Gosalawit-Utke, R.; Mulas, G.; Jepsen, J.; Dornheim, M.; Klassen, T.; Marini, A. XLI Congresso di Chimica Fisica, Alessandria (Italy), 23-27/06/2013. "Chemico-physical characterization and hydrogen sorption properties of chemical hydrides confined into mesoporous scaffolds". Poster presentation.
67. Milanese, C.; Girella, A.; Berbenni, V.; Bruni, G.; Soru, S.; Garroni, S.; Enzo, S.; Mulas, G.; Jepsen, J.; Pistidda, C.; Bellosta von Colbe, J.; Dornheim, M.; Klassen, T.; Marini, A. XLI Congresso di Chimica Fisica, Alessandria (Italy), 23-27/06/2013. "Thermodynamic and kinetic properties of the LiBH4 – MgH2 and LiBH4 – MgH2 – LiAlH4 systems for solid state hydrogen storage". Oral presentation.
68. Milanese, C.; Girella, A.; Soru, S.; Garroni, S.; Enzo, S.; Mulas, G.; Jepsen, J.; Pistidda, C.; Bellosta von Colbe, J.; Dornheim, M.; Klassen, T.; Marini, A. Gordon Research Conference on "Hydrogen-Metal systems. Hydrogen Interactions in Energy Storage", Il Ciocco Resort (Barga, Italy), 14-19/07/2013. "Chemico-physical characterization and sorption properties of reactive hydride composites for hydrogen storage". Flash oral presentation + poster presentation.
69. Milanese, C.; Jepsen, J.; Girella, A.; Bellosta von Colbe, J.M.; Dornheim, M.; Klassen, T.; Marini, A. "Materials and Processes for Energy Applications" - Joint meeting of MP1004, MP1103 and MP1106 COST Actions, Prague (Czech Republic), 20-22/03/2013. "Thermodynamic and kinetic characterization of the catalysed LiBH4 - MgH2 system". Invited Oral presentation.
70. Milanese, C.; Jepsen, J.; Girella, A.; Garroni, S.; Bellosta von Colbe, J.M.; Mulas, G.; Dornheim, M.; Klassen, T.; Marini, A. NIS Colloquium "Materials for hydrogen storage", Torino (Italy), 15/02/2013. "Physico-chemical properties and sorption behaviour of the catalysed LiBH4 - MgH2 reactive hydride composite". Invited Oral presentation.
71. Mulas, G.; Garroni, S.; Masolo, E.; Pilo, M.; Guccini, V.; Pellicer, E.; Baró, M.D.; Gatto, I.; Milanese, C.; Campesi, R. Gordon Research Conference on "Hydrogen-Metal systems. Hydrogen Interactions in Energy Storage", Il Ciocco Resort (Barga, Italy), 14-19/07/2013. "Nanosized systems and mesoporous materials for hydrogen production, storage, and conversion". Flash oral presentation + poster Presentation.
72. Murgia, S. Nanomed Workshop - Dalla Nanomedicina al brain imaging, Pula (CA) 17-19/04/2013. "A Novel Nanocarrier for an Effective Dermal Drug Release". Oral presentation.
73. Paduano, L; Mangiapia, G.; D'Errico, G.; Irace, C.; Radulescu, A.; Frielighaus, H.; Fragneto, G.; Montesarchio, D. International Conference on Neutron Scattering, Edinburgh (UK) 08-12/07/2013. "Nanodevices for neoplastic diagnosis or therapy". Oral presentation.
74. Parisi, M.L.; Maranghi, S.; Sinicropi, A.; Basosi, R. VII Congresso Nazionale dell'Associazione Italiana Gestione Energia, Rende (CS), 10-11/06/2013. "Development of dye sensitized solar cells: a life cycle perspective for the environmental and market potential assessment of a renewable energy production technology". Oral presentation.
75. Parisi, M.L.; Spinelli, D.; Pogni, R.; Basosi, R. VII Convegno della Rete Italiana LCA, Milano (MI) 27-28/06/2013. "LCA comparativa di processi di tintura di fibre tessili". Poster presentation.
76. Parisi, M.L.; Spinelli, D.; Pogni, R.; Basosi, R. VII Italian LCA Network, Milan (Italy) 27-28/06/2013. "LCA comparativa di processi di tintura di fibre tessili". Poster presentation.
77. Pentimalli, M.; Milanese, C.; Indriyati; Padella, F. Third International Conference on Multifunctional, Hybrid and Nanomaterials (Hybrid Materials 2013), Sorrento (Italy), 03-07/03/2013. "Disordered boron nitride-graphite composite for hydrogen storage". Poster presentation.
78. Pogni, R.; Sinicropi, A.; Baratto, M.C.; Basosi, R. XLI Congresso Nazionale di Chimica Fisica, Alessandria, 23-27/06/2013. "Investigation of redox-active aminoacids in oxidative enzymes: the role of the combined EPR and computational approach". Poster presentation.
79. Ristori, S.; Gelli, C.; Maurel, S.; Giordano, C.; Capozzoli, L.; Colzi, I.; Di Cola, E.; Lyonnard. S.; Gonnelli, C; "Nanoparticles synthesis by using water extracts from Ni hyperaccumulator and Ni excluder plants" 11th International Conference on Biology and Synchrotron Radiation. Hamburg (Germany). 08-11/09/2013. Poster presentation.
80. Sciacca, M.F.M.; Milardi, D.; Messina, G.M.L.; Marletta, G.; Brender, J.R.; Ramamoorthy, A.; La Rosa, C. 57th Annual Meeting of the Biophysical-Society, Philadelphia, PA (USA) 02-06/02/2013.

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"Pores Versus Fibrils: Calcium Ions Regulate Different IAPP-Mediated Membrane Damage Mechanisms". Poster presentation.

81. Soru, S.; Pistidda, C.; Milanese, C.; Bonatto Minella, C.; Marini, A.; Karimi, F.; Dornheim, M.; Baró, M.D.; Enzo, S.; Mulas, G.; Garroni, S. 20th International Symposium on Metastable, Amorphous and Nanostructured Materials (ISMANAM 2013), Torino (Italy), 30/06-05/07/2013. "Multicomponent LiBH4-LiAlH4-MgH2 hydrogen storage system: in-situ synchrotron radiation powder diffraction studies". Oral presentation.
82. Spinelli, D.; Fatarella, E.; Basosi, R.; Pogni, R. National Physical-Chemistry Congress, Alessandria (Italy) 23-27/06/2013. "Immobilization of laccase on nylon 6: a comparison between film and nanofiber". Poster presentation.
83. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R. Giornata Gruppo Sensori - GS2013, Sestri Levante, 19-20/09/2013. "A biosensor technology to investigate drug interactions with membrane transporters". Oral presentation.
84. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R. XL Congresso Nazionale di Chimica Fisica, Alessandria, 23-27/06/2013. "Study of copper transport mechanism in human copper ATPases (ATP7A/B)". Oral presentation.
85. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Arnesano, F.; Natile, G. 38th FEBS Congress, St. Petersburg, Russia, 6-11/07/2013. "Transport of platinum-based anticancer drugs by recombinant human copper ATPases (ATP7A/B)". Poster presentation.
86. Torrisi, V.; Ruffino, F.; Grimaldi, M.G.; Marletta, G. "European Materials Research Society Conference", Strasburgo 14-18/05/2013. "Hybrid Multilayers: transition effect in bipolar conduction behavior". Oral presentation.
87. Torrisi, V.; Ruffino, F.; Grimaldi, M.G.; Marletta, G. "Third International Conference on Multifunctional, Hybrid and Nanomaterials", Sorrento (NA) 03-07/03/2013. "Hybrid Multilayers: Schottky diode behaviour and transition effect in bipolar conduction behavior". Poster presentation.
88. Torrisi, V.; Ruffino, F.; Licciardello, A.; Grimaldi, M.G.; Marletta, G. "European Materials Research Society Conference", Nizza 9-13/05/2013. "Hybrid multilayer by sputtered gold nanoparticles onto diblock-copolymer template". Poster presentation.
89. Vitiello, G.; Paduano, L.; D'Errico, G. XL Congresso Nazionale di Chimica Fisica, Alessandria 23-27/06/2013. "The role of omega-3 fatty acids in the biomembrane processes". Poster presentation.
90. Zappalà, G.; Puntoriero, F.; Sartorel, A.; Bonchio, M.; Campagna, S.; Licciardello, A. Chimica Fisica 2013. XLI Congresso Nazionale di Chimica Fisica. Alessandria, 23-27/06/2013. "Self-assembly of a supramolecular bi-layer for photo-induced water splitting". Oral presentation.
91. Zappalà, G.; Puntoriero, F.; Sartorel, A.; Bonchio, M.; Campagna, S.; Licciardello, A. EMRS 2013 Spring Meeting, Strasbourg, Francia, 27-31/05/2013. "Self assembly of a tetranuclear Ru(II) dendrimer and polyoxotungstate catalyst on oxide substrates for photo-induced water splitting". Poster presentation.
92. Albers, W.A.; Cotrone, S.; Magliulo, M.; Mallardi, A.; Wang, X.; Nilsson, D.; Munter, T.; Tappura, K.; Palazzo, G.; Torsi, L.; Norberg, P.; Vikholm-Lundin, I. E-MRS 2012 Spring Meeting, 15-18/05/2012-Strasburg, France. "Functionalization of Electrolyte-Gated Organic Field-Effect Sensors". Oral presentation.
93. Angelico, R.; Ceglie, A.; He, J-Z.; Palumbo, G.; Colombo, C. EUROSOIL-2012: 4th International Congress of the European Confederation of Soil Science Societies (ECSSS), Bari 02-06/07/2012. "Characterization of ferrihydrite-humic substance (Fe-HS) coprecipitates by transmission electron microscopy (TEM) and dynamic light scattering (DLS)". Poster presentation.
94. Angelico, R.; Ceglie, A.; Murgia, S.; Olsson, U.; Palazzo, G.; Amin, S. 26th Conference of the European Colloid and Interface Society (ECIS 2012), Malmö / Lund (Sweden) 02-07/09/2012. "Tuning microstructure of non-ionic micellar networks: rheology and self-diffusion investigations". Poster presentation.
95. Angelico, R.; Ceglie, A.; Murgia, S.; Olsson, U.; Palazzo, G.; Amin. S. 26th ECIS Conference, Malmö & Lund, Svezia, 02-07/09/2012. "Tuning Microstructure of Non-Ionic Micellar Networks: Rheology and Self-Diffusion Investigations". Poster presentation.
96. Angione, M.D.; Cotrone, S.; Magliulo, M.; Mallardi, A.; Palazzo, G.; Torsi, L. 2012 MRS Spring Meeting, 09-13/04/2012, San Francisco, CA. "A new strategy for highly performing OFET biosensors development". Oral presentation.
97. Angione, M.D.; Cotrone, S.; Magliulo, M.; Mallardi, A.; Palazzo, G.; Torsi, L. Biosensors 2012-22nd Anniversary World Congress on Biosensors, 15-18 May 2012 - Cancun, Mexico. "A new strategy for highly performing OFET biosensors development". Oral presentation.
98. Baglioni, P. Colloids and Nanomedicine 2012, Amsterdam, The Netherlands, 15-17/07/2012. "Magnetic effects on DNA-mediated nanoparticles clusterisation". Invited lecture.
99. Baglioni, P. 26th Conference of the European Colloid and Interface Society – ECIS, Malmö, Sweden. "Magnetic effects on DNA-mediated nanoparticles clusterisation". Invited lecture.
100. Baglioni, P. E-MRS 2012 Spring Meeting, Strasbourg, France, 15/05/2012. "Magnetic effects on

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DNA-mediated nanoparticles clusterisation". Invited lecture.

101. Baglioni, P. Nanotech Italy 2012, Venezia, 21-23/11/2012. "Nanoscience for cultural heritage conservation". Invited lecture.
102. Baglioni, P. Universidad Autónoma de San Luis Potosí, Mexico, 20/03/2012. "Microemulsions and Micellar Solutionsfor the Conservation of Cultural Heritage". Invited lecture open to public for Cátedra de Investigación Científica del Instituto de Física 2012.
103. Baglioni, P. Universidad Autónoma de San Luis Potosí, Mexico, 21/03/2012. "Hybrid-Lipid-DNA Self Assemblies". Invited lecture open to public for Cátedra de Investigación Científica del Instituto de Física 2012.
104. Baglioni, P. Universidad Autónoma de San Luis Potosí, Mexico, 22/03/2012. "Cement: a two thousand year old nano-colloid". Invited lecture open to public for Cátedra de Investigación Científica del Instituto de Física 2012.
105. Baglioni, P. Meeting of the Italian Neutron Society, Firenze, 31/06/2012. "Neutrons and Cultural Heritage: Nanoparticles, Microemulsions, Gels and Responsive Gels. Invited lecture.
106. Baglioni, P. Conference on Science and Technology for the Conservation of Cultural Heritage, Santiago de Compostela (Spain), 01-05/10/2012. "New products and materials for conservation and maintenance of cultural heritage". Invited lecture.
107. Baglioni, P. Workshop on Structure and Dynamics of Water in Gas, Liquid and Solid Phases, Institute of Atomic and Molecular Sciences, Academia Sinica in Taipei (Taiwan), 28-30/11/2012. "Cement hydration and nanostructure". Invited lecture.
108. Baglioni, P. National Palace Museum, Taipei (Taiwan), 30/11/2012. "Nanomaterials for the conservation and preservation of movable and immovable artworks". Invited lecture.
109. Baratto, M.C. Emory@Unisi Summer School, Chemistry for Life&Environment Education, Collaboration, Innovation, IX Edition, Siena, 28/05-04/07/2012. "EPR spectroscopy for radical detection in food and antioxidants". Oral presentation.
110. Bartolommei, G.; Inesi, G.; Moncelli, M.R.; Tadini-Buoninsegni, F. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "Distinctive features of transport mechanisms in sarcoplasmic reticulum Ca2+-ATPase (SERCA) and Cu+-ATPases (ATP7A/B)". Poster presentation.
111. Bernini, C.; Andruniów, T.; Olivucci, M; Pogni, R.; Basosi, R.; Sinicropi, A. XXXI Congresso Interregionale TUMA 2012, Francavilla al Mare (CH) 18-20/06/2012. "Calcolo degli shifts nei parametri EPR, UV-Vis and RR di radicali triptofano immersi in diversi ambienti a partire da modelli QM/MM dell'Azzurrina da Pseudomonas aeruginosa". Poster presentation.
112. Bernini, C.; Andruniów, T.; Olivucci, M; Pogni, R.; Basosi, R.; Sinicropi, A. 1st National Meeting of the Theoretical and Computational Chemistry of the Italian Chemical Society, Pisa (PI) 22-23/02/2012. "EPR, UV-VIS and RR spectral parameter shifts of tryptophan radicals embedded in contrasting hydrophobic and hydrophilic environments computed from QM/MM Models of Pseudomonas aeruginosa azurin". Poster presentation.
113. Bernini, C.; Pogni, R.; Basosi, R.; Sinicropi, A. 1st National Meeting of the Theoretical and Computational Chemistry of the Italian Chemical Society, Pisa (PI) 22-23/02/2012. "QM/MM characterization of redox-active Trp radicals in LiP and LiP-like systems". Poster presentation.
114. Bortolussi, S.; Ciani, L.; Postuma, I.; Protti, N.; Bruschi, P.; Ferrari, C.; Cansolino, L.; Ristori, S.; Altieri, S. 14th International Congress on Neutron Capture Therapy, Tsukuba (Japan), 09-14/09/2012. "Boron concentration measurement by α spectrometry and quantitative neutron autoradiography in cell and tissue samples treated with different boronated formulations and administration protocols". Oral presentation.
115. Boscagli, C.; Gambinossi, F.; Busa', C.; Caminati G. 14th International Conference on Organized Molecular Films ICOMF14 (LB14), Paris (France) 10-13/07/2012. "Nanofabrication of polymer capsules arrays for 3rd generation solar cells. Poster presentation.
116. Bravi, M.; Parisi, M.L.; Basosi, R. VI Convegno della Rete Italiana LCA, Bari (BA) 07-08/06/2012. "Analisi del ciclo di vita in serie storica di un sistema integrato di gestione dei rifiuti: il caso della Provincia di Siena". Oral presentation.
117. Campesi, R.; Garroni, S.; Pellicher, E.; Baró, M.D.; Milanese, C.; Girella, A.; Dolci, F.; Mulas, G. 6th International Symposium Hydrogen & Energy, Stoos (Switzerland), 22-27/01/2012. "SANS and TEM characterization of MgH2-NaBH4 nanoparticles confined in silica based mesoporous scaffold SBA-15". Poster presentation.
118. Cavigli, P.; Baglioni, P.; Caminati, G. 14th International Conference on Organized Molecular Films ICOMF14 (LB14), Paris (France) 10-13/07/2012. "Langmuir-Blodgett nanoassemblies of PVKIridium complexes for Phosphorescent Organic Light Emitting Diodes" Oral presentation.
119. Cavigli, P.; Gambinossi, F.; Baglioni, P.; Caminati, G.; Materials Today Virtual Conference: Nanotechnology, 11-13/12/2012 "LB films of PVKIridium complexes for PhOLED devices". Poster presentation.
120. Ciani, L.; Bortolussi, S.; Ferrari, C.; Panza, L.; Altieri, S.; Ristori, S. 14th International Congress on

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Neutron Capture Therapy, Tsukuba (Japan), 09-14/09/2012. "Increasing tumor uptake of Boron: bioactive compounds and vectors". Oral presentation.

121. Cotrone, S.; Magliulo, M.; Angione, D.; Mallardi, A.; Palazzo, G.; Torsi, L.; Albers, W.A.; Munter, T.; Tappura, K.; Vikholm-Lundin, I.; Suspène, C. E-MRS 2012 Spring Meeting, 15-18/05/2012- Strasburg, France. "Analytical performance of BioEGOFET sensors". Oral presentation.
122. Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman B. "Colloids and Nanomedicine", Amsterdam (Netherland) 15-17/07/2012. "Hollow polyelectrolyte nanocapsules assembled on liposome templates". Poster presentation.
123. Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman B. 26th Conference of the European Colloid and Interface Society (ECIS). Malmö / Lund (Sweden) 02-07/09/2012. "Polyelectrolyte nanocapsules assembled onto liposome templates". Oral communication.
124. D'Errico, G. 26th Conference of the European Colloid and Interface Society, Malmö (Sweden) 02-07/09/2012. "Nanostructured polymeric hydrogels containing surfactant aggregates for drug delivery". Oral presentation.
125. Diaz-Fernandez, Y.A.; Moth-Poulsen, K.; Malavasi, L.; Milanese, C. Materials for tomorrow, Gothenburg (Sweden), 23-25/10/2012. "Occurrence of hcp and fcc diffraction domains within capped silver nanoparticles". Poster presentation.
126. Ferrari, S.; Grandi, S.; Bini, M.; Capsoni, D.; Galinetto, P.; Ugolotti, E.; Pirzio F. European Materials Research Science E-MRS, Varsavia (Polonia), 17-21/09/2012. "Transparent carbon nanotube incorporated sol-gel glasses as saturable absorbers for ultrafast lasers". Oral presentation.
127. Ferrari, S.; Spreafico, C.; Tealdi, C.; Bini, M.; Capsoni, D.; Mustarelli, P.; Canton P. 63rd Annual Meeting of the International Society of Electrochemistry, Praga, 19-24/08/2012. "Li2Mn0.5Fe0.5SiO4 cathode material: structural and electrochemical characterization". Oral presentation.
128. Fierro, A.; Spinelli, D.; Bardi, L.; Jez, S.; Zucaro, A.; Forte, A.; Basosi, R. 2nd Dire Meeting, Roma, (Italy) 27/09/2012. "The primary importance of more precise and locally available data for the evaluation of net GHG emissions of N2O by means of LCA applied to agricultural production". Poster presentation.
129. Fratini, E.; Faraone, A.; Muller, A.; Baglioni P. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce (LE) 11-16/09/2012. "The strange world of polyoxomolybdate". Poster presentation.
130. Fratini, E.; Liu, Y.; Porcar, L.; Baglioni P. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce (LE) 11-16/09/2012. "Proteins Cluster Phases". Oral presentation.
131. Garroni, S.; Pistidda, C.; Sale, M.; Taras, A.; Napolitano, E.; Milanese, C.; Campesi, R.; Karimi, F.; Dornheim, M.; Enzo, S.; Mulas, G. International Symposium on Metal-Hydrogen Systems MH 2012, Kyoto (Japan), 21-26/10/2012. "In Situ Synchrotron Radiation Powder X-ray Diffraction study of the 2LiNH2+LiH+KBH4 system". Poster presentation.
132. Gosalawit-Utke, R.; Pistidda, C.; Milanese, C.; Dornheim, M.; Klassen, T. International Symposium on Metal-Hydrogen Systems MH 2012, Kyoto (Japan), 21-26/10/2012. "Nanoconfined 2LiBH4-MgH2 in Nanoporous Carbon Aerogel Scaffolds for Reversible Hydrogen Storages". Oral presentation.
133. Gualdani, R.; Materazzi, S.; Nassini, R.; Fusi, C.; Geppetti, P.; Moncelli, M.R. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "Insight into the mechanism of the desensitization of TRPA1 channels by the anti-inflammatory compound Parthenolide". Poster presentation.
134. Jepsen, J.; Milanese, C.; Girella, A.; Lozano, A.; Bellosta von Colbe, J.; Marini, A.; Klassen, T.; Dornheim, M. World Hydrogen Energy Conference 2012, Toronto (Canada), 03-07/07/2012. "Compaction pressure influence on density, sorption behaviour & surface morphology for LiBH4-MgH2 composite". Oral presentation.
135. Lampis, S. La Parola ai Giovani 2012, Sassari (SS) 19/09/2012. "Nucleotide Recognition and Phosphate Linkage Hydrolisis at a Lipid Cubic Interface." Oral presentation.
136. Licciardello, A. Convegno congiunto delle sezioni SCI Calabria e Sicilia 2012, Arcavacata di Rende, 06-07/12/2012 "Engineering and characterization of molecular surfaces and thin films". Invited lecture.
137. Licciardello, A. Berner Fachhochschule-Haute école specialisée bernoise, 05/03/2012. "Anwendung der Sekundär-Ionen Massenspektrometrie auf Oberflächen und Dünnenschichten von technologischem Interesse" (Application of secondary ion mass spectrometry to surfaces and thin films of technological interest). Invited seminar.
138. Li Destri, G.; Torrisi, V.; Marletta, G. International Conference on Time of Polymers 2012 (TOP 2012), 10-14/06/2012, Ischia, Italy. "Electroactive functional hybrid layered nanocomposites". Invited lecture.
139. Lopez, F.; Cuomo, F.; Mosca M.; Ceglie, A. "Colloids and Nanomedicine", Amsterdam (Netherland) 15-17/07/2012. "Nucleic acids condensation onto nucleolipids doped liposomes". Poster presentation.
140. Magliulo, M.; Pistillo, B.R.; Mulla, M.Y.; Cotrone, S.; Cioffi, N.; Favia, P.; Sabbatini, L.; Palazzo,

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G.; Torsi, L. 2012 MRS Spring Meeting, 9-13/04/2012, San Francisco, CA. "PE-CVD P3HT surface modification for biomolecules integration in OFET devices". Oral presentation.

141. Magliulo, M.; Pistillo, B.R.; Mulla, M.Y.; De Tullio, D.; Manoli, K.; Cioffi, N.; Sabbatini, L.; Mallardi, A.; Palazzo, G.; Favia, P.; Torsi, L. XXIII Congresso Nazionale di Chimica Analitica, 16-20/09/2012, Hotel Hermitage, Biodola, Isola d'Elba. "PE-CVD as a powerful tool for P3HT surface modification in EGOFET biosensors development". Oral presentation.
142. Magliulo, M.; Pistillo, B.R.; Mulla, M.Y.; De Tullio, D.; Manoli, K.; Cioffi, N.; Sabbatini, L.; Mallardi, A.; Palazzo, G.; Favia, P.; Torsi, L. Convegno Nazionale della Divisione di Chimica dei Sistemi Biologici, DCSB 2012, Napoli 24-25/09/2012. "Integration of biomolecules in EGOFET devices by plasma assisted organic semiconductor surface modification". Oral presentation.
143. Manoli, K.; Dumitru, L.M.; Mulla, M.Y.; De Tullio, D.; Magliulo, M.; Intranuovo, F.; Mallardi, A.; Palazzo, G.; Favia, P.; Torsi, L. Avogadro Colloquia. 29/10/2012. Aula Prodi - Bologna. "Integration of biomolecules in EGOFET devices-Organic semiconductor surface modification". Oral presentation.
144. Marletta, G.; Ciapetti, G. CAARI Conference 2012, Forth Worth, USA, 10-14/08/2012. "Ion Beam-Induced Biofunctional Surfaces". Invited lecture.
145. Marletta, G. IUMRS-International Conference on Electronic Materials (IUMRS-ICEM 2012), 23-28/09/2012, Yokohama, Japan. "Smart Biocompatible Surfaces by Ion Beams". Invited lecture.
146. Martina, M.R.; Caminati, G. Materials Today Virtual Conference: Nanotechnology, 11-13/12/2012. "Nanolayers for diagnostics of proteins involved in degenerative amyloidosis". Poster presentation.
147. Martina, M.R.; Mercatelli, E.; Baglioni, P.; Caminati, G. 14th International Conference on Organized Molecular Films ICOMF14 (LB14), Paris (France) 10-13/07/2012. "Nanolayers for diagnostics of proteins involved in degenerative amyloidosis". Oral presentation.
148. Martini, S.; Bonechi, C.; Ciani, L.; Figura, N.; Rebmann, H.; Ristori, S.; Rossi, C. XXVIth International Conference on Polyphenols, Florence (Italy), 22-26/07/2012. "In- vitro Activity of Liposomal Resveratrol against Helicobacter Pylori". Poster presentation.
149. Martini, S.; Bonechi, C.; Ciani, L.; Figura, N.; Ristori, S.; Rossi, C. XXVI International Conference on Polyphenols in Florence, Italy 22-26/07/2012. "In-vitro Activity of Liposomial Resveratrol against Helicobacter Pylori". Poster presentation.
150. Materazzi, S.; Fusi, C.; Gualdani, R.; Moncelli, M.R.; Appendino, G.; Geppetti, P.; Nassini, R. 14th World Congress on Pain, Milano, 27-31/08/2012. "The antimigraine compound Parthenolide, contained in the feverfew herb, selectively activates and desensitizes the Transient Receptor Potential Ankyrin 1 (TRPA1) channel". Poster presentation.
151. Messina, G.M.L.; Dettin, M.; Marletta, G. Materials Research Society, Boston, MA (USA) 25-30/11/2012. "Charge-dependent Nano-Mesoscale Self-Organization Processes of Amphiphilic Peptides". Poster presentation.
152. Messina, G.M.L.; Lettieri, R.; Venanzi, M.; Formaggio, F.; Toniolo, C.; Marletta, G. Congresso Nazionale Biomateriali, Lecce 18-20/06/2012. "Peptide confinement in nanopores for antibacterial surfaces". Poster presentation.
153. Messina, G.M.L.; Lettieri, R.; Venanzi, M.; Formaggio, F.; Toniolo, C.; Marletta, G. Nanomaterials for biomedical technologies 2012, Frankfurt am Main (Germany) 06-07/03/2012. "Peptide-mediated confinement of liposomes in nanopores". Poster presentation.
154. Milanese, C.; Girella, A.; Marini, A. International Symposium on Metal-Hydrogen Systems MH 2012, Kyoto (Japan), 21-26/10/2012. "Thermal conductivity as a function of temperature for the most common metallic and complex hydrides". Poster presentation.
155. Monduzzi, M. Bjorn Lindman Symposium, Malmo, September 2012. "From self-assembly fundamental knowledge to nanomedicine developments". Invited lecture.
156. Mulas, G.; Campesi, R.; Garroni, S.; Delogu, F.; Milanese, C. 6th International Symposium Hydrogen & Energy, Stoos (Switzerland), 22-27/01/2012. "Hydrogenation of carbon monoxide over nanostructured systems: mechanochemical approach". Poster presentation.
157. Mulas, G.; Garroni, S.; Peru, F.; Campesi, R.; Dolci, F.; Milanese, C.; Girella, A.; Marini, A.; Pellicer, E.; Baró, M.D. Materials Research Society MRS Spring Meeting-Symposium P: Advanced Materials and Nanoframeworks for Hydrogen Storage and Carbon Capture, San Francisco (USA), 9-13/04/2012. "Sorption properties of chemical hydrides confined into mesoporous scaffolds". Oral presentation.
158. Mulla, M.Y.; Pistillo, B.R.; Magliulo, M.; Cotrone, S.; Palazzo, G.; Favia, P.; Sabbatini, L.; Torsi, L. Convegno Nazionale Sensori Innovazione, attualità e prospettive, Roma 15-17/02/2012. "Modifying organic semiconductor active layer of EGOTFT using PE-CVD for biosensors development". Oral presentation.
159. Murgia, S.; Falchi, A.M.; Carboni, M.; Lampis, S.; Sinico, C.; Manca, M.L.; Schmidt, J.; Talmon, Y.; Monduzzi, M. 26th ECIS Conference, Malmö & Lund, Sweden, 02-07/09/2012. "A Novel Nanocarrier for an Effective Dermal Drug Release". Oral presentation.
160. Musumeci, C.; Zappalà, G.; Orgiu, E.; Quici, S.; Licciardello, A.; Samorì, P. 6th International

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Symposium SUPRACHEM2012, "Supramolecular Systems in Chemistry and Biology", Strasbourg 5-8/09/2012. "Nanoscale investigation on single molecules conductive properties and their modulability through chemical design". Poster presentation.

161. Paduano, L. JCNS Workshop 2012 - Trends and Perspectives in Neutron Scattering for Soft Matter and Biophysics, Tutzing (Germany), 08-11/10/2012. "Nanodevices for antineoplastic diagnosis or therapy." Oral presentation.
162. Palazzo, P.; Angione, M.D.; Cotrone, S.; Magliulo, M.; Mallardi, A.; Torsi, L. Association in Solution III, ECI conference, Bifrost University, Iceland, 23-27/07/2012. "Phospholipids and proteins as active components of transistors: Where soft matter and organic electronics meet".
163. Palazzo, G. Scuola Nazionale di Chimca Analitica per Dottorandi 2012, Roma, Società Chimica Italiana, Divisione di Chimica Analitica, 04/10/2012. Lezione: "Nanotecnologie e Nanomateriali in Chimica Analitica: nanoanalisi vs analisi di nanostrutture".
164. Parisi, M.L.; Basosi, R. 8th Biennal International Workshop on Advances in Energy Studies, Mumbai (India) 25-27/10/2012. "Environmental life cycle analysis of non-conventional thin film photovoltaics: the case of dye-sensitized solar devices". Oral presentation.
165. Parisi, M.L.; Maranghi, S.; Basosi, R. 2nd DIRE Meeting, Roma (RM) 27/11/2012. "Life cycle Analysis of dye sensitized solar cell technology". Poster presentation.
166. Parisi, M.L.; Sinicropi, A.; Basosi, R. 25th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, Perugia (PG) 26-29/06/2012. "Life cycle assessment of thin film non conventional photovoltaics: the case of dye sensitized solar cells". Oral presentation.
167. Picciolo, F.; Squartini, T.; Ruzzenenti, F.; Basosi, R.; Garlaschelli, D. Eighth International Conference on Signal Image Technology and Internet Based Systems, SITIS 2012, Sorrento, Naples, Italy, 25-29/11/2012. "The Role of Distances in the World Trade Web". Oral presentation.
168. Pistidda, C.; Milanese, C.; Dornheim, M.; Klassen, T. International Symposium on Metal-Hydrogen Systems MH 2012, Kyoto (Japan), 21-26/10/2012. "Effect of a Partial Replacement of CaH2 by CaF2 in the Mixed System CaH2 + MgB2". Oral presentation.
169. Pogni, R.; Baratto, M.C.; Sinicropi, A.; Basosi, R. XI Convegno Nazionale GIRSE & 1st Joint Meeting ARPE-GERPE-GIRSE, Palermo, 03-06/10/2012. "Insights into the LRET mechanism of Ligninolytic Peroxidases and variants: an EPR-QM/MM approach". Poster presentation.
170. Ruzzenenti, F.; Bravi, M.; Tempesti, D.; Salvatici, E.; Manfrida, G.; Basosi R. 8th Biennal International Workshop on Advances in Energy Studies, Mumbai (India) 25-27/10/2012. "Assessment of micro CHP systems fueled by low-temperature geothermal and solar energy". Oral presentation.
171. Ruzzenenti, F.; Picciolo, F.; Basosi, R. 8th Biennal International Workshop on Advances in Energy Studies, Mumbai (India) 25-27/10/2012. "Rebound effect and structural change". Oral presentation.
172. Sacconi, A.; Moncelli, M.R. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "Study of the adsorption process of ATPases on Solid Supported Membrane". Poster presentation.
173. Sacconi, A.; Moncelli, M.R. 3rd PhD-Day, Firenze, 16/07/2012. "Studio di proteine di membrana con tecniche elettriche e spettroscopiche combinate". Poster presentation.
174. Sacconi, A.; Moncelli, M.R. Echems 8th, Bertinoro, Italy, 28/06-01/07/2012. "Characterization of model system on gold surface to study biological molecules". Oral presentation.
175. Sadafi, F.Z.; Tadini-Buoninsegni, F.; Bartolommei, G.; Messori, L.; Scaletti, F.; Massai, L.; Moncelli, M.R. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "Interaction of an anticancer drug with SERCA1a". Poster presentation.
176. Sapuppo, D.; Cristaudo, V.; Zappalà G.; Licciardello, A. SIMS EUROPE 2012, Münster, Germania, 08-12/09/2012. "Nitric oxide dosing in C60-SIMS depth profiling of polymer/inorganic hybrid multilayers". Oral presentation.
177. Sciacca, M.F.M.; Milardi, D.; Messina, G.M.L.; Marletta, G.; Brender, J.R.; Ramamoorthy, A.; La Rosa, C. Gordon Research Conference-Biointerface Science, Les Diablerets (Switzerland), 20-25/05/2012. "Membrane Disruption mechanism by Self-assembling of Peptides". Poster presentation.
178. Sinicropi, A. HRSMC EPA Summer School on Photochemistry, Fundamentals and Applications, Wijk aan Zee, The Netherland, 15-19/09/2012. "Computational Photochemistry - Lectures 1-4".
179. Sinicropi, A.; Bernini, C.; Pogni, R.; Basosi, R. Oxizymes in Marseille. 16-19 settembre 2012, Marsiglia "Investigation of redox-active aminoacids in oxidative enzymes: the role of the combined EPR and computational approach". Poster presentation.
180. Sinicropi, A.; Bernini, C.; Pogni, R.; Basosi, R. XXXI Congresso Interregionale TUMA 2012, Francavilla al Mare (CH) 18-20/06/2012. "Studio computazionale di radicali amminoacidici coinvolti in cammini di trasferimento elettronico in proteine". Oral presentation.
181. Smeazzetto, S.; Montis, C.; Berti, D.; Moncelli, M.R. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "Ion channel activity of Phospholamban reconstituted in Giant Unilamellar Vescicles (GUVs)". Poster presentation.

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182. Smeazzetto, S.; Saponaro, A.; Young, H.S.; Moncelli, M.R.; Thiel, G. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "Structure-function relation of Phospholamban: modulation of channel activity as a potential regulator of SERCA activity". Poster presentation.
183. Sostegni, S.; Gualdani, R.; Dragoni, E., Nativi, C.; Moncelli, M.R. 3rd International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze, 23-27/09/2012. "ADM_09 as a new TRPA1 selective antagonist to relieve chemotherapy-related pain". Poster presentation.
184. Speltini, A.; Merli, D.; Dondi, D.; Milanese, C.; Galinetto, P.; Longhi, D.; Profumo, A. XXIII Congresso Nazionale della Divisione di Chimica Analitica, Isola d'Elba (Italy), 16-20/09/2012. "Multi-walled carbon nanotubes-modified silica microspheres: a new HPLC stationary phase". Poster presentation.
185. Spinelli, D.; Fatarella, E.; Martorana, A.; Bernini, C.; Sinicropi, A.; Baratto, M.C.; Basosi R.; Pogni, R. Oxyzymes, Marseille (France) 16-19/09/2012. "Immobilized Fungal Laccases for biotransformation processes". Poster presentation.
186. Spinelli, D.; Martorana, A.; Baratto, M.C.; Basosi, R.; Pogni, R. Environmental Microbiology and Biotechnology 2012 (EMB 2012), Bologna (Italy) 10-12/04/2012. "Synthesis of textile dyes by laccase biotransformations". Contribute for the Congress Acts.
187. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Inesi, G. XXI Congresso Nazionale della Società Italiana di Biofisica Pura e Applicata, Ferrara, 17-20/09/2012. "Pre-steady state charge transfer in recombinant ATP7A and ATP7B". Oral presentation.
188. Tolu, E.; Peru, F.; Campesi, R.; Dolci, F.; Milanese, C.; Marini, A.; Pellicer, E.; Baró, M.D.; Garroni, S. Mulas, G. International Symposium on Metal-Hydrogen Systems MH 2012, Kyoto (Japan), 21-26/10/2012. "Ordered Mesoporous Scaffolds for the Confinement of Nanosized Complex and Metal Hydrides". Oral presentation.
189. Torsi, L.; Magliulo, M.; Mallardi, A.; Cioffi, N.; Sabbatini, L.; Scamarcio, G.; Palazzo, G. XXIII Congresso Nazionale di Chimica Analitica, 16-20/09/2012, Hotel Hermitage, Biodola, Isola d'Elba. "A new OFET device configuration for highly performing bio-electronic sensors". Oral presentation.
190. Torsi, L.; Magliulo, M.; Mallardi, A.; Palazzo, G. Convegno Nazionale della Divisione di Chimica dei Sistemi Biologici, DCSB 2012, Napoli 24-25/09/2012. "Novel strategies in organic field-effect transistor Bio-sensors". Oral presentation.
191. Wang, X.; Nilsson, D.; Norberg, P.; Cotrone, S.; Magliulo, M.; Palazzo, G.; Torsi, L.; Suspène, C.; Yassar, A.; Albers, W.M.; Tappura, K.; Vikholm-Lundin, I. E-MRS 2012 Spring Meeting, 15-18/05/2012-Strasburg, France. "Printed Electrolyte-Gated Organic Field-Effect Transistors on Flexible Substrates with Immobilized Bioreceptors on Semiconductor Surface for Sensing Applications". Oral presentation.
192. Zappalà, G.; Sapuppo, D.; Amato, M.E.; Licciardello, A. SIMS EUROPE 2012 Münster, Germania, 08-12/09/2012. "ToF-SIMS characterization of self assembled rhodamine-derivatives on quartz". Poster presentation.
193. Angelico, R.; Ceglie, A.; He, J-Z.; Palumbo, G.; Colombo, C. The Italian Chapter of the International Humic Substances Society (IHSS), Portici (NA) 05-07/12/2011. "Nature of ferrihydrite-humic substances (Fe-HS) coprecipitate: scanning and transmissions electron microscopy (SEM, TEM) and dynamic light scattering (DLS) analysis". Oral presentation.
194. Angelico, R.; Losito, I.; Introna, B.; Cuomo, F.; Ceglie, A.; Palmisano, F.; XXIV Congresso Nazionale della Società Chimica Italiana-Divisione di Chimica Fisica, Lecce 11-16/09/2011. "Role of base-pairing in the synthesis of nucleolipids obtained through alkylation of Cytidine and Guanosine". Oral presentation.
195. Angione, D.; Cioffi, N.; Cotrone, S.; Magliulo, M.; Mallardi, A.; Sabbatini, L.; Palazzo, G.; Torsi, L. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16 Settembre 2011. "Protein integrated into organic field effect transistor as electronic biosensors". Oral presentation.
196. Angione, D.; Cotrone, S.; Magliulo, M.; Mallardi, A.; Palazzo, G.; Torsi, L. MRS Spring Meeting, 25-29/04/2011, San Francisco (CA). "In water label-free pico-molar detection with innovative bio-electronic OFET sensors". Oral presentation.
197. Angione, D.; Dumitru, L.; Magliulo, M.; Cotrone, S.; Mallardi, A.; Cioffi, N.; Palazzo, G.; Torsi. L. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011 "Reliability testing in OFET Biosensors". Poster presentation.
198. Angione, M.D.; Magliulo, M.; Cotrone, S.; Mallardi, A.; Dumitru, L.M.; Mulla, M.Y.; Palazzo, G.; Torsi, L. ICOE, 22-24/06/2011, Roma, Italy. "Integration of bio-molecules in OFET sensors". Oral presentation.
199. Ballistreri, A.; Impallomeni, G.; Carnemolla, G.M.; Guglielmino, S.P.P; Nicolò, M.S.; Cambria, M.G. Europolymer Conference 2011-Biobased Polymers and Related Biomaterials, Gargnano, (BS) 29/05-03/06/2011. "Biosynthesis and structural characterization of biodegradable plastics from Brassica carinata oil and from very long chain fatty acids". Poster presentation.
200. Baratto, M.C.; Martorana, A.; Bernini, A.; Valensin, D.; Sinicropi, A.; Pogni, R.; Basosi, R.

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Emory@Unisi Summer School, Chemistry for Life&Environment Education, Collaboration, Innovation, VIII Edition, Siena, 30/05-04/07-2011. "Characterisation of Laccase-Catalysed Homocoupling Reaction of 4-Methylamino Benzoic Acid". Poster presentation.

201. Baratto, M.C.; Martorana, A.; Bernini, C.; Valensin, D.; Sinicropi, A.; Pogni, R.; Basosi, R. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce, 11-16/09/2011. "Insights on the homocoupling reaction of 4-methylamino benzoic acid mediated by Trametes versicolor laccase". Poster presentation.
202. Bonechi, C.; Martini, S.; Ciani, L.; Lamponi, S.; Ristori, S. 25th European Colloid and Interface Society (ECIS), Berlino 04-09/09/2011. "Resveratrol loaded liposome: a strategy for delivering natural antioxidants". Poster presentation.
203. Bonechi, C.; Martini, S.; Ciani, L.; Lamponi, S.; Setzer, C.; Rebmann, H.; Ristori, S. 25th Conference European Colloid and Interface Society, Berlin (Germany) 04-09/09/2011. "Resveratrol loaded liposome: a strategy for delivering natural antioxidants". Poster presentation.
204. Boscagli, C.; Gambinossi, F.; Caminati, G. 25th European Colloid and Interface Society Conference, Berlin (Germany) 04-09/09/2011. "Nanofabrication of mesoporous architectures for Dye Sensitized Solar Cells (DSSCs)". Oral presentation.
205. Cabo, M.; Garroni, S.; Pellicer, E.; Milanese, C.; Girella, A.; Marini, A.; Rossinyol, E.; Suriñach, S.; Baró, M.D. Euromat 2011, Montpellier (France), 12-15/09/2011. "Effects of nanocast mesoporous NiO, NiCo2O4 and Co3O4 additives on the hydrogen sorption performance of MgH2". Oral presentation.
206. Cambria, M.G.; Bottari, R.; Ballisteri, A.; Impallomeni, G.; Guglielmino, S.P.P. 29° Convegno SIMGBM Pisa (PI) 21-23/09/2011. "Rhamnolipid biosurfactants from Brassica carinata oil: synthesis and characterization". Poster presentation.
207. Campesi, R.; Milanese, C.; Girella, A.; Delogu, F.; Garroni, S.; Napolitano, E.; Doppiu, S.; Mulas, G. 2nd Symposium Advanced Dutch H2 and FC Research, Eindhoven (Holland), 24/03/2011. "Hydrogen Sorption properties of nanocomposites NaBH4-MgH2 confined by melting impregnation into SBA-15". Oral presentation.
208. Capsoni, D.; Boiocchi, M.; Bruni, G.; Bini, M.; Ferrari, S.; Maietta, M.; Berbenni, V. XL Congresso Nazionale dell'Associazione Italiana di Cristallografia, Siena 19-22/09/2011. "Preparation and characterization of Carprofen-4,4'Dipyridil co-cristals". Poster presentation.
209. Carboni, M.; Murgia, S.; Lampis, S.; Falchi, A.M.; Fadda, A.M.; Sinico, C.; Lai, F.; Talmon, Y.; Monduzzi, M. 25th ECIS Conference, Berlin, Germany, 04-09/09/2011. "Fast Preparation and Characterization of Innovative Cationic Small Unilamellar Liposomes". Poster presentation.
210. Carretti, E. Convegno di Studi Scienza e Beni Culturali Governare l'innovazione Processi, strutture, materiali e tecnologie tra passato e futuro, Bressanone, 21-24/06/2011. "Sistemi nano tecnologici per la conservazione: stato dell'arte e prospettive". Oral presentation.
211. Consumi, M.; Matteucci, M.; Leone, G.; Bonechi, C.; Rossi, C.; Kusmic, C.; Menichetti, L.; L'Abbate, A.; Magnani, SIMS-XVIII International Conference on Secondary Ion Mass Spectrometry, Riva del Garda 18-23/09/ 2011. "ToF-SIMS characterization of ischemic murine heart tissue". Poster presentation.
212. Cotrone, S.; Mulla, M.Y.; Ambrico, M.; Ligonzo, T.; Magliulo, M.; Palazzo, G.; Mallardi, A.; Angione, M.D.; Cioffi, N.; Torsi, L. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "Dieletric properties of lipid layers integrated in OTFT". Poster presentation.
213. D'Errico, G.; Vitiello, G.; Galdiero, S.; Busi, E.; Merlino, A.; Picone, D.; D'Ursi, A.M.; Paduano, L. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "On the role played by the pre-TM domain of viral fusion glycoproteins in the infective process". Oral Presentation.
214. Diaz Fernandez, Y.A.; Amato, E.; Pasotti, L.; Taglietti, A.; Pallavicini, P.; Milanese, C.; Girella, A.; Grisoli, P.; Dacarro, C.; Necchi, V. Dalla scienza dei materiali allo sviluppo di nuovi dispositivi per la diagnosi e la cura di patologie associate all'invecchiamento, Pavia (Italy), 17/06/2011. "Biomimetically Coated Silver Nanoparticles: Synthesis, Characterization and Antibacteric Activity". Poster presentation.
215. Donà, A.; Cabrini, E.; Milanese, C.; Pallavicini, P. X Congresso Nazionale di Chimica Supramolecolare, Perugia (Italy), 25-28/09/2011. "Synthesis of anisotropic gold nanoparticles with accurately tunable LSPR in the 700-1500 nm range". Poster presentation.
216. Falsini, S.; Ristori, S.; Ciani, L.; Fortunato, A.; D'Amico, M.; Arcangeli, A. Joint National Ph.D Meeting organized by ABCD, Gubbio 20-22/10/2011; "Properties of complexes formed by siRNA and cationic Gemini surfactants". Poster presentation.
217. Ferrari, S.; Agnesi, A.; Pirzio, F.; Reali, G.; Bini, M.; Capsoni, D.; Massarotti, V. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "Carbon Nanotube Saturable Absorbers for Ultrafast Pulsed Lasers". Oral presentation.
218. Ferrari, S.; Bini, M.; Capsoni, D.; Massarotti V. SSI18th - International conference on Solid State Ionics, Warszawa (Poland) 03-08/07/2011. "Electrochemical behaviour of the doped Li3V2(PO4)3

cathode material". Poster presentation.

219. Ferrari, S.; Bini, M.; Capsoni, D.; Massarotti, V.; Mustarelli, P.; Spina, G.; Leonelli, C. SSI18th - International conference on Solid State Ionics, Warszawa (Poland) 3–8/07/2011. "Study of defects in LiFePO4 by using PDF analysis and Mössbauer spectroscopy". Oral presentation.
220. Ferrari, S.; Bini, M.; Capsoni, D.; Massarotti, V.; Mustarelli, P.; Spina, G.; Leonelli, C.; Rizzuti, A.; Del Giallo, F.; Lantieri, M. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "Anti-site defects formation in LiFePO4 cathode material prepared by microwave-assisted hydrothermal synthesis". Poster presentation.
221. Fratini, E. Workshop on C-S-H, Lausanne (Swiss) 03-04/10/2011. "Neutron Scattering on C-S-H". Oral presentation.
222. Garroni, S.; Milanese, C.; Girella, A.; Marini, A.; Campesi, R., Suriñach, S.; Baró, M.D.; Mulas, G. Faraday Discussion 151: Hydrogen Storage Materials, Rutherford Appleton Laboratory, Didcot, (UK), 18-20/04/2011. "Kinetic, thermodynamic and spectroscopic exploration on the NaBH4-MgH2 RHC system". Poster presentation.
223. Ghezzi, M.; Gambinossi, F.; Caminati, G. 25th Conference of the European Colloid and Interface Society, Berlin (Germany) 04-09/09/2011. "Hybrid nanoarchitectures for PhOLED devices". Poster presentation.
224. Gualdani, R.; Moncelli, M.R.; Ottolia, O.; Philipson, K.D.; Olcese, R. EMBO/FEBS Lecture Course on Channels and Transporters, Erice (TP), 11-17/05/2011. "Structural rearrangements of NCX1 revealed by Voltage Clamp Fluorometry". Poster presentation.
225. Jepsen, J.; Bellosta von Colbe, J.; Lozano, G.A.; Milanese, C.; Klassen, T.; Dornheim, M. Gordon Research Conference on Hydrogen-Metal Systems, Stonehill College (Easton, Massachusetts, USA), 17-22/07/2011. "Potentials and challenges of a Li-RHC based Tank". Poster presentation.
226. Licciardello, A. Département de Physique, Université de Namur (FUNDP), Namur, 21/10/2011. "Dynamic SIMS of molecular materials: nitric oxide-assisted cluster-SIMS depth profiling of polymers". Invited seminar.
227. Liviu, D.; Daniela, A.; Maria, M.; Cotrone, S.; Antonia, M.; Cioffi, N.; Palazzo, G.; Torsi, L. ECRO XXI Congress 7-10/09/2011, Manchester (UK). "Reliability tests performed on OFET Biosensors". Poster presentation.
228. Loiselle, S.A.; Bracchini L.; Dattilo A.M.; Rossi, C. (conference organisers) "The Aquatic Ecosystem Puzzle: Threats, Opportunities & Adaptation", Siena, Italy June 2011, participation - 120 scientists from 35 countries.
229. Magliulo, M.; Angione, M.D.; Cotrone, S.; Sabbatini, L.; Mallardi, A.; Palazzo, G.; Torsi, L. GS2011, 15-17/06/2011, Teramo (IT). "Innovative electronic OFET biosensors". Oral presentation.
230. Marletta, G. MRS-Mexican MRS, Cancun (Mexico), 14-19/08/2011. "Orienting Biomolecules onto Irradiated Surfaces: From Epitope Orientation to Cell Hunting". Invited lecture.
231. Marletta, G. E-MRS Spring Meeting, Symposium P on "Bioinspired and Biointegrated materials as new frontier nanomaterials II", Nice (France), 9-13/05/2011. "New Strategies for bioengineering". Invited lecture.
232. Marletta, G. Italian-Swedish Workshop on "Nanoscience and Medical Technology", Stockholm, 28-30/09/2011. "Nano-confinement: A Strategy for Biofunctional Surfaces". Invited lecture.
233. Matteini, P.; Ratto, F.; Rossi, F.; Pini, R.; Tiribilli, B.; Giambastiani, G.; Luconi, L.; Dei, L.; Caminati, G. International workshop BioPhotonics 2011, Parma (Italy) 08-10/06/2011. "Hybrid laser-activatable gold nanorods-loaded hydrogels for photothermal applications". Poster presentation.
234. Mazzaglia, A; Castriciano, M.; Martel, B.; Romeo, A.; Monsù Scolaro, L.; Ingo, G.M.; Padeletti, G.; Villari, V.; Sciortino, M.T.; Grasso, L.; Guglielmino, S.P.P. 2nd European Conference on Cyclodextrins Asti (AT) 02-04/10/2011. "Entrapment of anionic porphyrins in nanofabrics modified by cyclodextrin: spectroscopy, morphological investigation and antimicrobial photosensing activity". Poster presentation.
235. Medda, L.; Salis, A.; Magner, E. La Parola ai Giovani 2011, Cagliari 24/06/2011. "Effetti iono-specifici sulle proprietà elettrochimiche del citocromo c". Oral presentation.
236. Medda, L.; Salis, A.; Magner, E. XXV ECIS Conference, Berlin (Germany) 4-9/09/2011. "Specific Ion effects on the Electrochemical Properties of Cytochrome c". Poster presentation.
237. Messina, G.M.L.; Lettieri, R.; Venanzi, M.; Formaggio, F.; Toniolo, C.; Marletta, G. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "Peptide-mediated confinement of liposomes in nanopores". Oral presentation.
238. Messina, G.M.L.; Lettieri, R.; Venanzi, M.; Marletta, European Materials Research Society, Nice (France) 9-13/05/2011. "Peptide trapping in nanopores for antibacterial surfaces". Poster presentation.
239. Milanese, C. Helmholtz- Zentrum Geesthacht (Germany) - Zentrum für Material-und Küstenforschung GmbH, 6/06/2011. "Thermodynamic and kinetic investigation on hydrogen storage materials". Invited seminar.
240. Milanese, C.; Girella, A.; Berbenni, V.; Bruni, G.; Cofrancesco, P.; Marini, A.; Colella, A.; Bianchin, A.; Matteazzi, P. Workshop "Energia e Fonti rinnovabili" – Celebrazioni per i 650 anni

dell'Università di Pavia, Pavia (Italy), 15/06/2011. "Progetto Nanostore: dall'ideazione di un materiale per lo stoccaggio idrogeno alla realizzazione di un prototipo dimostrativo". Poster presentation.

241. Milanese, C.; Girella, A.; Campesi, R.; Garroni, S.; Doppiu, S.; Napolitano, E.; Mulas, G. 5th International Symposium Hydrogen & Energy, Stoos (Switzerland), 23-28/01/2011. "Investigation of the H2 sorption properties of NaBH4 – MgH2 nanocomposites confined into mesoporous SBA-15". Poster presentation.
242. Milanese, C.; Girella, A.; Garroni, S.; Mulas, G.; Campesi, R.; Pellicer, E.; Baró, M.D.; Marini, A. Gordon Research Conference on Hydrogen – Metal Systems, Stonehill College (Easton, Massachusetts, USA), 17-22/07/2011. "Preparation and characterization of borohydrides-based reactive hydride composites (RHCs)". Poster presentation.
243. Milanese, C.; Girella, A.; Garroni, S.; Mulas, G.; Suriñach, S.; Baró, M.D.; Marini, A. 5th International Symposium Hydrogen & Energy, Stoos (Switzerland), 23-28/01/2011. "Kinetic and Thermodynamic Investigations on Pure and Doped NaBH4 - MgH2 System". Oral presentation.
244. Milanese, C.; Girella, A.; Garroni, S.; Mulas, G.; Suriñach, S.; Baró, M.D.; Marini, A. Bunsentagung 2011, Deutsche Bunsen-Gesellschaft für Physikalische Chemie, Berlin (Germany), 2-4/06/2011. "Thermodynamic and kinetic investigations on pure and doped NaBH4-MgH2 hydrogen storage system". Oral presentation.
245. Milanese, C.; Girella, A.; Marini, A.; Garroni, S.; Mulas, G. Workshop "Energia e Fonti rinnovabili" – Celebrazioni per i 650 anni dell'Università di Pavia, Pavia (Italy), 15/06/2011. "Preparazione e caratterizzazione di materiali innovativi a base di idruri complessi per lo stoccaggio idrogeno". Poster presentation.
246. Milanese, C.; Marini, A. Workshop "Energia e Fonti rinnovabili" – Celebrazioni per i 650 anni dell'Università di Pavia, Pavia (Italy), 15/06/2011. "Impacchettare l'idrogeno". Poster presentation.
247. Milanese, C.; Marini, A. Workshop "Energia e Fonti rinnovabili" – Celebrazioni per i 650 anni dell'Università di Pavia, Pavia (Italy), 15/06/2011. "Veicoli a idrogeno: passato, presente e…". Poster presentation.
248. Monduzzi, M. Italy-Sweden Nanomed Meeting, Stockolm, September 2011. "3D vision of human lysozyme adsorbed onto a SBA-15 nanostructured matrix: a potential depot system". Invited lecture.
249. Mulas, G.; Garroni, S.; Campesi, R.; Napolitano, E.; Milanese, C.; Girella, A.; Pellicer, E.; Baró, M.D. International Symposium on Metastable, Amorphous and Nanostructured Materials ISMANAM 2011, Gijón (Spain), 26/06-1/07/2011. "Hydrogen sorption properties and structural characterization of the NaBH4/MgH2 system confined into SBA-15 mesoporous matrix". Oral presentation.
250. Mulla, M.Y.; Pistillo, B.R.; Magliulo, M.; Cotrone, S.; Cioffi, N.; Palazzo, G.; Favia, P.; Sabbatini, L.; Torsi, L. ECRO XXI Congress 7-10/09/2011, Manchester (UK) "Biomolecules integration in OTFT devices for biosensors development". Poster presentation.
251. Murgia, S.; Palazzo, G.; Mamusa, M.; Lampis, S.; Monduzzi, M. XXIV Congresso Nazionale Società Chimica Italiana, Lecce, Italia, 12-16/06/2011. "Modulazione della curvatura interfasale del tensioattivo Aerosol-OT in acqua attraverso i liquidi ionici 1-butil-3-metilimidazolo BF4-/Br-". Oral presentation.
252. Naldini, M.; Natali, I.; Carretti, E.; Baglioni, P.; Dei L. Convegno di Studi Scienza e Beni Culturali Governare l'innovazione Processi, strutture, materiali e tecnologie tra passato e futuro, Bressanone, 21-24/06/2011. "Sistemi compositi silicato-calcici TEOS-nanocalce per la conservazione di superfici architettoniche". Poster presentation presentation.
253. Natali, I.; Marinelli, F.; Carretti, E.; Angelova, L.; Weiss, R.G.; Baglioni, P.; Dei L. Convegno di Studi Scienza e Beni Culturali Governare l'innovazione Processi, strutture, materiali e tecnologie tra passato e futuro, Bressanone, 21-24/06/2011. "Sistermi polimerici a base acquosa con peculiari proprietà viscoelastiche: pulitura di superfici pittoriche con sistemi ad alta compatibilità ambientale". Poster presentation.
254. Nuccio, A.; Carretti, E.; Baglioni, P.; Dei, L. Convegno di Studi Scienza e Beni Culturali Governare l'innovazione Processi, strutture, materiali e tecnologie tra passato e futuro, Bressanone, 21-24/06/2011. "Sistemi compositi inorganico-organici nanocalce-copolimeri acrilici per la conservazione di superfici architettoniche". Poster presentation.
255. Palazzo, G.; Angione, D.; Cotrone, S; Magliulo, M.; Mallardi, A.; Torsi, L. SPIE 2011, 21-25/08/2011, San Diego (CA). "What we can learn from the integration of biological membranes into OTFT sensors". Oral presentation.
256. Palazzo, G. Accademia dei Lincei, 13ª Edizione delle Giornate Lincee della Chimica, Bari, Università di Bari, 21/11/2011. Seminario: "Nanomateriali per le scienze della vita: un approccio interdisciplinare".
257. Pallavicini, P.; Cabrini, E.; Donà, A.; Diaz Fernandez, Y.A.; Falqui, A.; Genovese, A.; Milanese, C.; Taglietti, A. X Congresso Nazionale di Chimica Supramolecolare, Perugia (Italy), 25-28/09/2011. "Beyond the CTAB paradigm: using zwitterionic and non-ionic surfactants to access new asymmetric gold nanoparticles". Oral presentation.

Conferences

258. Parisi, M.L.; Sinicropi, A.; Basosi, R. V Congresso Nazionale dell'Associazione Italiana Gestione Energia, Modena (MO) 08-09/06/2011. "Life Cycle Assessment of Gratzel-type cell production for non conventional photovoltaics from novel organic dyes". Oral presentation.
259. Parisi, M.L.; Spinelli, D.; Berzi, L.; Delogu, M.; Pierini, M.; Basosi, R. Ecomondo, Rimini (RN) 9/11/2011. "Analisi LCA integrata di scenari per lo sviluppo di metodi di riciclaggio e riuso dei residui plastici dagli ELV". Oral presentation.
260. Pogni R.; Miki Y.; Calvino F.R.; Giansanti S.; Ruiz-Duenas F.J.; Martinez M.J.; Basosi R.; Romero A.; Martinez A.T., Atti XXIV Congresso Nazionale della Società Chimica Italiana "Crystallographic, kinetic and spectroscopic study of the first ligninolytic peroxidase presenting a catalytic tyrosine". Lecce 11-16/09/2011, 573- 573. Poster presentation.
261. Ristori, S.; Ciani, L.; Falsini, S.; Candiani, G.; Di Cola, E.; Grillo, I.; In, M. 25th Conference European Colloid and Interface Society, Berlin (Germany) 04-09/09/2011. "Complexing a Small Interfering RNA with cationic micelles". Poster presentation.
262. Ristori, S.; Ciani, L.; Falsini, S.; Candiani, G.; Di Cola, E.; Grillo I.; In M. Conference on Nanotechnology for Biological and Biomedical Applications (Nano-Bio-Med), Trieste 10-14/10/2011. "Complexing a Small Interfering RNA with divalent cationic surfactants". Poster presentation.
263. Sabbatini, L.; Angione, D.; Cotrone, S.; Magliulo, M.; Cioffi, N.; Torsi, L. NanoEnergy 11, 03-06/04/2011, Natal, Brasil. "Surface architectures for Bio-Chem sensing". Oral presentation.
264. Sacconi, A.; Moncelli, M.R. II Scuola Nazionale di Chimica Bioinorganica, Siena, 03-06/07/2011. "Electrochemical and Spectroscopy study of ATPase". Poster presentation.
265. Salis, A; Cugia, F.; Monduzzi M. XXV ECIS Conference, Berlin (Germany) 4-9/09/2011. "Specific ion effects on lysozyme adsorption on ordered mesoporous silica". Poster presentation.
266. Sapuppo, D.; Zappalà, G.; Spampinato, V.; Licciardello, A. 18th International Conference on Secondary Ion Mass Spectrometry SIMS 18, Riva del Garda, Italy, 18-23/09/2011. "Molecular depth profiling of polycarbonate by nitric oxide-assisted C60 SIMS". Poster presentation.
267. Sapuppo, D.; Zappalà, G.; Spampinato, V.; Tuccitto, N.; Raudino, A.; Torrisi, A.; Licciardello, A. 18th International Conference on Secondary Ion Mass Spectrometry SIMS 18, Riva del Garda, Italy, 18-23/09/2011. "Nitric oxide-assisted SIMS depth profiling of polymers with C60 primary ions". Oral presentation.
268. Schiavo, B.; Girella, A.; Joseph, B.; Milanese, C. Faraday Discussion 151: Hydrogen Storage Materials, Rutherford Appleton Laboratory, Didcot, (UK), 18-20/04/2011. "Hydrogen Storage Properties of the CaH2-MgB2-AlB2 System". Poster presentation.
269. Sinicropi, A.; Bernini, C.; Pogni, R.; Basosi, R. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce, 11-16/09/2011 "QM/MM characterization of redox-active Trp radicals in LiP and LiP-like systems". Poster presentation.
270. Smeazzetto, S.; Schröder, I.; Thiel, G.; Moncelli, M.R. 36th FEBS Congress, Torino, 25-30/06/2011. "Phospholamban can act a san ion channel". Poster presentation.
271. Spampinato, V.; Vitale S.; Quici, S.; Torrisi, A.; Würthner, F.; Licciardello, A. 18th International Conference on Secondary Ion Mass Spectrometry SIMS 18, Riva del Garda, Italy, 18-23/09/2011. "ToF-SIMS of metal-complex-based supramolecular architectures on oxide surfaces". Poster presentation.
272. Spinelli, D.; Basosi, R. National Congress AIGE, Modena (Italy) 08-09/06/2011. "Biofuels from microalgae". Oral communication.
273. Tadini Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce, 11-16/09/2011. "Drug interactions with cation transport ATPases investigated on solid supported membranes". Oral presentation.
274. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Pilankatta, R.; Inesi, G. 13th International ATPase Conference, Asilomar, California, USA, 27/09-02/10/2011. "ATP-dependent charge transfer in recombinant copper ATPases ATP7A and ATP7B investigated on solid supported membranes". Poster presentation.
275. Taglietti, A.; Cucca, L.; Dacarro, G.; Diaz Fernandez, Y.A.; Donà, A.; Grisoli, P.; Milanese, C.; Necchi, V.; Pallavicini, P.; Pasotti, L. X Congresso Nazionale di Chimica Supramolecolare, Perugia (Italy), 25-28/09/2011. "Functionalization of nano-objects with glutathione". Oral presentation.
276. Taglietti, A.; Cucca, L.; Dacarro, G.; Diaz Fernandez, Y.A.; Grisoli, P.; Milanese, C.; Necchi, V.; Pallavicini, P.; Pasotti, L. X Congresso Nazionale di Chimica Supramolecolare, Perugia (Italy), 25-28/09/2011. "Antibacterial action of Glutathione coated Silver Nanoparticles against Gram positive and Gram negative bacteria". Poster presentation.
277. Vaselli, E.; D'Errico, G.; Sartorio, R.; Vitiello, G.; Zanardi, F.; Manzoni, L.; Paduano, L.; Mangiapia, G. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. Targeting RGD-recognizing integrins: aggregation behavior of a novel class of amphiphilic RGD integrin binders". Poster presentation.
278. Vaselli, E.; D'Errico, G.; Silipo, A.; Molinaro, A.; Lanzetta, R.; Radulescu, A.; Paduano, L.;

Conferences

Mangiapia, G. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "Characterization of vesicles formed by lipopolysaccharides:from the molecular structure to the aggregate architecture". Poster presentation.

279. Vignali, F.; Baratto, M.C.; Basosi, R.; Müller, K.; Callone, E.; Palanti, E.; Feci, E.; Elviri, L.; Predieri, G. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce, 11-16/09/2011. "Synthesis and characterization of wood-silica gel nanocomposites anchoring copper complexes active against biotic decay". Poster presentation.
280. Vitiello, G.; D'Errico, G.; Silipo, A.; Mangiapia, G.; Radulescu, A.; Molinaro, A.; Lanzetta, R.; Paduano, L. 16th European Carbohydrate Symposium, Sorrento (NA) 03-07/07/2011. "Characterization of liposomes formed by lipopolysaccharides from Burkholderia cenocepacia, Burkholderia multivorans and Agrobacterium Tumefaciens: from the molecular structure to the aggregate architecture". Poster presentation.
281. Vitiello, G.; Fragneto, G.; D'Ursi, A.M.; Paduano, L.; D'Errico, G. Workshop BILL-Bilayer at ILL, Grenoble (France) 25-31/02/2011. "Neutron Reflectivity study on the interaction between an octapeptide deriving from glycoprotein gp36 of Feline Immunodeficiency Virus and lipid membranes: the role of cholesterol". Poster presentation.
282. Vitiello, G.; Fragneto, G.; D'Ursi, A.M.; Paduano, L.; D'Errico, G. XXIV Congresso Nazionale della Società Chimica Italiana, Lecce 11-16/09/2011. "Lipid composition regulates the biomembranes micro-structural properties and modulates the interaction with a peptide deriving from the viral glycoprotein gp36". Poster presentation.
283. Zanchi, C.; Capsoni, D.; Licchelli, M.; Mustarelli, P.; Tomasi, C.; Weththimuni, M. 5° International Congress-Science and Technology for the Safeguard of Cultural Heritage in the Mediterranean Basin-Istambul (Turkey) 22-25/11/2011. "Fluorinated poolyurethane montmorillonite nanocomposites for the protection of Lecce Stone". Poster presentation.

Organized/Chaired

- -MRS SPRING Meeting 2011, Co-Chairman of Symposium B on "Functional Biointerfaces" (Co-Chairmen: K.Jandt, C.Ortiz), Strasbourg (France) - 2011.
- nternational Joint Meeting of the European Materials Research Society (E-MRS) International Union of Materials Research Societies (IUMRS) 2011, Chairman of the Conference (Co-Chairmen: H.U.Habermaier, J.Lindner, Hai-Ling Tu), Nice (France) - 2011.
- RS Spring Meeting 2011, Co-Chairman of the Symposium II on "Ion Beams – New Applications from Mesoscale to Nanoscale", San Francisco (USA) - 2011.
- -MRS SPRING Meeting 2012, Co-Chairman of Symposium B on "Functional Biomaterials" (Co-Chairmen: K.Rezwan, M.Manso Silvan), Strasbourg (France) - 2012.
- -MRS SPRING Meeting 2013, Co-Chairman of Symposium R on "nano-engineered bioactive interfaces" (Co-Chairmen: P. Netti, M.Lensen), Strasbourg (France) - 2013.
- -MRS Fall Meeting 2013, Co-Chairman of the Symposium G on "Bioinspired and Biointegrated Materials as frontier Nanomaterials III" (Co-Chairmen: P. Scharff, K.Arzum Erdem Gursan; E.Buzaneva; H.Fenniri); Warsaw (Poland) - 2013.

Guests

- r. Mathis Wackernagel, Ph.D. Global Footprint Network, "Ecological footprint" - 2011.
- r. Michela Ottolia, Ph.D. University of California at Los Angeles, Department of Physiology, Cardiovascular Research Laboratories, Los Angeles, U.S.A., "Probing structural rearrangements of the cardiac Na+-Ca2+ exchanger during its operation" - 2011.
- r. Stefano Giurgola, Responsabile Laboratorio e Controllo Qualità di Richard Ginori 1735 SpA, "Il Laboratorio Richard Ginori: dalla tradizione verso l'innovazione" - 2011.

Conferences

- rof. Mette Geiker, Ph.D. Technical University of Denmark, Department of Civil Engineering, “Porosoty development and porosity characterisation in cement pastes” - 2011.
- rof. Seema Bhadauria, Ph.D. Raja Balwant Singh College, Agra (India), “Microbiological analysis of biofilms on stone artifacts and their conservation by sol-gel and biologically synthesized nanomaterials” - 2011.
- rof. Antonio Zaza, M.D. Università di Milano-Bicocca, Dipartimento di Biotecnologie e Bioscienze, “Modulazione di SERCA e stabilità dello "store" cellulare di calcio” - 2012.
- rof. Krister Holmberg, Ph.D. Director Materials Science, Chalmers University of Technology, Chemical and Biological Engineering, “The use of mesoporous materials for organic and bioorganic synthesis” - 2012.
- rof. Poul Nissen, Ph.D. Department of Molecular Biology and Genetics, Centre for Membrane Pumps in Cells and Disease PUMPKIN - Aarhus University, Denmark, “Structural and functional studies of transmembrane transport proteins” - 2012.
- rof. Richard G. Weiss, Ph.D. Georgetown University, Washington, Department of Chemistry, “Simple molecules and simple chemistry yield complex materials through self-assembly” - 2012.
- r. Barbara Lonetti, Ph.D. Chargée de Recherche CNRS, Laboratoire des IMRCP, Université Paul Sabatier - Narbonne (France), “Liquid Crystals and Nanoparticles : a fruitful combination” - 2013.
- r. Nidhi Gour, Ph.D. University of Geneva, Switzerland, Department of Inhorganic and Analytical Chemistry, “Self-assembling Biomaterials” - 2013.
- r. Roman Polishchuk, Ph.D. Telethon Institute of Genetics and Medicine (TIGEM), “Pathogenesis of Wilson disease: From ATP7B trafficking to new therapeutic approaches” - 2013.
- rof Helmut Möewald, Ph.D. Max Plank Institute of Colloids and Interfaces, Potsdam-Golm (Germany), “Langmuir monolayers as physical models in bio- and nanosciences” - 2013.
- rof. Adrian R. Rennie, Materials Physics, Uppsala University, Sweden, “Understanding what molecules are doing in environmental processes: looking at materials with neutrons” - 2013.
- rof. Luis M. Liz-Marzan, Ph.D. Bionanoplasmonics Lab., San Sebastian (Spain), Ikerbasque, Basque Foundation for Science, Bilbao (Spain), Hybrid Nanomaterials for Plasmonic (Bio)Sensing” - 2013.
- rof. Stefan Stoll, Ph.D. University of Washington, Department of Chemistry, “Conformational transitions in proteins determined by DEER spectroscopy” - 2013.

Theses (undergraduate, master and PhD)

U.O. Bari

Bachelor in Chemistry (Laurea triennale)

- Inchingolo, A.V.: "Applicazioni di Microscopia a Scansione di Sonda su Sistemi Nanostrutturati e Biologici" (2012).
- Macchia, E.: "Dispositivi Bio-Elettronici: Realizzazione, Studio e Modeling" (2012).

Master in Chemistry of Materials (Laurea magistrale)

- Alberga, D.: "Modelli Molecolari per i Semiconduttori Polimerici P3HT e PBTTT" (2012).
- De Tullio, D.: "New Strategie to Improve EGOFET Biosensor Performance" (2012).
- Fucci, E.: "Nanomateriali per Sensori di Ossido di Azoto" (2012).

PhD in Materials Science and Technology

- Angione, M.D.: "Supramolecular Structures for Organic Electronic Devices" (2011).
- Crotone, S.: "Multilayer Structure of Biomolucules Immobilized on Organic Semiconductors for Advance Analytical Devices" (2011).

U.O. Bologna

Bachelor in Chemistry (Laurea triennale)

- Andergassen-Solva, P.: "Purificazione del core catalitico della DNA polimerasi III di Escherichia coli" (2012).

Master in Chemistry of Materials (Laurea magistrale)

- Caracausi, M.: "Costruzione di un sistema di co-espressione in Escherichia coli" (2012).
- Cimino, M.: "Costruzione di un sistema gnetico per l'isolamento di ceppi mutatori associati a mutanti del dominio PHP della DNA polimerasi III di Escherichia coli" (2012).
- Longanesi, L.: "Studio dei fenomeni aggregativi coinvolti nel processo di purificazione della variante della tossina difterica CRM197" (2012).
- Buglione, S.: "Problematiche connesse al processo di purificazione della variante della tossina difterica CRM197" (2011).
- Gratani, F.: "Analisi funzionale del dominio PHP della DNA polimerasi III di Escherichia coli" (2011).
- Landolfi, G.: " Sovraespressione e purificazione del core catalitico della DNA polimerasi III di Escherichia coli" (2011).
- Pellicani, B.: "Sintesi e caratterizzazione funzionale di acidi peptido-nucleici (PNAs)" (2011).

PhD in Materials Science and Technology

- Conte, E.: "Funzioni della subunità θ e del dominio PHP della subunità α nel core catalitico della DNA polimerasi III di Escherichia coli" (2012).

U.O. Cagliari

Bachelor in Chemistry (Laurea triennale)

- Serventi, F.: "Sistemi micellari per il restauro di pitture murali" (2013).
- Varotto, M.: "Studio degli effetti iono-specifici sulla Carica Superficiale della BSA" (2013).
- Carucci, C.: "Effetti iono-specifici sulla carica superficiale e la solubilità dell'emoglobina" (2011).

Master in Chemistry of Materials (Laurea magistrale)

- Cocco, G.M.: "Uno studio comparativo tra biodegradazione biomimetica ed enzimatica dell'idrogeno solforato" (2012).
- Loi, M.: "Studio comparativo delle polifenolo ossidasi estratte dai due chemotipi di Ferula communis L." (2012).
- Meli, V.: "Nanoparticelle cubiche fluorescenti per applicazioni in campo teranostico" (2012).
- Montaldo, N.P.: "Peptidi antimicrobici: una possibile risposta alla farmacoresistenza" (2012).
- Zucca, A.: "Preparazione e proprietà di un catalizzatore porfirinico biomimetico" (2012).
- Zurru, I.: " Caratterizzazione metabolica del lievito ambientale nitrofilo Sakaguchia dacryoidea" (2012).
- Trudu, M.: "Degradazione ossidativa biomimetica di reflui e scarti agroindustriali" (2011).

PhD in Materials Science and Technology

- Medda, L.: "Ion specific effects on charged interfaces" (2013).
- Carboni, M.: Nanostructures for protection and vehiculation of bioactive molecules" (2011).
- Cugia, F.: "DNA based biosensorfor envirnmental and medical applications" (2011).
- Hiwale, P.: "Smart nanostructured drug delivery systems based on non ionic surfactants" (2011).
- Lampis, S.: "Monoolein based cubic liquid crystals: specific interactions, evolution and applications" (2011).
- Zucca, P.: "Supported Metalloporphines As Novel and Bioinspired Ligninolytic Peroxidase–Like Catalysts". Doctor Europaeus (2011).

U.O. Campobasso

Bachelor in Chemistry (Laurea triennale)

- Passarella, S.: "Sviluppo di nuovo metodo estrattivo per la determinazione di pesticidi in prodotti apistici" (2013).

Master in Chemistry of Materials (Laurea magistrale)

- Di Matteo, N.: "Effetto degli antiossidanti naturali sull'ossidazione lipidica in sistemi mimetici di membrana" (2012).
- Mosca, J.: "Autocombustione e combustione dei prodotti alimentari nella valutazione dei rischi per la sicurezza industriale" (2012).
- Pomponio, A.: "Determinazione di acaricidi in prodotti apistici mediante tecniche ifenate" (2012).
- Sacco, P.: "Sviluppo di nanovettori per l'inclusione e veicolazione di molecole farmacologicamente attive" (2012).
- Oliva, D.: "Effetti degli antiossidanti e del metodo di cottura sulla formazione delle ammine eterocicliche aromatiche e del benzo(a)pirene nella carne cotta" (2011).

U.O. Catania

Bachelor in Chemistry (Laurea triennale)

- Spampinato, N.: "Adsorbimento di Laminina su superfici nanostrutturate" (2013).
- Calvagna, C.: "Processi di organizzazione di polietilenossido alle interfacce solide" (2012).
- Eredia, M.: "Processi di adsorbimento selettivo di proteine su superfici nanostrutturate" (2012).
- Franco, P.: "Sintesi e ancoraggio su superfici di derivati della rodamina B" (2012).
- Leanza, D.: "Spettrometria di massa di ioni secondari a tempo di volo (ToF-SIMS) per lo studio di sistemi polimerici complessi" (2012).
- Oddo, A.: "Proprietà elettriche di multistrati nanometrici polimero/metallo" (2012).
- Sorriso, G.: "Processi di Self-Assembly di peptidi anfifilici dipendenti da parametri di superficie" (2012).
- Tummino, A.: "Nanostrutturazione di superfici per eterogiunzioni in bulk" (2012).
- Cappello, E.: "Metodi di deposizione iterativa per nanostrati metallici ultrafat" (2011).
- Di Bari, I.: "Film di nanoparticelle auto-organizzanti all'interfaccia acqua/idrocarburo" (2011).
- Giuffrida, A.: "Struttura e proprietà di film ultrasottili di PCBM" (2011).
- Motta, V.: "Preparazione e caratterizzazione di superfici molecolari nano- e micro-strutturate" (2011).

Master in Chemistry of Materials (Laurea magistrale)

- Cappello, E.: "Funzionalizzazione e caratterizzazione chimico-fisica di superfici di ossidi con molecole fotoattive" (2013).
- Griffo, A.: "Studi chimico-fisici sulla struttura dei gel polimerici" (2013).
- Motta, V.: "Profili di profondità molecolari di multistrati polielettrolitici ottenuti mediante spin assembly" (2013).

- Rapisarda, A.: "Studio delle interazioni biomolecola-superfici mediante Localized Surface Plasmon Resonance (LSPR)" (2013).
- Squillaci, M.A.: "Studio delle proprietà elettriche di multistrati ibridi polimero/metallo" (2013).
- Cristaudo, V.: "Metodologie per l'ottenimento di profili di profondità di multistrati polimerici" (2012).
- Mannino, S.: "Miscele epossidiche complesse: influenza dei monomeri epossidici e del tenacizzante" (2012).
- Messina, A.: "Effetto del solvente sull'ordine molecolare di film sottili polimerici". (2012).
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U.O. Messina

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U.O. Napoli

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- Vassalini, I.: "Sintesi del metastannato di bario, BaSnO3. Descrizione e Confronto tra le metodologie di preparazione" (2011).

U.O. Siena

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- Boni, P.: "Liposomi come carriers per antiossidanti polifenolici" (2013).
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RESEARCH PROJECTS

1A – Visualization of lysozyme in Ordered Mesoporous Materials and effect of ionic strength on adsorption and release

A. Salis, D. Steri, M. Piras, M. Piludu, M. Monduzzi

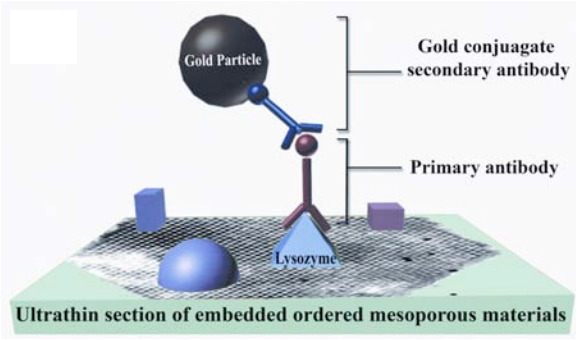
Aims

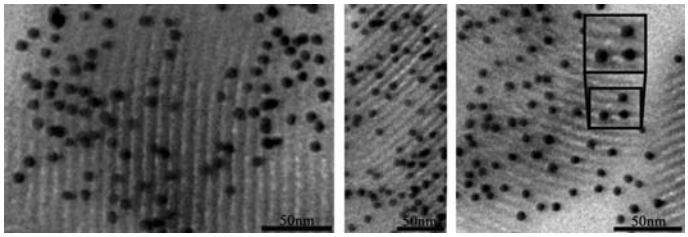
Protein adsorption on nanostructured silica. Immunogold staining. TEM characterization. Sustained Release.

Results

Ordered Mesoporous Materials (OMMs) have outstanding textural and structural features, such as high surface area, high pore volume, a highly ordered, and hence a highly reproducible structure, with uniform pore size. These peculiarities make them ideal hosts for proteins/enzymes and other bioactive molecules. This fact has led to a wide range of nanobiotechnological applications based on the immobilization of proteins/enzymes such as biocatalysis and biosensing. Innovative emerging applications are the use of OMMs in different nanomedicine topics as carriers for the sustained release of drugs and bioactive agents, and for tissue engineering. A huge number of papers have been devoted to protein adsorption onto ordered mesoporous materials. A key question concerns the location of proteins after adsorption. Available physico-chemical techniques of material characterisation (FTIR, BET, TGA) can give only indirect information on the presence of proteins adsorbed inside the pores of the material. To the best of our knowledge, no one has shown if the protein is effectively adsorbed on the internal pore surface of an OMM through a direct visualization method. Here we show, for the first time, the real location of human lysozyme protein molecules adsorbed onto SBA-15 mesoporous silica. This result was obtained by a suitable combination of an immunochemical technique that involves the post-embedding immunogold staining (IGS) and transmission electron microscopy (TEM). IGS is based on the use of colloidal gold particles conjugated to specific antibodies as markers against several cellular constituents (A). The advantages of this technique are the high resolution of the staining, its unmistakable signature that can easily be distinguished and observed by electron microscopy and its high detection level that allows the visualization of extremely low concentrations of the antigens. Samples of human Lysozyme loaded SBA-15 were embedded with LR Gold resin and cut in ultrathin sections, then two consecutive incubation steps of the sections with specific antibodies were carried out. First the incubation with the unlabelled primary antibody specific to Human Lysozyme protein was performed, and then secondary colloidal gold conjugated antibodies were added.

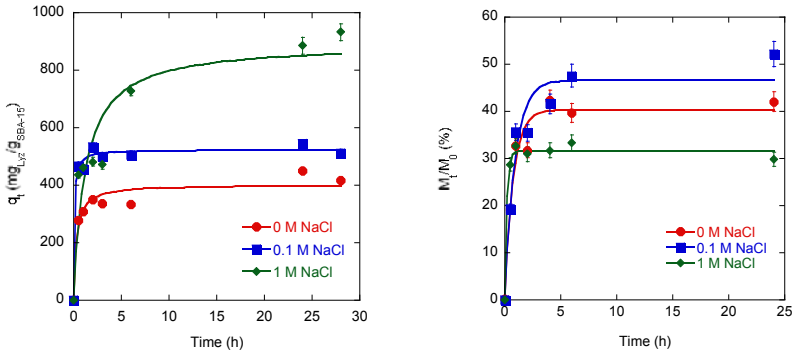
A





The samples were then observed and photographed by TEM (B). In the TEM micrographs the typical hexagonal array of the pores and cylindrical parallel channels of SBA-15 are clearly visible. Remarkably, each black spot can easily be associated to the presence of a Lysozyme molecule. The joined use of the IGS method and TEM gives evidence of the exact location of protein molecules on SBA-15 surface.

Then the effect of ionic strength on the adsorption and release of lysozyme as a model therapeutic protein from SBA-15 was investigated. The lysozyme adsorption kinetics on SBA-15 can be described through a pseudo-second order model or, alternatively, with an intraparticle diffusion model. The sustained release of lysozyme from SBA-15, carried out at 37°C in a buffer solution at the physiological pH (7.4) and salt concentration (0.15 M NaCl), was measured both in terms of released amount of protein and released enzymatic activity (not shown). We found that the ionic strength of the immobilizing solution strongly affects lysozyme adsorption (C) and release trends (D). These effects are likely due to the interaction of electrolytes with both the biological and the inorganic surfaces, which results in the modulation of the forces at the basis of adsorption and release processes.



These results show the importance of the adsorbing solution composition in modulating the adsorption and release kinetics. In the case of Lysozyme-SBA-15system, here examined, it can be concluded that the use of NaCl 0.1 M as the immobilizing solution is likely to represent the best compromise between adsorption and desorption (release) in terms of kinetic aspects, keeping into consideration also that enzymatic activity must be preserved at the possible highest level.

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1A – Synthesis, characterization and functional evaluation of light hydrides-based nanostructured composites for solid state H_2 storage (PRIN Project 2008)

C. Milanese, A. Girella, V. Berbenni, G. Bruni, A. Marini, S. Garroni, E. Napolitano*, S. Enzo*, G. Mulas**
*(*University of Sassari, Dept. of Chemistry and Pharmacy)*

Aims

Ideation and preparation of novel light hydrides-based composites for solid-state H_2 storage; evaluation of their sorption properties; determination of the thermodynamic and kinetics characteristics of the sorption reactions.

Results

In the frame of this PRIN project, started in 2009 and closed in 2012, many innovative composites for solid-state hydrogen storage have been ideated and tested, following the Reactive Hydride Composite (RHC) approach, that consists in mixing two or more high gravimetric capacity hydrides during the preparation step. Upon heating, an exothermic reaction between the components of the mixture takes place, lowering both the total desorption enthalpy of the composite and the desorption temperature (with respect to the pure hydrides). The other advantage of the approach is that the compounds obtained after desorption can be recharged at lower temperature and pressure with respect to the desorption products obtained by the pure hydrides, leading to a system closer to the practical applications targets. The most promising systems obtained during the research project are the binary $LiBH_4$ – MgH_2 and the ternary $LiBH_4$ – MgH_2 – $LiAlH_4$ composites. For both, for the first time in literature, a deep thermodynamic and kinetic investigation and a mechanistic study on the desorption mechanism have been made. The powders were prepared by high energy ball milling under Ar for 20 h and 30 h respectively with a ball to powder ratio of 10:1. Concerning the binary system, after the borohydride phase transformation and melting (well reported in literature at about 95 °C and 120 °C), two desorption steps are evident, corresponding to the two hydrides decomposition, taking place at 290 °C and 360 °C respectively. These temperature values are sensibly lower than those for the pure components. The coupled manometric – calorimetric analysis (Figure 1a) allowed to demonstrate the efficiency of the RHC approach: the desorption enthalpy of $LiBH_4$ decrease of more than 40 kJ/mol H_2 thanks to the MgH_2 presence (the value in the RHC is 54 kJ/mol). The total gravimetric capacity of the system is more than 9 wt %, i.e. compatible with practical applications. Concerning absorption, one only step, beginning at about 260 °C, is evident in the manometric measurements. The corresponding absorption enthalpy, measured for the first time in literature, is -40 kJ/mol H_2. Calorimetric measurements performed at different scanning rates allowed to obtain an absorption activation energy of 120 kJ/mol, i.e. considerably lower than the corresponding values for the pure hydrides (around 180 – 200 kJ/mol). The system exchanges hydrogen in a perfectly reversible way, with the absorption rate improving

from 18 h to obtain the full charge in the first cycle to less than 1 h in the subsequent runs. The desorption time scale is in the same range.
The milled system has been also encapsulated in high surface area matrices, such as C aerogel, in order to study the effect of nanoconfinement of the hydrides on their sorption properties. Encapsulation was made by both melting infiltration and wet chemical methods. Two strong effects on the sorption properties are evident with respect to the bulk material: desorption takes place in one only step and at temperature 50 °C lower. The reversibility of the system is still very good, but the gravimetric capacity falls to 3.5 wt % (the decrease of this parameter is due to the matrix "load").
Concerning the $LiBH_4$ – MgH_2 – $LiAlH_4$ ternary system, the sorption mechanism has been elucidated for the first time in literature thanks to the combination of the coupled calorimetric – manometric results (Figure 1b) and the in situ synchrotron X-Ray powders radiation analysis. The evolution of the reactions is quite complex and interesting: the first steps, taking place between 100 ° C and 200 °C, involve $LiAlH_4$ melting and decomposition to Li_3AlH_6, with the first H_2 release. Subsequently, this last phase decomposes, with hydrogen release and the formation of pure Al and LiH. Starting from 260 °C, after $LiBH_4$ melting, the MgH_2 dehydrogenation take places, with contextual formation of Mg_2Al_3 and $Mg_{17}Al_{12}$. Finally, at 320 °C, these last intermetallic compounds react with melted $LiBH_4$, leading to the formation of the ternary phase $Al_xMg_{1-x}B_2$. It is to note that, also in this case, the RHC approach is working: the desorption temperature of the three hydrides in the composite is consistently lower than for the pure ones (105 °C vs 120 °C for $LiAlH_4$, 260 °C vs 300 °C for MgH_2 and 320 °C vs 370 °C for $LiBH_4$).

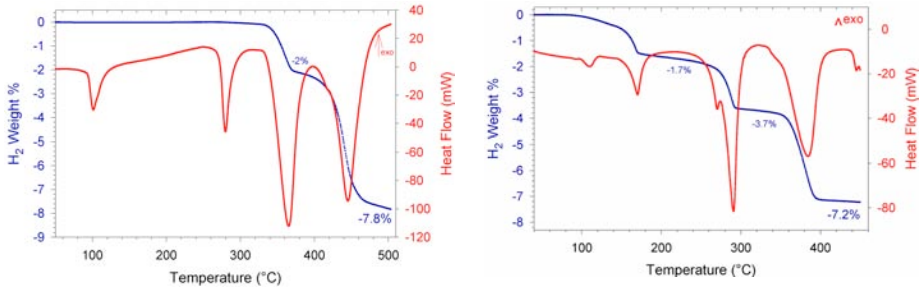

Figure 1: Coupled manometric – calorimetric measurements for the $LiBH_4$ – MgH_2 (left, a) and the $LiBH_4$ – MgH_2 – $LiAlH_4$ (right, b) systems.

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1A – The catalysed $LiBH_4$ – MgH_2 system for solid state hydrogen storage: from basic research to application scale (Vigoni-DAAD Project 2012-2013)

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Aims

Deep investigation on the H_2 sorption properties of the $LiBH_4$-MgH_2 reactive hydride composite; optimization of the properties by catalysing agents addition; pre-technological research on powders and pellets with increasing density; realization of the first RHC-based tank reported in literature.

Results

In the frame of this Vigoni-DAAD Project, funded by the Italian – German University and concerning the researchers exchange and travels, the attention was focused on the $LiBH_4$-MgH_2 system. This is the most promising RHC explored up to now in literature, thanks to its high gravimetric capacity (about 13 wt %) and full reversibility. First of all, the preparation procedures, (high-energy ball milling of the starting powders 2LiH-MgB_2 (molar ratio)), were optimized. The milling duration and balls to powder ratio leading to the best sorption performance were found as 20 h and 10:1 respectively (under Ar atmosphere). Subsequently, we tested different substances concerning their catalytic activity and $TiCl_3$ (5 mol %) gave the best results: after the first activation cycle, about 9 wt % of H_2 can be stored and released by the system in about half an hour on lab scale (300 °C; H_2 pressure = 15 bar for charging and 2 bar for discharging). For the first time in literature, the thermal conductivity and the specific heat C_P were measured for the system in both the charged and the discharged state. The thermal conductivity was measured also as a function of the temperature (from 25 °C to 200 °C, Figure 1) and the density of the samples.

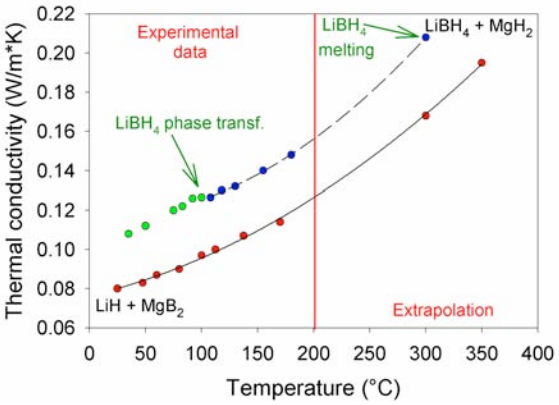

Figure 1: Thermal conductivity as a function of T for the charged and the discharged RHC system. Note, for the first one, the slope change due to $LiBH_4$ phase transition.

Pellets compacted at pressure increasing from 75 MPa to 600 MPa were cycled in the manometric instrument to investigate the influence of the density on the sorption properties. Differently from the powder sample, that was able to absorb the maximum hydrogen content already in the first charging step, even if with very slow kinetics, all the pellet samples need some activation cycles before reaching their highest gravimetric capacity (see Figure 2). Such a gravimetric capacity is the same of the corresponding powdered sample for all the pellets compacted at pressures up to 300 MPa, and the number of activation cycles increases with the compaction pressure up to 9. The sorption rates improve too, up to the values of the powdered samples. On the contrary, the pellets compacted at pressure higher than 300 MPa reach a maximum H_2 content of 3.5 wt % also after 10 sorption cycles. Scanning electron microscopy analysis performed on pellets compacted at 50 MPa, 300 MPa and 950 MPa after each of five activation cycles shows the formation of small cracks and a porosity increase (likely responsible of the improving in the sorption performance in the first cycles); however, the total break or changes in the cylindrical shape of the pellet have never been observed. This result is very interesting, considering that during desorption a liquid phase, i.e. $LiBH_4$, forms. This means that the Mg-containing phases, that remain always in the solid state at the working temperature of the system, form a sort of skeleton able to contain the Li based melting phase. By cycling, the changes in density and height of the pellets are very considerable, about 20 % decrease and 15 % increase of the starting values respectively. The changes in diameter of the pellets are about 4 times lower than those in height, according to the literature for the Mg/MgH_2 system.
The studies performed up to now allowed the realization of a tank containing 500 g of catalyzed powders, able to store 50 g of H_2: this is the first RHC-based tank for solid-state hydrogen storage reported in literature. Its overall gravimetric capacity is the same as on lab scale, and full reversibility is obtained. In the same working temperatures of the lab scale measurements, the sorption kinetics becomes a little bit worse (some hours are needed for full absorption and desorption). Work is in progress to optimize the working conditions of the tank to improve its sorption kinetics.

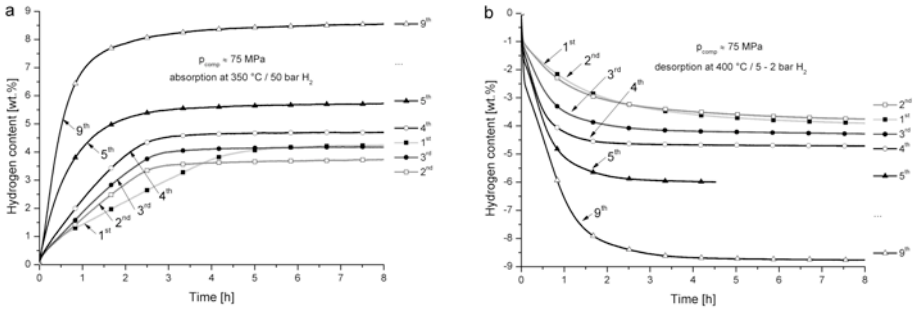

Figure 2: Absorption (a; T = 350 °C, starting H_2 pressure = 50 bar) and desorption (b; T = 350 °C, starting H_2 pressure = 2 bar) runs for the pellet prepared at 75 MPa.

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1A – Morphological characterization of nanosized Iron oxide particles

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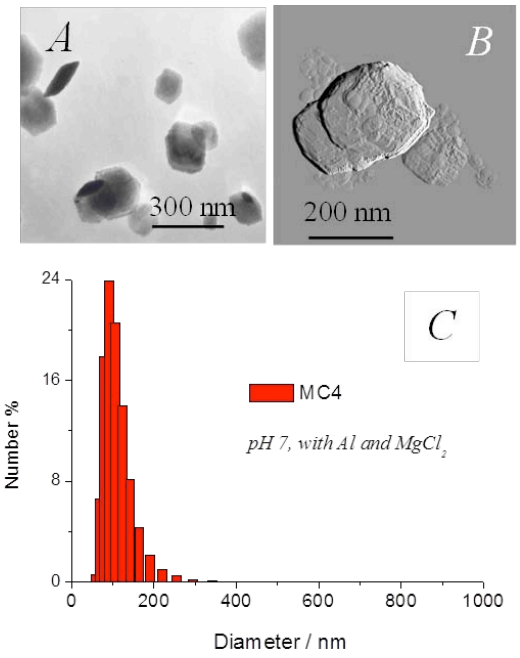
Aims

Iron oxides at submicron dimension show important applications in optics, electronics, magnetics, catalysis, nanosensor technology and biotechnology. In the present research project, we characterize the size and morphology of hematite (α-Fe_2O_3) nanoparticles using TEM, AFM and DLS techniques, and correlate the observed dimensional parameters with the synthesis conditions (type of salt used, aluminium substitution and pH). Moreover, we extend our investigation to the coprecipitation process of Fe(II) with humic acid (HA) and study its effect on Fe (hydr)oxide crystallinity.

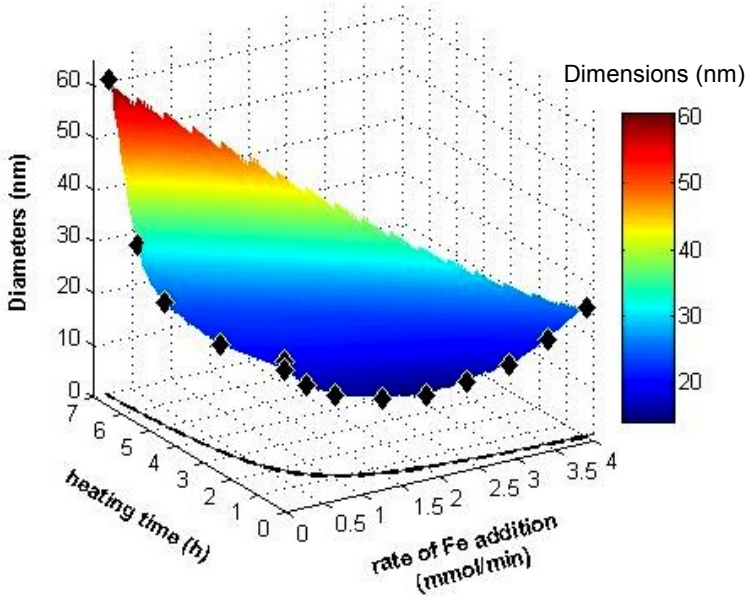
Results

For several types of synthetic hematites TEM images reveal large differences of morphological nature while AFM data provide accurate analyses of microstructure and surface roughness. These data should turn useful for a potential surface functionalization of iron oxide nanoparticles. Basically, DLS, AFM, and TEM techniques furnish complementary information on the average particle dimensions, whose variation could be attributed to the morphological difference of hematites, ranging from platy to regular or irregular hexagonal or ellipsoidal shape. On the right are illustrated data for a sample of hematite synthetized by aging ferrihydrite at pH 7.0 and at 371 K in presence of $MgCl_2$ and aluminum. Representative TEM (**A**) and AFM (**B**) micrographs of the hematite sample. (**C**) The number distribution of aggregate size obtained from DLS is described by a mean peak diameter of 107 nm and a narrow width of distribution of 33 nm.



Considering the influence of the reaction conditions on the average dimensions of

nanoparticles, it has been assessed that high rates of iron(III) nitrate addition coupled with short heating times represent the most favorable experimental conditions to produce 14-16 nm sized nanocrystals. This is better appreciated if we consider the 3D graph shown below where the mean diameters measured with DLS (Z-axis) are plotted as a function of the rate of iron(III) addition expressed in mmol/min (X-axis) and the heating time in hours (Y-axis).



Finally, several types of ferrihydrite-HA complexes have been synthetized through coprecipitation using leonardite at room temperature and pH 7 to explore a possible effect of organic matter on the morphology of iron nanophases.
TEM images show irregular subangular macroparticles with sponge-like structure, as an intermediate characteristic from ferrihydrite-coprecipitate products and iron-humic complex substances, with rough or irregular surfaces rounded by very small rounded particles.

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1A – Hydrogels for bone and tooth remineralization: synthesis, characterization and potential evaluation

P. Tempesti, G. Nicotera, M. Bonini, E. Fratini, F. Ridi, P. Baglioni

Aims

Synthesis of hydrogels embedding inorganic micro- and nanoparticles. Characterization by means of FEG-SEM, SAXS, DSC, DLS and AFM. Investigation of remineralization potential on tooth and bone specimens.

Results

We synthesized different hydrogels embedded with calcium and strontium-based micro- and nanoparticles, such as amorphous calcium phosphate (ACP), calcium hydroxyapatite (HAP) and strontium-doped hydroxyapatite (Sr-HAP). We aimed at developing a responsive nanocomposite material able to favour the remineralization process under specific conditions. We used poly(n-isopropylacrylamide) (PNIPAAm) and poly(acrylic acid)-poly(acrylamide) (PAA-PAAm) as the organic matrix. Both PNIPAAm and PAA-PAAm hydrogels exhibit unique reversible swollen-shrunk phase transitions triggered by changes in temperature (PNIPAAm) or pH (PAA-PAAm). PNIPAAm was synthesized using n-isopropylacrylamide as monomer and N,N-methylene-bisacrylamide as cross-linker. Different amounts of HAP (0.3 – 3.6 % w/w) were added during the polymerization process in order to assess the maximum concentration which could be uploaded without significantly modify the hydrogel structure.

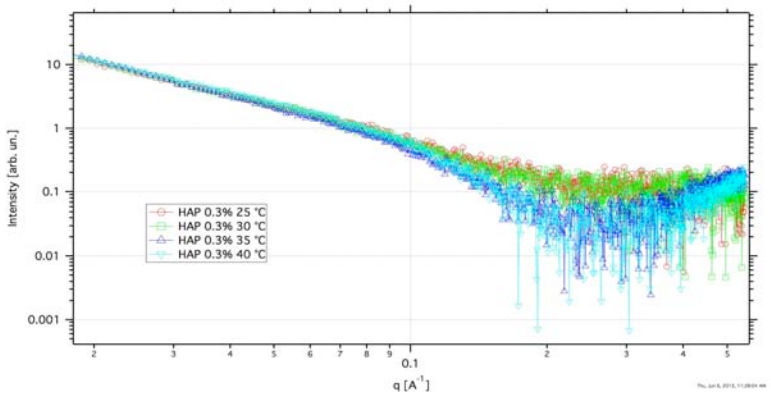

Figure 1: SAXS curves of a PNIPAM-HAP hydrogel collected at different temperatures.

The analysis of SAXS curves obtained at different temperatures (Figure 1) and DSC scans (not shown) highlighted the presence of a phase transition occurs at about 32°C. Figure 2 shows the macroscopical morphological changes occurring to the samples when from room temperature (A) they are heated above the phase transition (B) and cooled back to room temperature (C).

Figure 2: PNIPAM hydrogels with increasing HAP content going left to right at A) 20 °C, B) after heating at 50 °C and C) cooled from 50 °C to 20 °C.

The effect of the temperature during the synthesis on the hydrogel structure was investigated by performing the polymerization at 20 °C and at 50 °C. Figure 3 reports an example of the different structures as shown by FEG-SEM micrographs (examples reported in Figure 3).

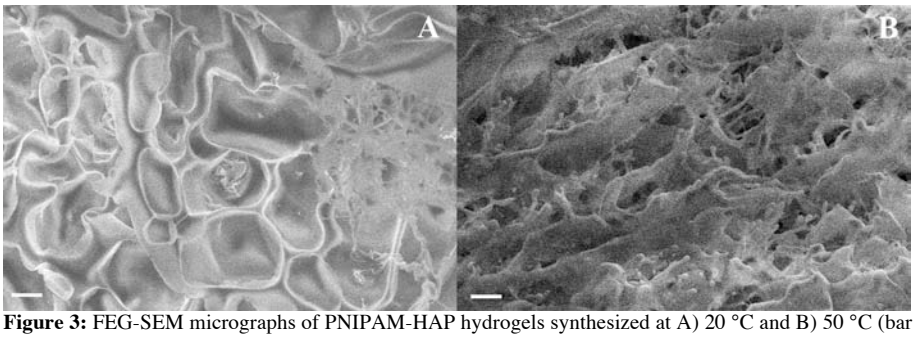

Figure 3: FEG-SEM micrographs of PNIPAM-HAP hydrogels synthesized at A) 20 °C and B) 50 °C (bar = 2 μm).

For PAA-PAAm gels a different approach was used. Aiming at obtaining different pore size distributions, ethylene glycol dimethacrylate and poly (ethylene glycol dimethacrylates) with 2 to 10 ethylene glycol units were investigated as cross-linkers for the synthesis of the poly(acrylamide) hydrogel. Longer chain cross-linkers provided better results for our purposes. The macroporosity of the poly(acrylamide) gel was controlled by adding monodisperse poly(methylmethacrylate) microparticles to the reaction mixture and eventually selectively dissolving them with dichloromethane after the polymerization.

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1A – Nanostructures for white-emitting OLED devices

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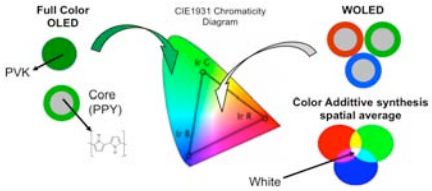
Aims

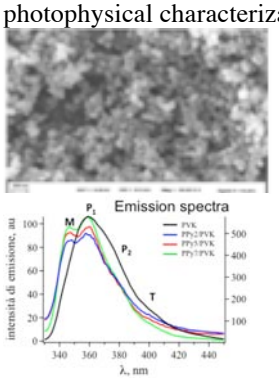
Design and realization of both single color and white-light emitting organic devices where dopant molecules are organized in conducting polymer nanostructures. Phosphorescent Organic Light Emitting Devices (PhOLED) composed of poly(9-vinylcarbazole) (PVK) nanostructures doped with Iridium(III) complexes emitting in the red, green and blue region of the visible spectrum. Single component polymeric nanoparticles as well as two-components core-shell systems doped with light-emitting iridium(III) complexes were prepared. Arrays of these nanostructures were assembled and characterized.

Results

Research on new fabrication procedures of phosphorescent nanomaterials revealed the leading role of nanofabrication on rigid and flexible surfaces. We realized Phosphorescent Organic Light Emitting Devices (PhOLED)composed of poly(9-vinylcarbazole) (PVK) nanostructures doped with Iridium(III) complexes emitting in the red, green and blue region of the visible spectrum.We employed two different kinds of nanostructured systems: PVK nanoparticles (NPs) and core–shell nanoparticles where a shell of PVK surrounds the surface of highly polypyrrole (PPy) NPs.

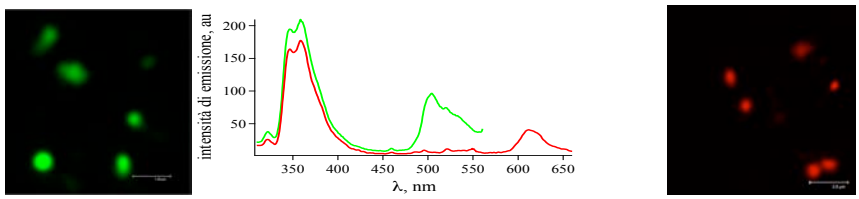


The rationale for the construction of the proposed nanodevices is reported above. Successful doping of the PVK NPs and of the PVK shell surrounding the PPY nanoparticles with Ir(III) complexes was obtained by the re-precipitation method as shown by a combination of different techniques, i.e. particle sizing, AFM, SEM and photophysical characterization of the system.

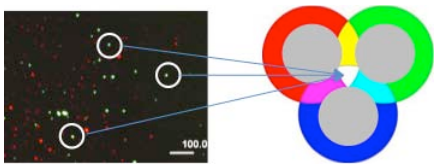


The results showed that the dimensions and morphology of the nanoparticles correlate with the experimental paramters used, i.e. choice of surfactant and reaction temperature, as well as the structure and concentration of the specific Iridium complex used. The carbazole moiety in PVK NP is mailnly in the excimeric form (P_i + T), with ground-state aggregates. Conversely, in core-shell PPY/PVK nanoparticles PVK in the outer shell adopts an extended conformation with monomeric carbazole units and excited state aggregates (M+P_i+T).

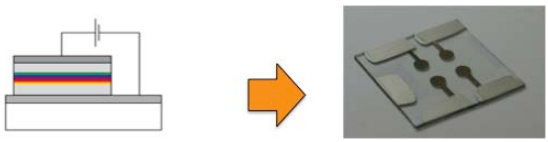
The photophysical characterization of the PVK/Ir NPs demonstrated that an energy transfer process between PVK and the Iridium complexes takes place both in aqueous suspension and after deposition of the nanostructures onto solid supports. Steady-state and time resolved fluorescence spectroscopy evidenced that energy transfer occurs in all cases but with efficiencies that depend on the concentration and geometry of the excimeric form of the fluorophore in the polymeric chain and thence on the polymer conformation.



Co-localization of the different Ir complexes in the NP system was obtained with two different procedures: incorporation of a balanced mixture of the complexes in the same NP shell or construction of single color nanoparticles further combined and closely immobilized onto a ITO covered flexible sheet.
Confocal Laser Scanning Microscopy allowed for the collection of the emission fingerprint on selected domains of the NP shell and, more importantly, showed that light-excitation of these systems resulted in the production of light with colors that followed the expected additive sinthesys rules in spatial average.



Immobilization of the emitting nanoparticles in a single layer was obtained by sedimentation, spin-coating and drop-casting techniques. Spin-Coating of nanoparticles on the PEDOT/PS/ITO slides resulted in poor and heterogeneous coverage of the surface whereas drop casting techniques allowed for efficient deposition of arrays of polymeric emitters. Proper choice of the RGB ratio of the monochromatic NP resulted in the fabrication of prototypes of produces white light Pholed.



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1A – Nanofabrication of polymer capsules arrays for third generation solar cells

G. Caminati, P. Baglioni, M. Banchelli

Aims

Fabrication of novel Graetzel-inspired nanoarchitectures based on mesoporous structures of hollow polymeric nanocapsules containing Ruthenium complexes as donor together with a fullerene derivative (NC60) selected as electron acceptor.

Results

Demand for new photovoltaic systems for the realization of low-cost solar cells in the near future has prompted the research for new technological solutions in the nanometer scale. One of the most studied III generation devices for the conversion of light into electrical energy is the dye-sensitized solar cell (DSSC) [Fig. 1].
We preliminary studied different LbL sequences of the selected polyelectrolytes on planar supports by means of QCM-Z experiments controlling the incorporation of both the donor and the acceptor in different positions of the layer sequence. Selected sequences were reproduced on $CaCO_3$ inorganic nanoparticles (NPs) with the redox couple immobilized in the PAH/PSS polyelectrolyte shell. Dissolution of the NPs core resulted in empty nanocapsules bearing the donors and the acceptor in different corona layers. The resulting nanocapsules were eventually deposited onto ITO covered surface to obtain a mesoporous array of polymer capsules as shown in figure 1.

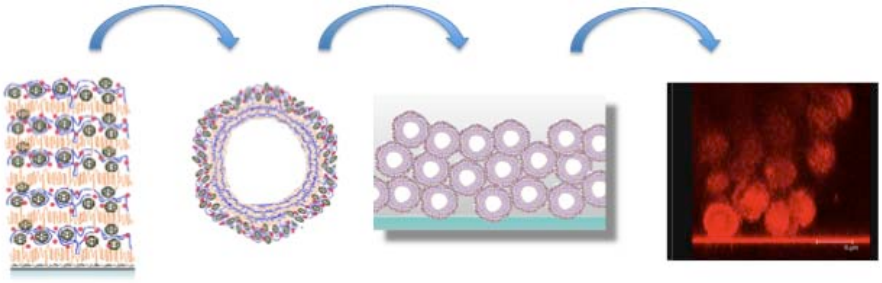

Fig. 1: Design and components of the proposed nanostructured solar cell.

Distribution of the donor and acceptor molecules on the capsule surface was monitored by zeta-potential and photophysical measurements. The results showed a peculiar dependence on NC60 concentration correlated to high propensity to nanocapsules aggregation. A critical threshold concentration of NC60 was found for the different donor/acceptor sequences studied as shown in fig. 2 (left).
Interestingly, the photophysical behaviour was found to strictly depend on the position of the acceptor along the polymeric sequence and thence on the aggregation of the nanocapsules.

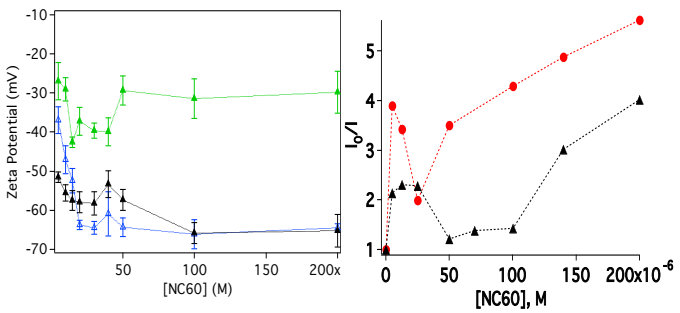

Fig. 2: (Left) Zeta potential behaviour for NC_{60} solution (blue), microcapsule/ acceptor (black) and microcapsule/ acceptor/ donor (green) system. (Right) Stern-Volmer plot for the decrease of fluorescence intensity in microcapsule/ acceptor (black) and microcapsule/ acceptor/ donor (red) system.

Combined AFM and Confocal Laser Scanning Microscopy provided information on the dimensions and morphology of the nanocapsule systems as a function of the shell thickness and surface charge, the study supported nanocapsules aggregation behaviour when the acceptor was located in the outer layer as shown in figure 3 (a and b).

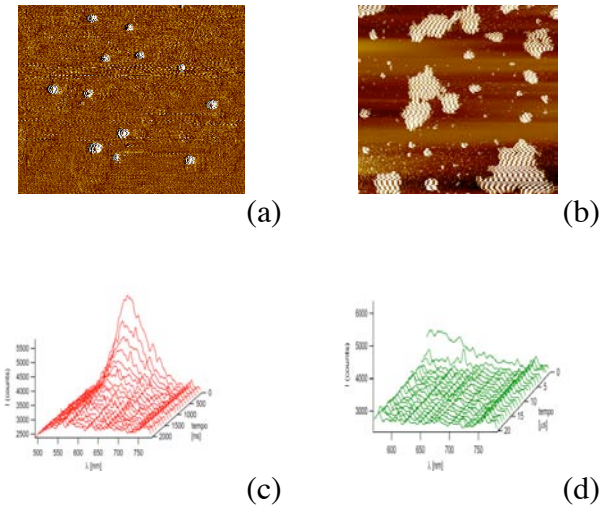

Fig. 3: AFM images and time-resolved fluorescence spectra as a function of NC60 for microcapsule/ acceptor/ donor system (a and c) and microcapsule/ acceptor (b and d) system.

Steady-state and time-resolved fluorescence investigation showed that efficient vectorial photoinduced electron transfer occurs between the donor and the acceptor in all cases but with different efficiencies that depend on the acceptor position in the layer sequence.

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1A – Nanosensors based on ultrathin films

G. Caminati, P. Baglioni, M.R. Martina

Aims

Design of nanosensors for early diagnostics of proteins involved in degenerative amyloidosis. New molecular devices for sensor applications by means of different nanotechniques tailored to meet the specific requirements of several detection systems. Hybrid architectures formed by a combination of Supported Lipid Bilayers (SLB), Langmuir-Blodgett (LB), Self-Assembly (SA) and Layer-by-Layer (LbL) systems as immobilizing scaffolds for protein ligands. Biomimetic systems for ligand delivery in the therapeutic stage.

Results

FK-506 binding protein (FKBP12) is a protein of the family of immunophilins, involved in many neurodegenerative diseases such as Alzheimer's syndrome where FKBP12 is known to be over-expressed in early stages of the disease. We designed and built phospholipid Langmuir-Blodgett films as well as Supported Lipid Bilayers incorporating ligands with high affinity for FKBP12, i.e. Tacrolimus (FK506) and Rifaximin, to detect low FKBP12 concentration in the initial phase of the amyloidosis. Several phospholipid nanoarchitectures differing in lipid composition, fluidity, number of layers and method of production (incubation versus co-spreading in the case of LB films) were screened.

Both ligands were successfully incorporated in the phospholipid scaffold although with different procedures. UV-Vis absorption and fluorescence spectra (see Fig. 1) for one DPPG LB layer incubated in Rfx solution unambiguously evidence the inclusion of the ligand in the nanolayer. Conversely, for z-type DPPG film, incubation with Rfx induces only a minor increase in the absorption and emission signal compared to 1 LB layer, suggesting a preferential localization of the ligand in the outer layer of the LB films.

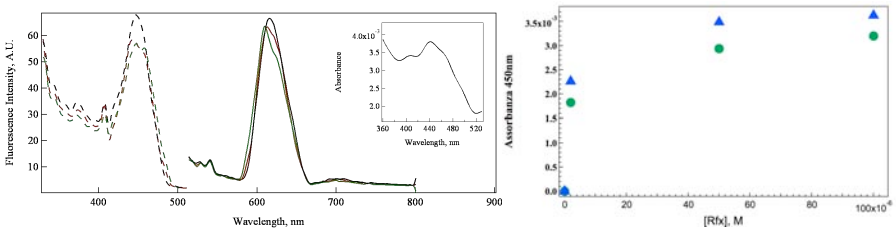

Fig. 1: Left. UV-Vis absorption (inset), fluorescence excitation (dotted line) and emission (solid line) spectra of DPPG LB incubated in Rfx= $1x10^{-5}$M (red), $0.8x10^{-5}$M (green), $1x10^{-6}$M (black). Right. Absorbance versus Rfx concentration for incubated 1 (green) or 2 (blue) layer LB film.

Co-spreading experiments for FK506 in monolayers of a DPPC/POPG (8:2) mixture result in efficient inclusion of the ligand as shown from the spreading isotherms and penetration studies as a function of FK506 concentration in the monolayer subphase (Fig.2). The specific FK506 emission band at 330 nm (see inset Fig. 2) confirms the presence of the ligand in the LB scaffolds.

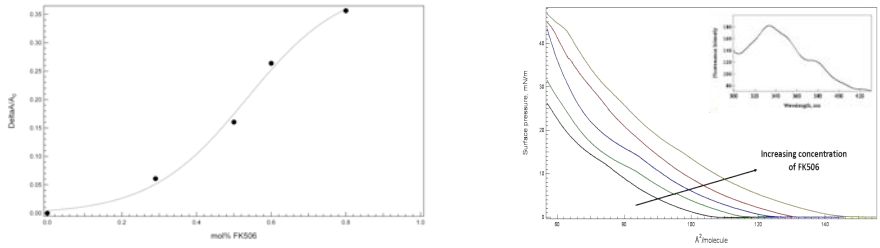

Fig. 2: Left. Change in the mean molecular area ($\Delta A/A_0$) of DPPC/POPG 8:2 monolayers with increasing concentration of FK506. Right. Spreading isotherms of pure DPPC/POPG 8:2 (black) and in presence of increasing concentration of FK506. Inset: fluorescence emission spectrum of FK506 in 1LB layer.

FKBP12-ligands interactions in the LB nanolayers were assessed from fluorescence quenching experiments Typical results for 1 LB layer (Fig. 3), show an efficient fluorescence quenching of FKBP12 fluorescence with both ligands. Higher quenching was found for the Rfx ligand, a result likely related to the larger ligand concentration obtained with the incubation procedure.

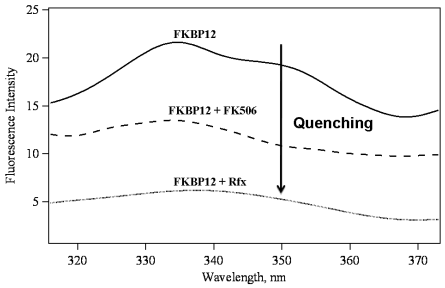

Fig. 3: Fluorescence emission spectra of FKBP12+Ligand free LB (solid line), FKBP12+LB/FK506 (dashed line) obtained by co-spreading and FKBP12 LB/Rfx (dotted line) obtained by incubation with ligand. FKBP12= 1μM.

The ligands were proved to insert quantitatively also in phospholipid liposomes, we therefore designed and fabricated a nanosensor device where the ligand is immobilized in a solid Supported Lipid Bilayer (SLB) formed by liposomes fusion on the QCM quartz slide. QCM sensors covered with SLB/FK506 system allows for the determination of traces of the protein in buffered solution by means of ligand-mediated binding of FKBP12 to the surface of the SLB. These results pave the way to design of phospholipid liposomal formulation for drug delivery as well as sensitive and specific nanosensors for FKBP12 for the early diagnosis of neurodegenerative amyloidosis. Studies of functionalized synthetic ligands with surface-anchors and suitable spacers are currently in progress for the preparation of chemically modified surfaces that can be directly coupled to sensing device for FKBP12.

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1A – Protein aggregation and misfolding at phospholipid monolayer/water interface

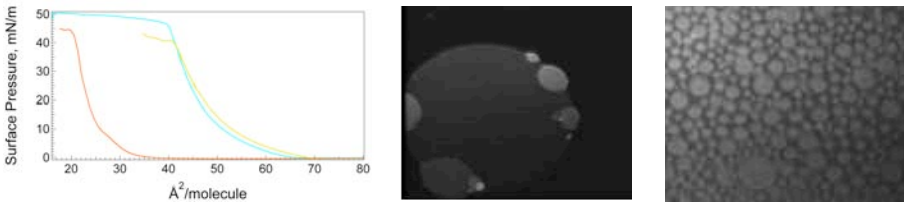
M.R. Martina, P. Baglioni, G. Caminati

Aims

Correlation between raft-like domains in membrane models and promotion of protein misfolding followed by formation of amyloid-like structures.

Results

The interactions between biomolecules and phospholipid membranes are recognized as a key topic to understand biological complexity with special emphasis on the role of lateral phase separation that produce transient domains, known as lipid raft. Increasing scientific reports evidence the implication of these domains in pathologically relevant phenomena. A vast number of severe neurodegenerative disorders including Parkinson's and Alzheimer's diseases are currently associated with the deposits of insoluble protein aggregates (amyloid fibrils). We investigated different models of cell membrane with different radii of curvature and composition to ascertain whether externally induced curvature changes may drive the lateral organization of the membrane components. The results suggest that all investigated biomimetic systems give comparable information although they can be studied by complementary techniques. In particular, we focused on planar membrane models, i.e. Langmuir monolayers, where direct visualization of the phase domains, flanked by the thermodynamic and spectroscopic characterization, is easily accomplished.
We reproduced and characterized lipid rafts for mixed phospholipid monolayers of DSPC/DOPC/Cholesterol at the water-air interface by means of surface-pressure area isotherms and Brewster Angle Microscopy as a function of monolayer composition and temperature.

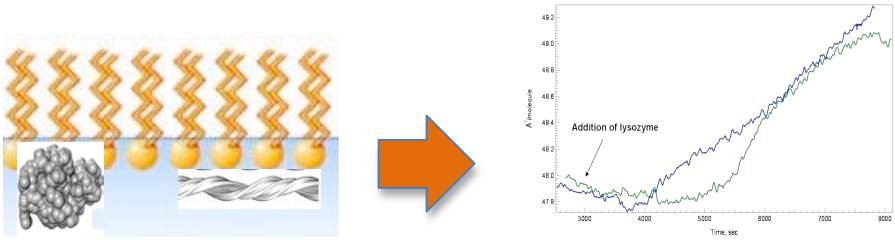


(a) (b) (c)

Fig. 1: (a) Spreading isotherm of DSPC/DOPC/Chol mixed monolayers of different composition exhibiting phase separations: small domains (blue, image b), large domains (yellow, image c), single phase (orange).

Furthermore, the same techniques were adopted to investigate the interaction of a water-soluble protein at the monolayer interface. Lysozyme was selected as model protein since lysozyme misfolding and pre-amyloid fibril-like aggregation was recently shown to occur at phospholipid liposome interface.

Native as well as preliminary fibrillated lysozyme was injected in the subphase under the phospholipid monolayer at selected lipid composition, temperature and surface pressure. Lysozyme insertion was studied for homogeneous expanded phases of the monolayer as well as in the presence of raft-like domains. For both native and fibrillated lysozyme, we observed that the protein is adsorbed at the monolayer/water interface but with different kinetics and mechanism.



BAM microscopy showed that the adsorbed lysozyme segregates along the border of the condensed domains eventually forcing a transition from a circular to a polygonal structure of the domains as shown in figure 2.

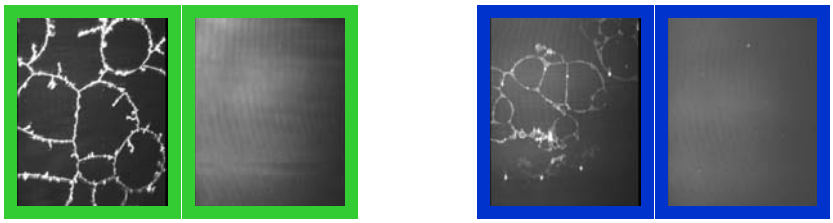
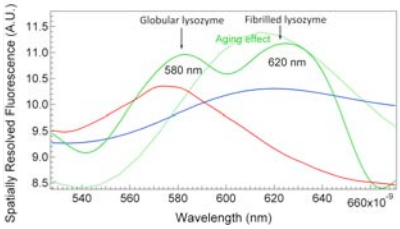


Fig. 2: BAM pictures of a DSPC/CHOL/DOPC monolayer of after addition of lysozyme in the subphase. Green: addition of globular lysozyme, Blue: addition of pre-fibrillated lysozyme.. Images b and d : addition of lysozyme to single phase monolayer.

Transfer of the monolayer/lysozyme system onto solid support allowed to characterize the resulting protein structure by means of circular dichroism and FT-IR/ATR spectroscopy that evidenced the presence of the characteristic features of β-sheet units also for the globular form after interaction with the raft-domains in the monolayer. Spatially resolved fluorescent spectra were collected by means of Confocal Laser Scanning Microscopy after staining of the monolayer/lysozyme film with Congo Red (CR).



The measurements evidenced the typical emission spectra of CR intercalated in β-sheet structures for all systems thus indicating the presence of aggregates enriched in β-structure providing direct evidence for the involvement of lipid rafts in amyloidogenic processes.

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1A – Design, synthesis and applications of new organic sensitizers for non-conventional photovoltaic cells

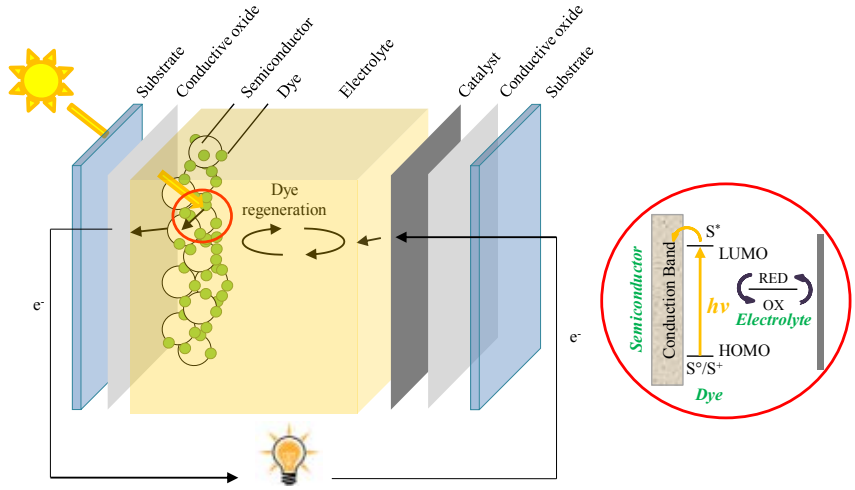
M.L. Parisi, A. Sinicropi, S. Maranghi, M. Taddei, R. Basosi

Aims

The aim of the project is the design, computational characterization and synthesis of new organic dyes for the production of Grätzel-type solar cells, along with the environmental assessment of their photovoltaic performances trough life cycle analysis.

Results

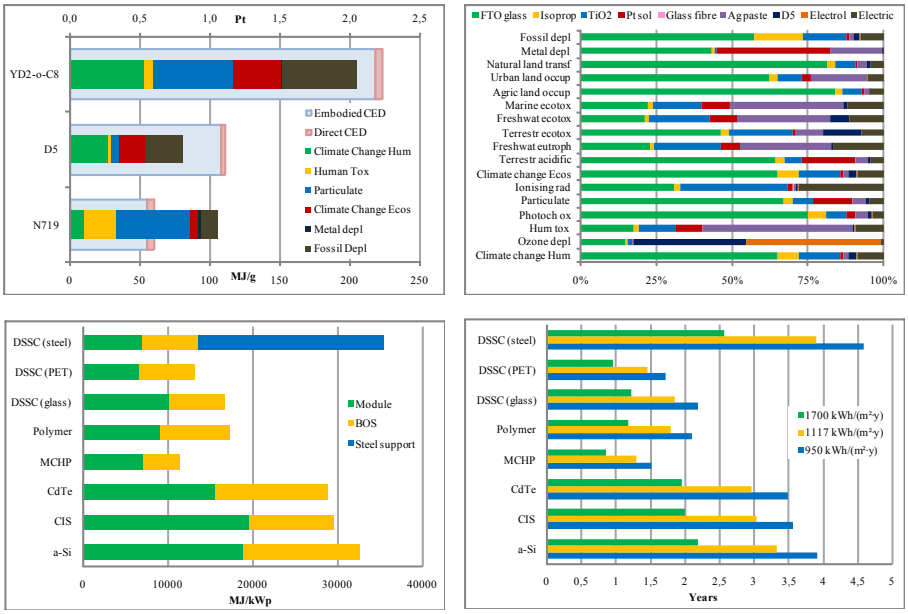
Since the pioneering work published by Grätzel and O'Reagan on the first efficiently assembled dye-sensitized solar cell (DSSC) in 1991, the research activity on photovoltaic cells based on hybrid sensitizer/nanocrystalline semiconductor systems has undergone some major developments. This present project is based on a multidisciplinary approach for the production of new organic dye sensitizers for DSSCs that could result to be competitive in comparison with the already available solar systems. This approach takes benefit from the synergic employment of state-of-the-art computational methods and innovative eco-compatible synthetic strategies that together with the spectro-, photo- and electrochemical characterization of the synthesized compounds allows the development of an accurate protocol for the design



and investigation of organic sensitizers to be employed in photovoltaic cells.

A life cycle analysis of the production process of each components of a solar cell has to be performed in order to achieve a systematic and in-depth assessment of environmental impacts and burdens (in energetic and pollution terms) deriving from

all input flows, and to highlight the critical points and hot spots of the process itself. Such an evaluation represents the starting point to draw a detailed eco-profile of innovative technologies. Major outcomes from the project are pivotal in understanding the environmental dynamics, the benefits and drawbacks associated with the



production of DSSCs in comparison with other photovoltaic crystalline silicon and other thin film technologies.

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1A – Nanostructured Magnesium Silicate Hydrates (M-S-H): new environmentally sustainable cements

G. Ferraro, E. Fratini, F. Ridi, P. Baglioni

Aims

Synthesis of a pure phase of magnesium silicate hydrates $(MgO)_x$-SiO_2-$(H2O)_y$ (shortly M-S-H). Study of chemical composition, morphology and microstructure as a function of the Mg/Ca ratio.

Results

According to recent studies[1], MgO-based cement can be obtained by a production process, which involves low CO_2 emissions. The main binding agent is M-S-H. The pure phase was prepared through a synthesis in solution starting from magnesium nitrate and sodium metasilicate[2]. A mixed sample with Ca/Mg target ratio 1:1 was also prepared to investigate the compatibility of both magnesium and calcium silicate hydrates. X-ray Diffraction (XRD) evidenced that M-S-H is mainly composed by Lizardite ($Mg_3SiO_5(OH)_4$) while C-S-H peaks are mainly due to Tobermorite ($Ca_5(Si_6O_{16}(OH)_2)\cdot 4(H_2O)$) crystalline structure. Fourier Transform Infrared Spectroscopy (FT-IR) signals and Mg/Si (or Ca/Si) ratios measured with Electron Dispersive Spectroscopy (EDS) analysis are in agreement with the presence of both these minerals. Differential Scanning Calorimetry (DSC) shows for M-S-H a characteristic peak centered at -40°C. This is due to the crystallization of the water confined in Small Gel Pores (pores with entrances of about 1-3 nm) [3]. The same measurements performed on the C-S-H sample show no peaks at -40°C probably because this system have a less porous structure. At the submicron level, M-S-H samples show an irregular porosity consisting of interconnected and densely packed globules (diameter between 30 and 40 nm) (Figure 1A). The C-S-H sample exhibited a leafy or sheet shape in a dense, laminar pattern (Figure 1B).

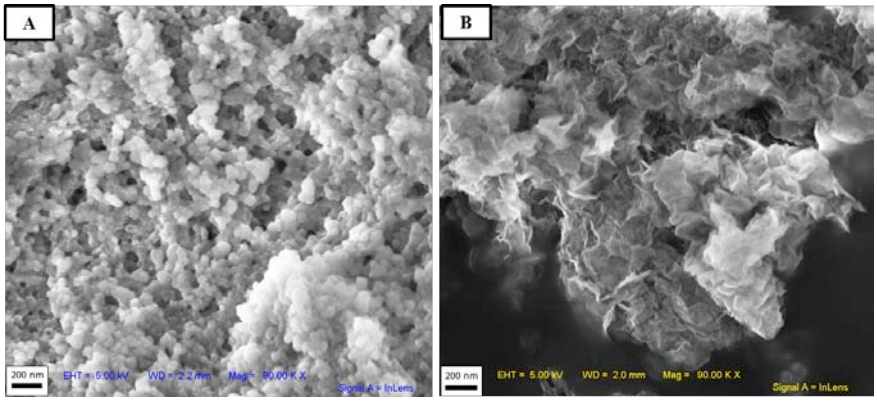

Fig. 1: SEM image of M-S-H (A) and C-S-H (B) at magnification 90 K. Scale bar is 200 nm.

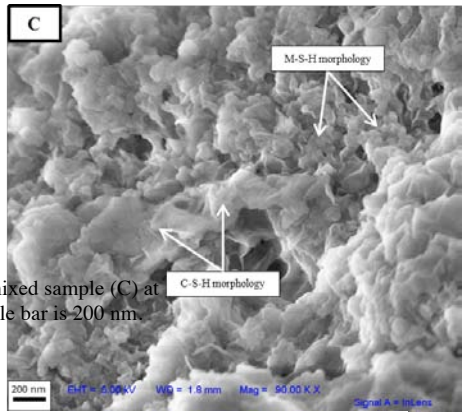

Fig. 2: SEM image of mixed sample (C) at magnification 90 K. Scale bar is 200 nm.

The mixed sample shows regions with typical M-S-H structure alternate to other regions with the C-S-H morphology (see Figure 2). Small Angle X-ray Scattering (SAXS) was performed to have information on the nano-structure of the samples. The results (see Figure 3) reveal that the magnesium and calcium silicate hydrates present subunits in the nanometer range as supposed in the Colloidal Model [3]. The subunit of the M-S-H sample has a diameter of 1.5 nm and aggregates in fractal objects with a mass fractal dimension between 2 and 3.

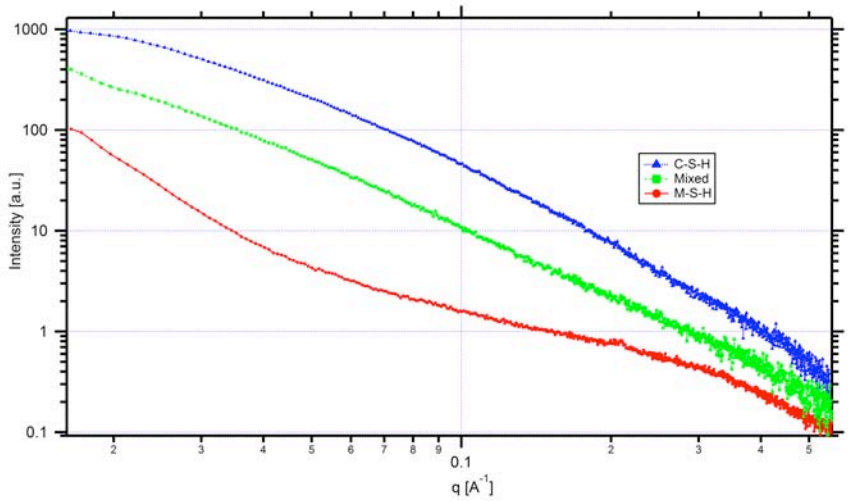

Fig. 3: SAXS curves associated to M-S-H, C-S-H and mixed.

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1A – Relaxation dynamics in polyoxomolybdate species

E. Fratini, A. Faraone (NIST), A. Müller (U. Bielefeld), P. Baglioni

Aims

Relaxation dynamics of hydration water, confined water and the inorganic cage in the case of three different polyprotic inorganic acids (i.e. nanocages): $\{Mo_{72}X_{30}\}$ (X=Fe, Cr, V).

Results

The dynamics of the nanocages (see figure 1), characterized by their isododecahedron shape and nanometer size, was investigated using neutron scattering.

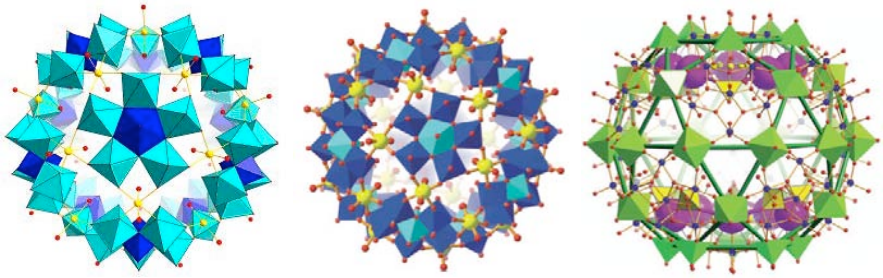
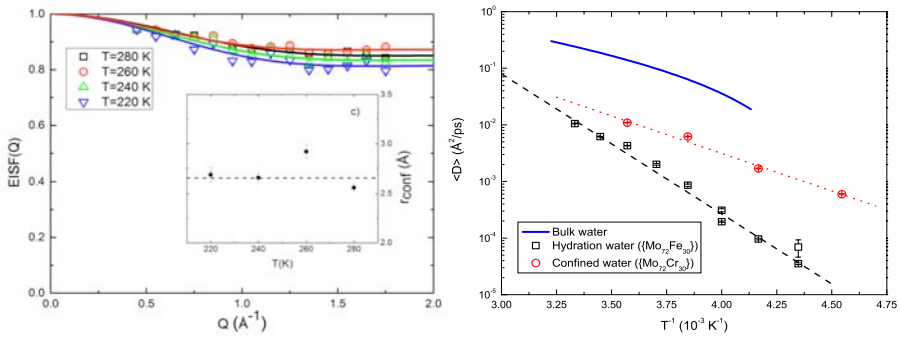


Fig. 1: Combined polyhedral and ball-and-stick representation of the structure of: Left) $\{Mo_{72}Fe_{30}\}$ Center) $\{Mo_{72}Cr_{30}\}$ and Right) $\{Mo_{72}V_{30}\}$ nanocapsules.

In the $\{Mo_{72}Cr_{30}\}$ sample both the relaxation dynamics of the methyl groups located inside the nanocage cavity, as well as that of the water molecules confined within it were studied. Due to the presence of these acetate groups, the cavity represents a unique hydrophobic subnanometer scale confining system for the water molecules. The CH_3 rotational dynamics is characterized by elevated activation energy comparable to the values found for methyl group rotations in the solid state. The dynamics of the water molecules confined within the cage follows the Volino-Dianoux model (scattering law of a system confined in a spherical potential well) with an in-cage diffusion coefficient and an activation energy similar to that of water hydrating oxide nanoparticles. The overall dynamics of the water molecules is much slower than that of bulk water and is qualitatively different as bulk water has a strong non-Arrhenius behavior (see figure 2). The breaking of the hydrogen bonds linking together the water molecules within the cavity is the most likely process activating the confined diffusive motion. Finally, using a hydrogenated and a partially deuterated $\{Mo_{72}V_{30}\}$ sample, a nanocage, which has not any methyl groups, the vibrational dynamics of the cage itself was studied. The motions of the atoms within the cage are harmonic. The mean square displacement of the atoms is of the order of ≈ 1 Å^2 around room temperature. Together with our previous publication [2] on the dynamics of water confined in the voids between $\{Mo_{72}Fe_{30}\}$ nanocages, these evidences provide a

rather complete picture of the single particle dynamics of the atoms in these systems relevant for their possible application in catalysis and as model systems. In this respect, the investigation of the water molecules confined within the hydrophobic



cavity of $\{Mo_{72}Cr_{30}\}$ is particularly relevant because of the interest for the behavior of water in contact with hydrophobic surfaces.

Fig. 2: Left) The Q dependence of the EISF at the four temperatures investigated for a dry $\{Mo_{72}Cr_{30}\}$ sample. Inset) Temperature dependence of the confinement radius. Right) Arrhenius plot of the diffusion coefficient of water hydrating $\{Mo_{72}Fe_{30}\}$ (squares) and confined within $\{Mo_{72}Cr_{30}\}$ (circles). The continuous blue line represents the diffusion coefficient of bulk water measured by NMR.

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1A – C-S-H gel nanostructure

E. Fratini, F. Ridi, S.H. Chen (MIT), P. Baglioni

Aims

Derive a detailed nanoscopic description of the globular primary units and relative clusters in cement based materials.

Results

We have synthesized a series of pure C–S–H (I) gels with three different water contents. Small-angle neutron scattering analysis indicates that C–S–H gel is more likely to be consisted of globules, whose dimensions are dependent on the total water content. A rigorous analytic model was derived taking into account the intraglobule structure factor ⟨P(Q)⟩orientation and the interglobule structure factor S(Q). The globules are basically disk-like objects consisting of alternate water and calcium silicate layers. The globules are packed in a fractal structure with a cutoff size of about 70 nm and a fractal dimension D of about 2.65.

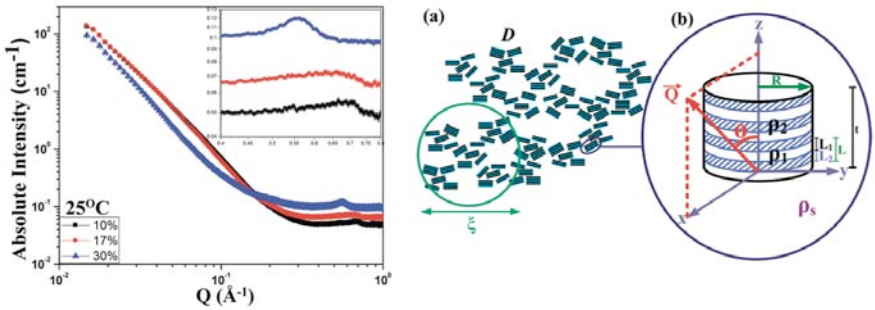
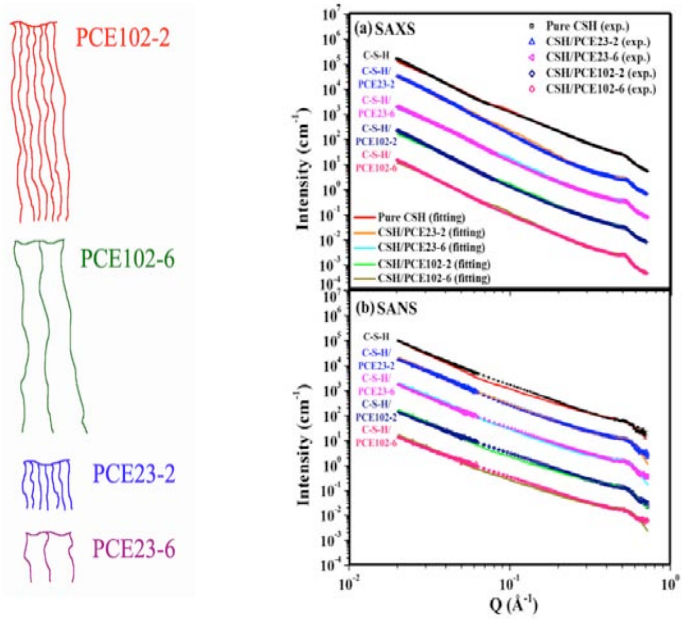


Fig. 1: Left) SANS curve of a pure synthetic phase of C-S-H. Right) Graphical description of the analytic model adopted for the fitting of the SANS data.

The developed model was applied to the investigation of the effect of comb-shaped polycarboxylic ethers (PCEs) with controlled molecular architectures on the microstructure and nanostructure of the synthesized C-S-H gel using the combination of SAXS and SANS techniques (see Figure 2). The combined data analysis gives additional fitting conditions to extract the structural parameters accurately. PCE additives can enhance the local stacking of the calcium silicate sheets by increasing the average number of repeating layers in the globules, which further pack into more open fractal-like structures in the range of a few hundred nanometers. The layer thickness of a globule is not significantly affected by the PCEs added. This is a clear proof of the lack of any intercalation phenomena in the C-S-H/PCE systems, in contrast to what is usually found in Al-rich phases. The investigation in the micrometer range evidences that the PCEs depress the fibril formation characteristic of the C-S-H phase in favor of a foil-like morphology, which is more compact and interconnected. The pastes containing PCE23-6, PCE102-6 and PCE23-2, which have higher adsorption propensity toward the calcium silicate phase, result more abundant in amorphous regions, showing less extended foils. A recent collaboration with the

group of M. Geppi (UNIPI) highlighted a linear correlation between the mean silicate chain length and the globule dimension in the C-S-H/PCE systems. [3] These findings are fundamental for understanding the effect of superplasticizers at a microscopic



level. In the future, this enhanced understanding could allow a fine tuning of the structure and mechanical properties of C-S-H, and in turn those of cement.

Fig. 2: Left) Molecular structure of the different PCEs investigated in this study. Right) Evolution of the (a) SAXS (b) SANS curves and relative fits as a function of the PCE added.

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1A – Rational design of gold nanoparticles functionalized with carboranes for application in Boron Neutron Capture Therapy

L. Ciani, S. Bortolussi, I. Postuma, L. Cansolino, C. Ferrari, L. Panza, S. Altieri, S. Ristori

Aims

Bottom-up approach to obtain new boron carriers built with ortho-carborane functionalized gold nanoparticles (GNPs) for applications in Boron Neutron Capture Therapy (BNCT).

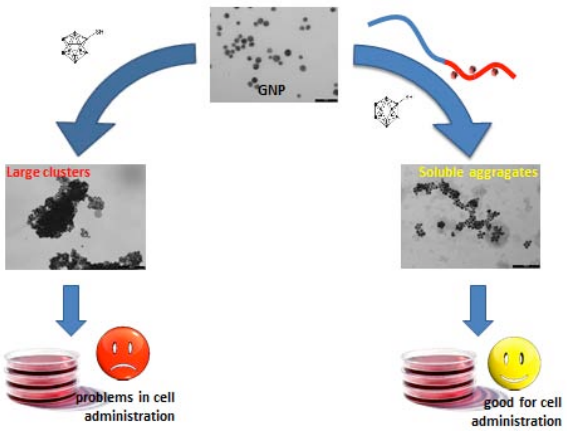
Results

One of the open questions of BNCT is the possibility to know the biodistribution and concentration of ^{10}B immediately before irradiation with neutron. These information are essential to set the treatment planning, i.e. the irradiation configuration and time, to optimize the dosimetry and the outcome of the therapy. In clinical practice radiotherapists infer the parameters needed for these calculations from the boron concentration measured in the blood stream. However, it is known that the real biodistribution and accumulation ability of tumor tissues are case-specific and should be treated accordingly. This is the same concern that underlines theranostic, a discipline combining imaging and therapeutic functions into one platform.

Nanomaterials engineered with multiple functions have great potentiality to solve the problem of locating drugs and performing treatment with a single agent. Among possible materials to be used for theranostics, gold nanoparticles have reached a "gold standard" position. In fact, they have been used for imaging, diagnosing and treating diseases. GNPs show peculiar physico-chemical properties such as surface plasmon resonance in the visible or near infrared region (the so called therapeutic window) and can be easily functionalized through bonding with thiol, amine or carboxylic groups. The absorbance in nanoscale gold particles is much stronger than in the bulk material and can be easily tuned by changing size and morphology.

So far, metallic nanoparticles have been scarcely used as vectors for boronated compounds in BNCT. This is probably due to the intrinsic difficulty of combining high boron uptake, water solubility and biocompatibility in the resulting formulation.

In this paper we propose a bottom up approach to design a new boron carrier, namely ortho-carborane functionalized GNPs. One or two thiol groups were



used to anchor the carborane cage on the gold surface in the effort of carrying a large quantity of boron atoms per single vector. A further step in this work was to increase the water solubility of carboranes functionalized GNPs and allow their safe use in biological test. For this purpose we chose an appropriately tailored diblock copolymer PEO-b-PCL bearing carborane pendants groups. Block copolymers of this type are known to enhance compatibility with biological fluids and show low protein adhesion. They were loaded onto the already functionalized AuGNPs by exploiting the attractive interactions which exist among carborane cages.

GNPs functionalization was followed through spectroscopic (UV-Vis and FTIR) and microscopy (TEM) techniques. It was found that in the case of carboranes bearing only one SH group, the clusters of nanoparticles formed in water were efficiently disrupted, allowing the administration of boron carriers with acceptable size (100-200 nm).

Overall, these composites show very good biocompatibility and high boron accumulation into osteosarcoma cells, which is encouraging evidenced to pursue applications in vivo.

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1B – Monoolein-based nanocarriers for drug delivery and imaging applications

S. Murgia, S. Lampis, M. Carboni, V. Meli, R. Angelico, M. Monduzzi

Aims

Preparation and characterization of cationic vesicles based on monoolein and lauroycholine chloride for topical drug delivery.
Preparation and characterization of monoolein based cubosomes doped with fluorescent probes for single living cell imaging.

Results

A novel cationic liposome nanocarrier, having interesting performance in topical drug delivery, is here presented and evaluated for its features. Two penetration enhancers, namely monoolein and lauroylcholine chloride, are combined to rapidly formulate (15 min) a cationic liposome nanostructure endowed of excellent stability (> 6 months) and skin penetration ability, along with low short-term cytotoxicity, as evaluated via the MTT test. Cytotoxicity tests and lipid droplet analysis give a strong indication that monoolein and lauroylcholine synergistically endanger long-term cells viability. The physicochemical features, investigated through SAXS, DLS, and cryo-TEM techniques, reveal that the nanostructure is retained after loading with diclofenac in its acid (hydrophobic) form. The drug release performances are studied using intact newborn pig skin.
Analysis of the different skin strata proves that the drug mainly accumulates into the viable epidermis with almost no deposition into the derma. Indeed, the
flux of the drug across the skin is exceptionally low, with only 1% release after 24 h. These results validate the use of this novel formulation for topical drug release when the delivery to the systemic circulation should be avoided.
Vesicle-based gel composed of monoolein and lauroylcholine chloride were also prepared and characterized. A number of vesicular formulations were prepared, in the range of 4–14 wt% of the dispersed phase, to investigate the system evolution from a dilute uni-lamellar vesicle dispersion to a vesicle lipid gel. Morphology, thermal stability up to 55 °C, and viscoelastic properties, along with the effect of acid diclofenac inclusion within the formulation, were evaluated by cryo-TEM, SAXS, and rheological measurements. Moreover, the nanostructure of the vesicle dispersion obtained upon gel dilution in water was assessed by cryo-TEM and SAXS, while DLS was used to monitor the formulation stability (size and z-potential). All the collected results lead to the conclusion that this new vesicle-based gel displays all the requirements needed for application in the pharmaceutical and cosmetic fields.

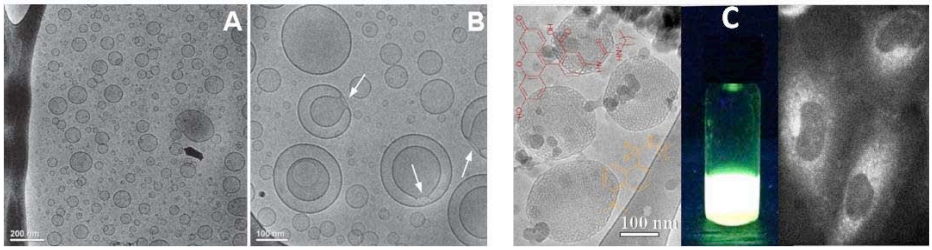

Fig. 1: Cryo-TEM images of (A) unilamellar, (B) bilamellar liposomes and cubosomes (C) doped with fluorescent probes.

The second type of monoolein-based nanocarrier consist of cubosomes doped with two fluorescent probes, namely, fluorescein and dansyl, properly modified with a hydrocarbon chain to increase their encapsulation efficiency within the monoolein palisade. The same nanocarriers were also loaded with quercetin, a hydrophobic molecule with potential anticancer activity. Particularly, the cubosomes doped with the modified fluorescein probe were successfully exploited for single living cell imaging. The physicochemical and photophysical characterizations, along with the well-known ability of cubosomes in hosting molecules with pharmaceutical interest, strongly encourage the use of these innovative fluorescent nanocarriers for theranostic purposes.

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1B – Soft matter for smart drug delivery systems

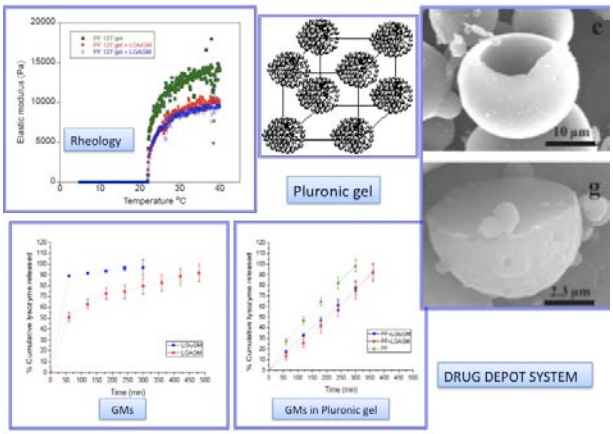
M. Monduzzi, S. Murgia, S. Lampis, R. Angelico, G. Colafemmina, G. Palazzo

Aims

Different kinds of surfactants were investigated for the phase behavior to prepare some innovative drug delivery systems

Results

A first work (1) was aimed to evaluate the microstructure and the performance of gelatin microspheres (GMs) cross-linked by two different crosslinkers viz. D-glucose and glutaraldehyde. New formulations were obtained, suspending the GMs in a thermoreversible Pluronic F127 (PF127) liquid crystalline gel. Lysozyme was used as a model biomacromolecular drug to evaluate release features. The lysozyme-loaded microspheres were characterized by scanning electron microscopy (SEM) for size distribution, shape, and surface texture. SEM revealed that both types of lysozyme-loaded GMs were spherical in shape and that the surface of glutaraldehyde cross-linked GMs was smoother than that of the glucose cross-linked GMs as shown in the Figure below. The in vitro release of lysozyme from both types of cross-linked GMs was successfully controlled when they were suspended in PF127 gel (a discrete cubic phase), thus suggesting the potential use of this new combined formulation as a drug-depot system.



A work in collaboration with a pharmaceutical group (2) focused on how composition and preparation method of Phospholipon-50 based vesicles affects their morphological features and delivery performances. Penetration Enhancer-containing Vesicles, PEVs, vesicles containing a water miscible penetration enhancer (Transcutol- P) and encapsulating sodium diclofenac, were formulated and compared with conventional liposomes.

The variations in vesicle structure, bilayer thickness, and number of lamellae were assessed by TEM and SAXS-WAXS. Interestingly, results showed that multi- and unilamellar vesicles provided improved diclofenac delivery to pig skin, whereas PEVs enhance drug transport by penetrating intact the stratum corneum, thanks to a synergic effect of vesicles and penetration enhancer.

A work in collaboration with Pharmaness explored the possibility to prepare solid lipid nanoparticles (SLP) for the delivery of hydrophobic drugs, using lipid based warm microemulsions (wμe). To this aim the lecithin(LCT)/water(W)/tripalmitin(TP) /1-butanol(B)/taurocholate sodium salt (ST) phase behavior at 70 ◦C was investigated. The LCT/B weight ratio, the replacement of 1-butanol with different alcohols, and the addition of ST at different LCT/ST weight ratios. The microstructure of the isotropic phase region obtained in the presence of ST was characterized by both ^{1}H NMR PGSE measurements and conductivity.

The results highlight the relevance of the microstructural characteristic of wμe to achieve SLNs with average diameter in the order of 100–200 nm and narrow size distribution.

Another work in collaboration with Pharmaness focused on the commercial non-ionic surfactant Solutol-HS15 phase behavior in water and on the possibility to solubilize Δ9-tetrahydrocannabinol. It was found that the cannabinoid molecules become entrapped within the surfactant hydrophobic tails, thus increasing the surfactant effective packing parameter and inducing a radical change of the micelle shape. At sufficiently low water content (18–35 wt.%), such alteration of the interfacial packing results in a lamellar organization of the surfactant molecules.

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1B – Hofmeister effects at the polar interface of Triton X-100 micelles

S. Murgia, G. Palazzo, M. Monduzzi

Aims

Specific anion effects according to Hofmeister series occur also in micellar systems formed by non ionic surfactants

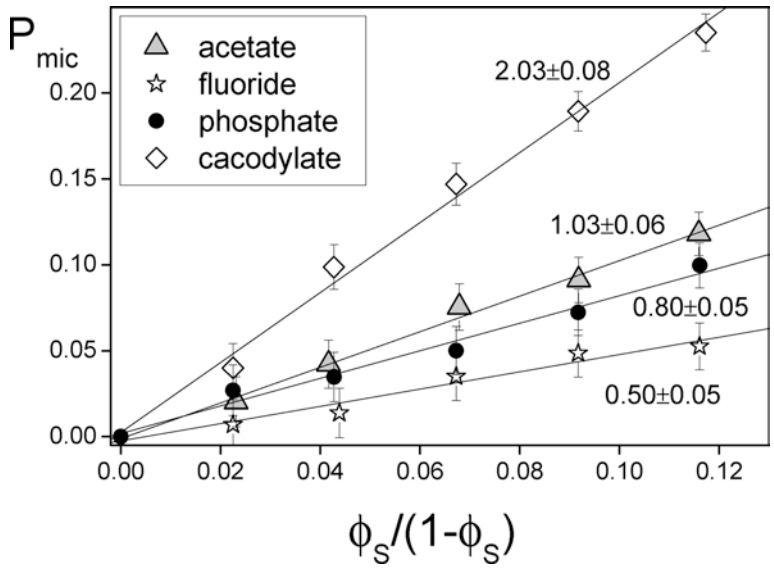
Results

Anion binding to nonionic micelles was quantified by selfdiffusion. Four anions were probed by multinuclear PGSTE NMR measurements in a Triton X-100 micellar aqueous solution. The salt concentration used was sufficiently low to avoid any micellar growth affecting surface curvature. The micellar aggregates that provide a model surface are uncharged with hydrophilic headgroups so that electrostatic ion surface interactions play little or no role in prescribing specific anion binding. Anionic affinity to the micellar surface followed a Hofmeister series:

$(CH_3)_2AsO_2^- \gg CH_3COO^- > H_2PO_4^- > F^-$.

The observed ion specificity is rationalized by calling into play the nonelectrostatic interactions occurring between the anions and the micellar surface.

Binding, expressed in terms of P_{mic}, depends on the surfactant volume fraction fS as shown in the figure below where the slope values obtained from linear regression represent the partition constants of the different anions between the bound and free states.



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1B – Ionic liquids and phase behavior

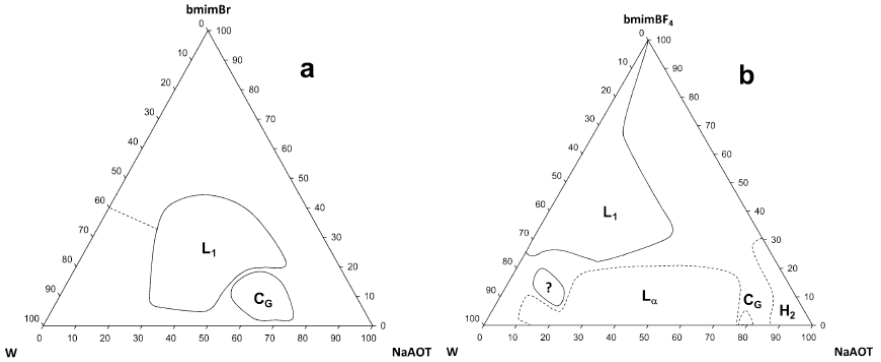
S. Murgia, G. Palazzo, S. Lampis, F. Lopez, M. Monduzzi

Aims

Ionic Liquids peculiar features are worthy to be explored at a molecular level either for their self-assembly characteristics or for the interactions with surfactant systems.

Results

A recent investigation on the sodium bis(2-ethylhexyl)sulfosuccinate/water/1-butyl-3-methylimidazolium tetrafluoborate (NaAOT/W/bmimBF_4) system showed that the anionic two-tailed surfactant NaAOT, that is known to form reverse micelles or planar interfaces (typically lamellar liquid crystals), can originate discrete spherical micelles of normal curvature because of strong interactions with the ionic liquid. The goal of the present paper was to detect macro- and microscopic modifications within such a system upon substitution of the ionic liquid's counter-ion tetrafluoroborate with



bromide. Firstly, the phase diagram of the NaAOT/water/bmimBr system was determined. Then, the monophasic regions were investigated by means of NMR self-diffusion and SAXRD experiments. The results obtained proved this system to be surprisingly different from that containing the similar Ionic Liquid (IL) bmimBF_4. The study focused mainly on the characterization of the micellar region, which turned out to be constituted of a bicontinuous nanostructure. This finding can be accounted for suggesting a decreasing of the NaAOT effective surfactant packing parameter, as in the case of NaAOT/water/bmimBF_4 system, although the effect in the presence of Br^- is less pronounced. Data modeling showed the same degree of interfacial adsorption for the $bmim^+$ cation in both systems, regardless of the particular counterion used, either BF_4^- or Br^-. Thus, the remarkable differences between the two systems, as shown in the Figure below, appear to be mainly due to a specific counterion effect. This result highlights once again the ions specificity, which is found ubiquitously in chemistry and biology.

In order to understand the role of the IL in addressing NaAOT phase behavior, it seemed important to highlight some peculiar aspects of ionic liquid self assembly in water, which is still a matter of wide debate. The whole water /1-butyl-3-methyl imidazolium ($bmim^+$) tetrafluoborate (BF_4^-) phase diagram was thoroughly re-investigated, at a molecular level, by means of ^1H and ^{19}F NMR PGSTE and ^{11}B NMR relaxation experiments performed at room temperature. The analysis of H_2O, $bmim^+$ and BF_4^- ions self-diffusion coefficients and the ^{11}B NMR relaxation times revealed that ion-pair dissociation is a progressive process starting at a H_2O molar fraction equal to 0.2 and ending at high water content. More importantly, the collected results indicate that H_2O and ions diffuse within different domains, strongly suggesting that the system under investigation is actually nanostructured. This fact agrees with some other recent works focusing on the possible mesoscopic order that ionic liquids possess when dissolved in water because of their hydrophobic tail segregation.

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1B – Stimuli responsive polyelectrolyte nanocapsules

F. Cuomo, F. Lopez, A. Ceglie, B. Lindman (Physical Chemistry, Lund Univ., Sweden), M.G. Miguel (Dept. Quimica, Coimbra University, Portugal)

Aims

Production of polyelectrolyte capsules with nanometer dimension bearing stimuli-responsive properties.

Results

Polymer capsules have been assembled by applying the Layer by Layer (LbL) deposition procedure onto cationic liposomes made of lecithin and didodecyldimethylammonium bromide (DDAB). Core-shell structures and hollow capsules with seven or eight layer of polyelectrolyte were produced and characterized by means of Dynamic Light Scattering, ζ potential, and SEM. The polyelectrolyte used were the alginate and the chitosan. The produced nanocapsules were sensitive to pH changes of the environment because of the behaviour of the polyelectrolytes composing the multishell walls; in fact they exhibit variations in size depending from the pH of the bulk solution. The nanocapsules having chitosan as outer layer are stable only at acidic pH, nanocapsules having alginate as outer layer remain stable at all the pHs used in this study (pH 4.6 to 8). The pH-optimum for the shrinking event is in the acidic range. The role of both the polymers in the shrinking/swelling event is demonstrated by comparing nanocapsule populations with alginate (7 layers) or chitosan (8 layers) as the outer layer.

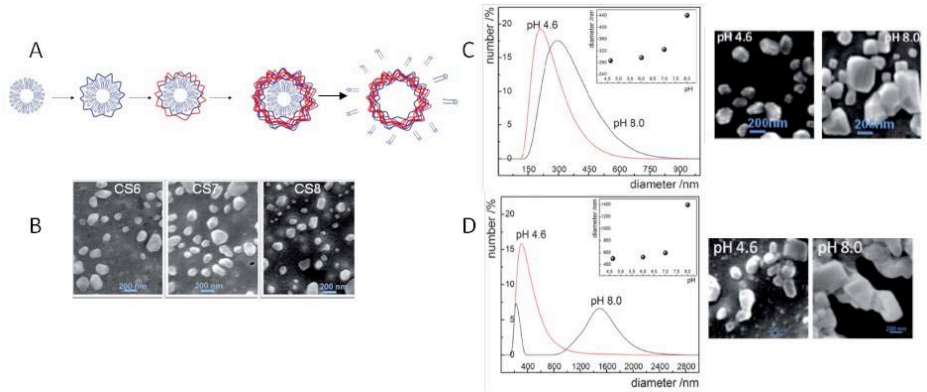

Fig. (A): LbL deposition and core removal scheme. **(B):** SEM photographs of core-shell assemblies with 6, 7 and 8 layers (CS6, CS7, CS8 respectively). **(C):** Size distributions of hollow capsules with 7 layers at pH 4.8 (red line) and 8.0 (black line). In the inset the capsule size as a function of pH is illustrated. The SEM photographs show the size of the capsules at pH 4.6 and 8.0. **(D):** Size distributions of hollow capsules with 8 layers at pH 4.8 (red line) and 8.0 (black line). In the inset the capsule size as a function of pH is illustrated. The SEM photographs show the size of the capsules at pH 4.6 and 8.0.

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1B – Network connectivity in physical gels.

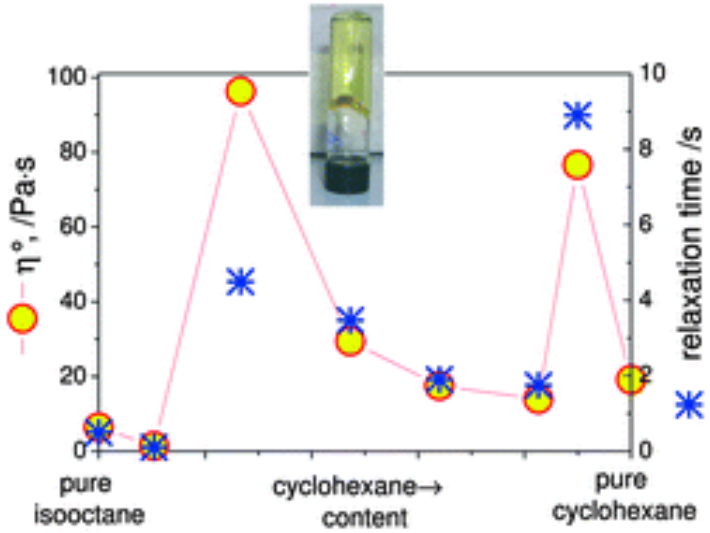
R. Angelico, A. Ceglie, S. Murgia, M. Monduzzi, G. Palazzo, U. Olsson (Chemical Center, Lund University, Sweden)

Aims

The goal of the present project is to investigate the effect of inter-micellar connections (branches) on the rheology of long and flexible self-assembled wormlike micelles.

Results

Lecithin and water self-assemble into wormlike reverse micelles that can be branched or unbranched depending on the oil composition (and on the water content). In this respect, cyclohexane favours disconnected reverse micelles while isooctane promotes the formation of branches. By using mixtures of cyclohexane and isooctane as the oil phase and different water/lecithin ratios, the branch density of the system can be finely tuned. PGSE-NMR experiments allowed us to distinguish between branch-free (unbranched) and branched systems and the response of the very same samples to mechanical stress was measured by rheology. This allows, for the first time, an experimental correlation between rheological properties and the presence of branches. It turned out that the presence of a few inter-micellar connections sensibly decreases the zero-shear viscosity measured in steady state flow curves. Comparison with oscillatory rheology experiments indicates that the main effect of branches is to shorten the terminal relaxation time by speeding-up the reptation.



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1B – Physicochemical characterization of self-assembled nanocarriers for medical drugs.

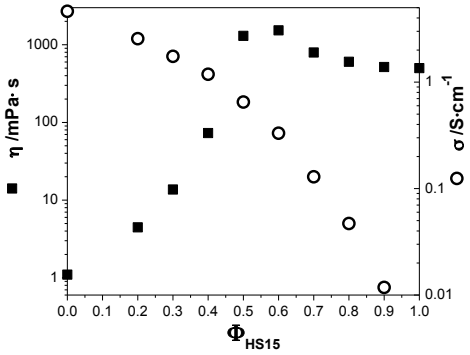
R. Angelico, G. Palazzo, G. Colafemmina, S. Murgia, S. Lampis, M. Monduzzi, A. Ceglie, A. Mangia (I.R.C.C.S. "Casa Sollievo della Sofferenza" S. Giovanni Rotondo Hospital, FG)

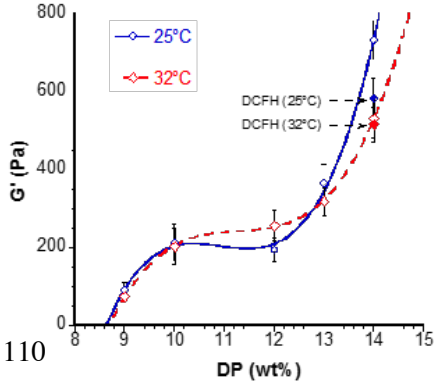
Aims

The therapeutic success of poorly water-soluble drugs strongly depends on the accurate design of delivery vehicles, most of them are self-assembled structures. In this research project, we emphasize the role played by the physicochemical characterization of different types of delivery vehicles selected for specific applications including micelles, vesicular phospholipid gels and liposomes, with the final goal of the optimization of drug therapeutic performance.

Results

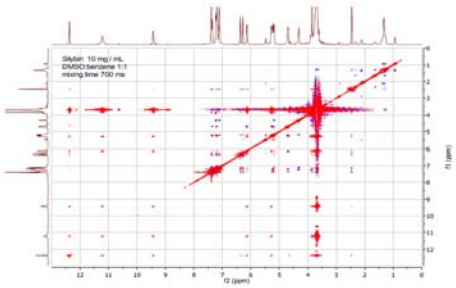
We investigated the phase behaviour upon water dilution of a commercial non-ionic surfactant (HS15), one of the most common components of drug delivery systems used in customary pre-clinical practice. From the analysis of rheology, SAXS, DLS, conductivity and NMR data, it was demonstrated that spherical micelles found in dilute surfactant solutions coalesce at a surfactant volume fraction close to 0.5 whereas no liquid crystalline phases were detected even at the highest HS15 concentrations in water. We also investigated the effect on the HS15 micelles microstructure of the solubilisation of a cannabinoid molecule as a model drug. The results indicated an increase in the surfactant effective packing parameter with a consequent alteration of the particle shape at low and intermediate HS15 content. A similar perturbation effect was observed in a different system based on cationic liposome nanocarriers, obtained by combining monoolein and lauroylcholine chloride.

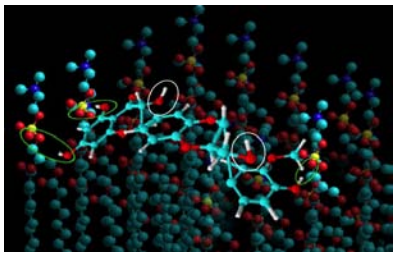




At low concentrations in water, the system is composed of small uni-lamellar vesicles characterised by low polydispersity and excellent stability, but above a critical volume fraction multi-walled vesicles start forming, giving rise to a macroscopic consistency typical of a stiff gel. Actually, it was proposed for topical drug delivery since skin penetration and permeation tests showed that the formulation was able to

deliver acid diclofenac (DCFH) into the viable epidermis. Viscoelastic parameters obtained from oscillatory rheology indicated that drug encapsulation gave rise to larger and less deformable (hence, worse packed) vesicular aggregates compared to the plain system. Another example of phospholipid nanocarrier has been obtained by co-aggregation with the cationic lipid DOTAP of several types of amphiphilic ruthenium complexes (that show a remarkable antitumoral and antimetastatic activity associated with a lower toxicity). A detailed microstructural characterization has been achieved by combining a variety of techniques including DLS, SANS, neutron reflectivity (NR), electron paramagnetic resonance (EPR), and zeta potential measurements. The in vitro bioactivity profile of the ruthenium-loaded nanoparticles was investigated on human and nonhuman cancer cell lines showing a marked tendency to accumulate in proximity of the nuclei. Finally, silybin, the bioactive component of Silybum Marianum, has been described to prevent HCV entry and to have a direct inhibitory activity on viral polymerase NS5B, with a variable efficacy depending on its pharmaceutical formulation and pharmacokinetic properties. Thus, the goal of our study was to design a suitable nanocarrier made by a mixture of non-ionic ad negatively charged phospholipids and comparing the pharmacological activity of this new silybin formulation with the compound dissolved in DMSO. From the analysis of 1H-NOESY-2D-NMR spectra carried out in apolar media, it was possible to identify several chemical residues on the bioactive molecule, directly involved with the phospholipid head groups via H-bonding, in accord with





preliminary molecular modelling results.

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1B – Nucleic Acid liposomes interactions

F. Cuomo, F. Lopez, A. Ceglie

Aims

The formulation of complexes obtained with liposomes and nucleic acid (lipoplexes) has been in the last few years and still is of major concern, because of the enormous utilization for items related to the investigation of biotechnological aspects. In the present investigation we intend to study the association behavior of lipoplexes made by oligo, polynucleotides and mononucleotides with cationic liposomes. Furtheremore the study is aimed to exploit on additional specific interactions at the polar head of nucleobases besides electrostatic interaction.

Results

The association behavior of different nucleic acids with cationic liposomes has been monitored, in order to find out how the polymer length, the type of base and the charge density affect the lipoplex formation. In particular the associative features displayed by the homopolymer 20-mer of adenine, Oligo (dA), of timine, Oligo (dT), and of guanine, Oligo (dG), were compared to understand the role of the base. The effects of the nucleic acid length and of the charge density were evaluated taking account of the association of the polyadenylic acid and of the DNA onto the liposomes. The results show that the homopolymer Oligo (dG) is able to interact with the cationic liposomes to the same extent as DNA, in spite of the fact that Oligo (dG) is a short polymer made of 20 residues and DNA is a longer and dual strand polymer having a higher charge density.

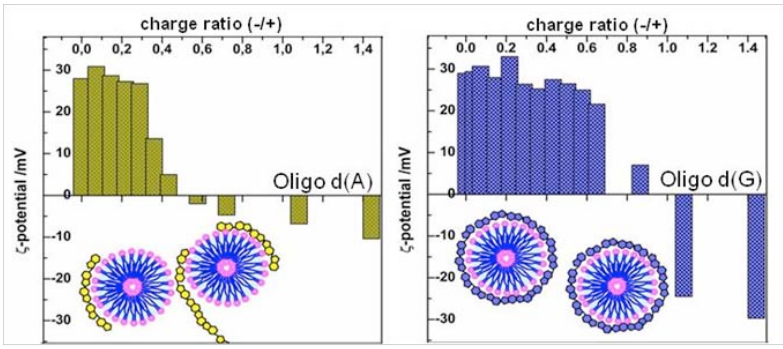

Fig.: Surface charge of liposome interacting with Oligo (dA) 20-mer (left) and Oligo (dG) 20-mer (right). The draw represents a sketch of the liposome–interaction. As illustrated the liposome surface is not fully covered with the Oligo (dA), while liposome surface is fully covered in the presence of Oligo (dG).

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1B – Alkylation of complementary ribonucleotides in nanoreactors.

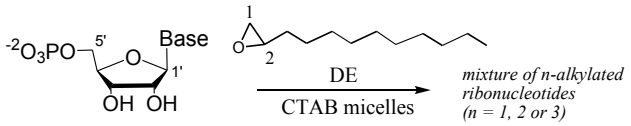
R. Angelico, A. Ceglie, F. Cuomo, I. Losito, F. Palmisano (Dip. Chimica, Univ. Bari)

Aims

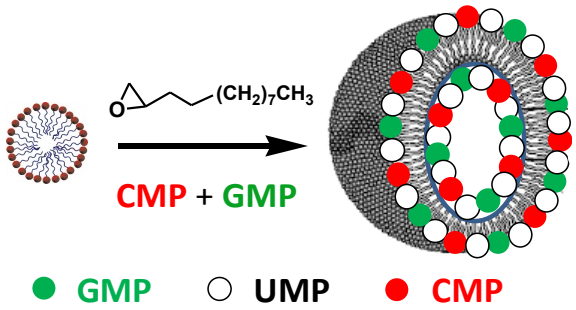
The pair of complementary ribonucleotides CMP and GMP react with the hydrophobic alkylating agent Dodecyl Epoxide DE dispersed in micellar nanoreactors to produce alkylated nucleobases. We intend to investigate the effect of base-pairing on the structure of modified nucleobases obtained from the reaction of alkylation.

Results

CMP and GMP reacting with DE dispersed in CTAB micelles yielded their lipophilic derivatives, which assembled in larger mixed aggregates (multi-lamellar-vesicles).



A partial deamination process occurred for CMP, which was spontaneously converted in UMP. Furthermore, both CMP and UMP alkylated products were affected by the presence of GMP through different chemical pathways. Indeed, a careful analysis of experimental data acquired with LC-Electrospray Ionization-single and sequential mass spectrometry (LC-ESI-MS and MS^n, with n = 2-3) allowed us to discover interesting properties of C-G base pair recognition. In particular, a reduced reactivity of the phosphate OH group of GMP and the absence of specific alkylated UMP species, i.e. those whose generation was related to the deamination of NH_2-alkylated Cytosine in mono- or bi-alkylated CMP, were found to be peculiar in mixtures initially containing both types of ribonucleotides.



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1B – Nucleolipid-Ruthenium complexes stabilized by lipid aggregates for antineoplastic therapy

G. Mangiapia, G. Vitiello, A. Luchini, G. D'Errico, L. Paduano

Aims

Metal complexes have an enormous impact in the treatment of cancer. This research is focused on the design and physico-chemical characterization of novel Ruthenium-based supramolecular aggregates with potential antineoplastic activity. The study was realized by combining Neutron Scattering techniques (SANS and NR), Dynamic Light Scattering (DLS) and Electron Spin Resonance (ESR) spectroscopy.

Results

A new organometallic ruthenium complex, named AziRu, along with three amphiphilic nucleoside-based ruthenium complexes, ToThyRu, HoThyRu and DoHuRu, incorporating AziRu in their skeleton, have been synthesized, stabilized in POPC phospholipid formulations and studied for their antineoplastic activity.

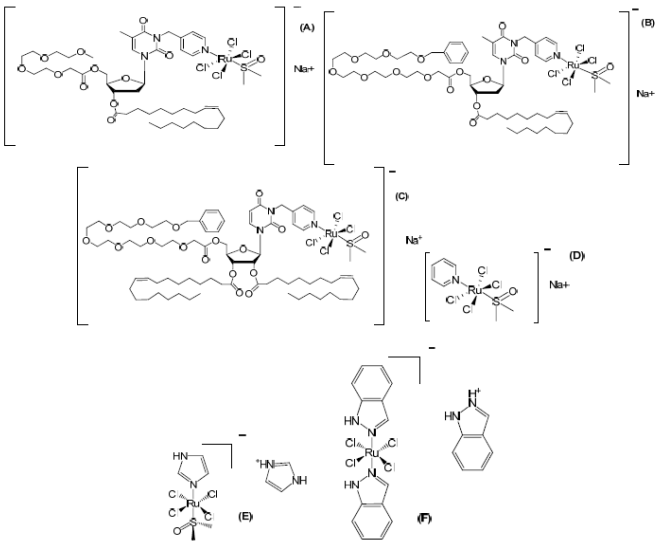


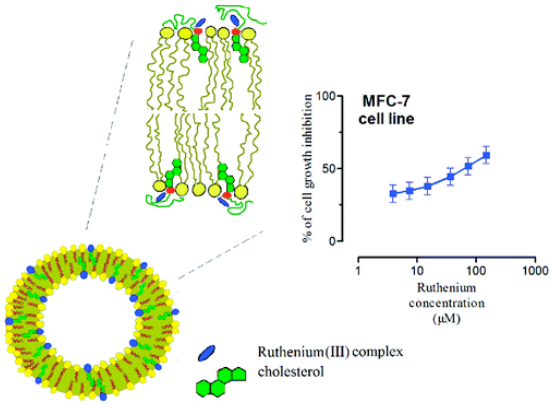
Fig. 1: Molecular structures of the Ruthenium-complexes: ToThyRu (A), HoThyRu (B) and DoHuRu (C), AziRu (D), along with the two anticancer drugs NAMI-A (E) and KP1019 (F).

Self-aggregation behavior of these complexes was investigated, showing that the three synthesized AziRu derivatives able to form liposomes and, under specific conditions, elongated micelles. The formulations prepared in POPC proved to be stable for months and showed high *in vitro* antiproliferative activity. These results introduce new perspectives in the design of innovative transition-metal-based supramolecular systems for anticancer drug vectorization.

Subsequently, we have developed an efficient drug delivery strategy for these novel anticancer amphiphilic ruthenium anionic complexes, based on the formation of stable

nanoparticles with the cationic lipid 1,2-dioleyl-3-trimethylammoniumpropane chloride (DOTAP). This strategy is aimed at ensuring high ruthenium content within the formulation, long half-life in physiological media, and enhanced cell uptake. An in-depth microstructural characterization of the aggregates obtained mixing the ruthenium complex and the phospholipid carrier at 50/50 molar ratio is realized by combining a variety of techniques, including dynamic light scattering (DLS), small angle neutron scattering (SANS), neutron reflectivity (NR), electron paramagnetic resonance (EPR), and zeta potential measurements. The in vitro bioactivity profile of the Ru-loaded nanoparticles is investigated on human and non-human cancer cell lines, showing IC_{50} values in the low μM range against MCF-7 and WiDr cells, that is, proving to be 10–20-fold more active than AziRu, a previously synthesized NAMI-A analog, used for control. The intracellular fate of the amphiphilic Ru-complexes was investigated in the same in vitro model by means of an ad hoc designed fluorescently tagged analog, which exhibited a marked tendency to accumulate within or in proximity of the nuclei.

Finally, a novel ruthenium complex, linked to a cholesterol-containing nucleolipid (named ToThyCholRu), stabilized by lipid aggregates for antineoplastic therapy is also studied. In order to retard the degradation kinetics typically observed for several ruthenium-based antineoplastic agents, ToThyCholRu is incorporated into a liposome bilayer formed by POPC. The resulting nanoaggregates contain up to 15% in moles of the ruthenium complex, and are shown to be stable for several weeks. The liposomes host the ruthenium–nucleolipid complex with the metal ion surrounded by POPC lipid headgroups and the steroid moiety inserted in the more external acyl chain region. These ruthenium-containing liposomes are more effective in inhibiting the growth of cancer cells than a model NAMI-A-like ruthenium complex, prepared for a direct evaluation of their anti-proliferative activity.



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1B – Interaction of peptides deriving from viral fusion glycoproteins with lipid membranes

G. Vitiello, G. D'Errico, L. Paduano

Aims

A synergic combination of different imaging techniques such as Electron Spin Resonance (ESR), Neutron Reflectivity (NR), Fluorescence spectroscopy and Molecular Dynamics (MD) simulations can be successfully used to describe the structural organization of lipid bilayers and their interaction with peptides involved deriving from viral fusion glycoproteins.

Results

We investigate the interaction between an octapeptide (C8) deriving from the MPER domain of gp36 of feline immunodeficiency virus and lipid bilayers with different lipid composition by combining experimental results with molecular dynamics simulations. In the case of POPC bilayers, our data indicate that C8 binds to the lipid bilayer adsorbing onto the membrane surface without deep penetration. As a consequence of this interaction, the bilayer thickness decreases. The association of the peptide with the lipid membrane is driven by hydrogen bonds as well as hydrophobic interactions that the Trp side chains form with the lipid headgroups.

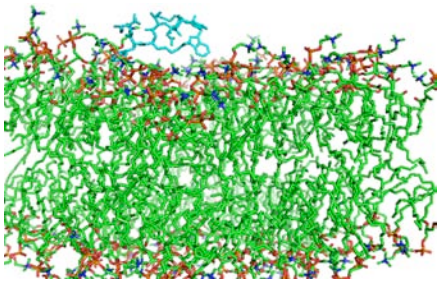


Fig. 1: Schematic representation of the destabilizing effect induced by C8 on POPC bilayer.

Upon peptide-bilayer interaction, C8 forms transient secondary structures ranging from 310 helices to turn conformations, while acyl chains of the peptide exposed POPC molecules assume a more ordered packing. At the same time, lipid headgroups' hydration increases. The asymmetric lipid bilayer perturbation is proposed to play a fundamental role in favoring the membrane fusion process.

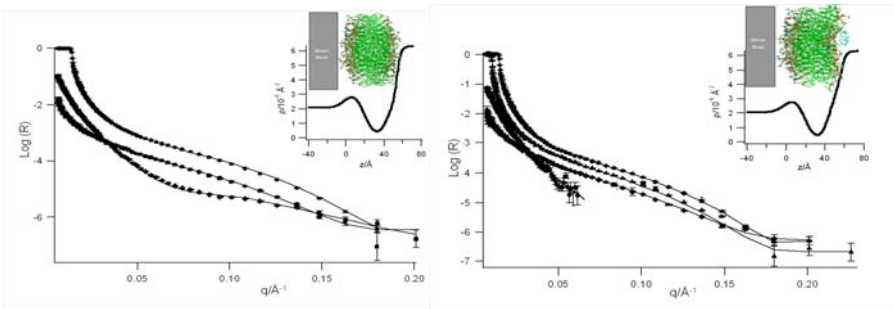


Fig. 2: Neutron Reflectivity profiles (points) and best fits (continuous lines) corresponding to pure POPC bilayer (*on the left*) and in the presence of C8 peptide (*on the right*) in (●) D_2O, (■) SMW and (♦) H_2O solvents. The inset shows the ρ profile for the POPC bilayer in D_2O.

Subsequently, we investigated the effect of sphingomyelin (SM) and cholesterol (CHOL) presence in the biomembranes on the interaction with the C8 peptide. A strict interplay among the different lipids in the peptide-induced fusion mechanism is highlighted.

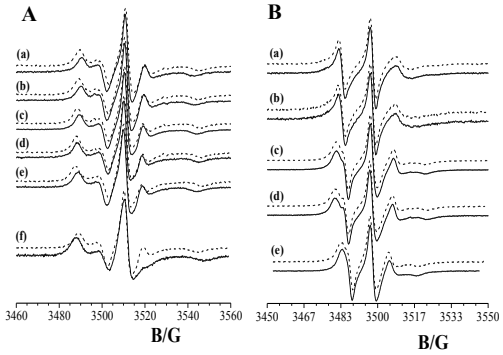
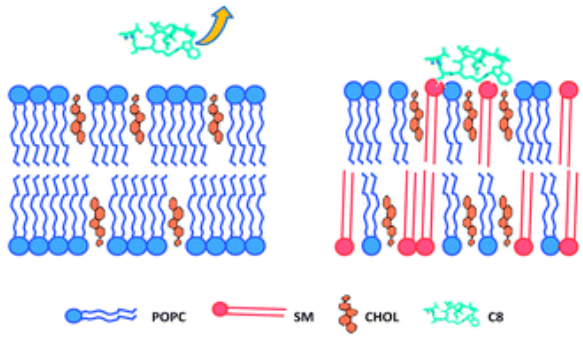


Fig. 3: ESR spectra of 5-PCSL (panel A) and 14-PCSL (panel B) in lipid bilayers of pure POPC (a), POPC/CHOL at weight ratios of 90:10 (b), 80:20 (c), 66:33 and (d) POPC/SM/CHOL (e) in the absence (continuous lines) and presence (dashed lines) of C8 peptide. ESR spectrum of 5-SMSL in POPC/SM/CHOL bilayer (f) is also reported in panel A in the absence (continuous lines) and presence (dashed lines) of C8 peptide.

Since CHOL preferentially locates close to SM, POPC molecules remain relatively free to interact with the peptide, driving its positioning at the membrane interface. Here, C8 comes in contact with CHOL-interacting SM molecules, causing a strong perturbation of acyl chain ordering, which is a necessary condition for membrane fusion. Our findings suggest that CHOL rules, by an indirect mechanism, the activity of viral fusion glycoproteins.



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1-3.

1B – Nanostructuring of novel saccharide-based synthetic ion transporters and their interaction with lipid bilayers

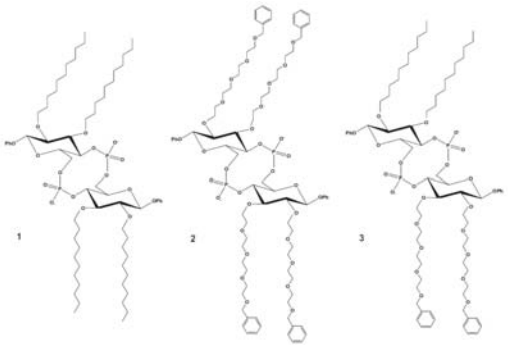
G. Vitiello, D. Ciccarelli, G. D'Errico, L. Paduano

Aims

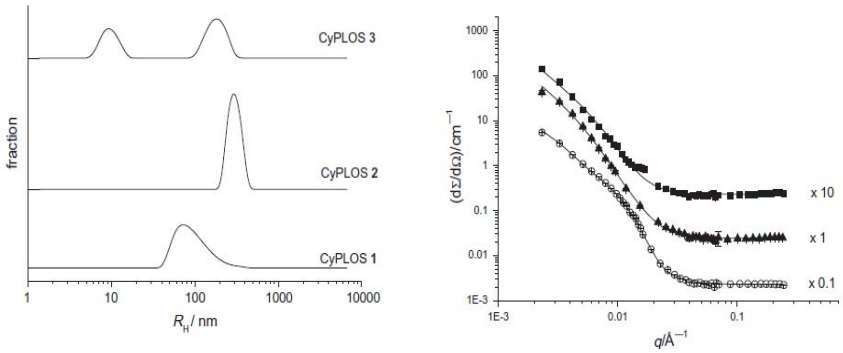
Ionophores are an important class of synthetic molecules which mimic natural ion channels or carriers. The

Results

We report the aggregation behavior in pseudo-physiological environment of three Cyclic Phosphate- Linked Oligosaccharides (CyPLOS) derivatives, synthetic ion transporters based on cyclic, phosphate-linked disaccharide skeleton differing for the nature of the tails (tetraethylene–TEG glycol and/or n-undecyl chains) attached to the C-2 and C-3 of the constitutive monosaccharides.



Their aggregation behaviour has been studied by a combined use of dynamic light scattering (DLS), electron paramagnetic resonance spectroscopy (ESR) and Small Angle Neutron Scattering (SANS). DLS measurements were performed to reveal the formation and size distribution of the CyPLOS aggregates. EPR measurements, by using 5-doxyl stearic acid (5-DSA) as spin-probe, showed that the aggregates are mainly due to the formation of double layers and allowed to analyze the local fluidity. Finally, SANS measurements allowed estimating the layer thickness of the double layers. Our results indicate that the three CyPLOS analogs show self-aggregation properties that depend



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on the different nature of the inserted tails.

Fig. 2: DLS curves (*on the left*) and SANS profiles (*on the right*) for the binary aqueous systems containing the synthesized CyPLOS 1-3.

The mechanism underlying the ionophoric activity of CyPLOS 2, a carbohydrate-based synthetic ion transporter decorated with four tetraethylene glycol (TEG) chains, has been investigated by an integrated Electron Spin Resonance approach. The mode of interaction of the ionophore with lipid bilayers has been studied by quantitatively analysing the perturbations in the ESR spectrum of an ad hoc synthesized spin-labeled CyPLOS analog, and, in parallel, in the spectra of spin-labeled lipids mixed with 2.

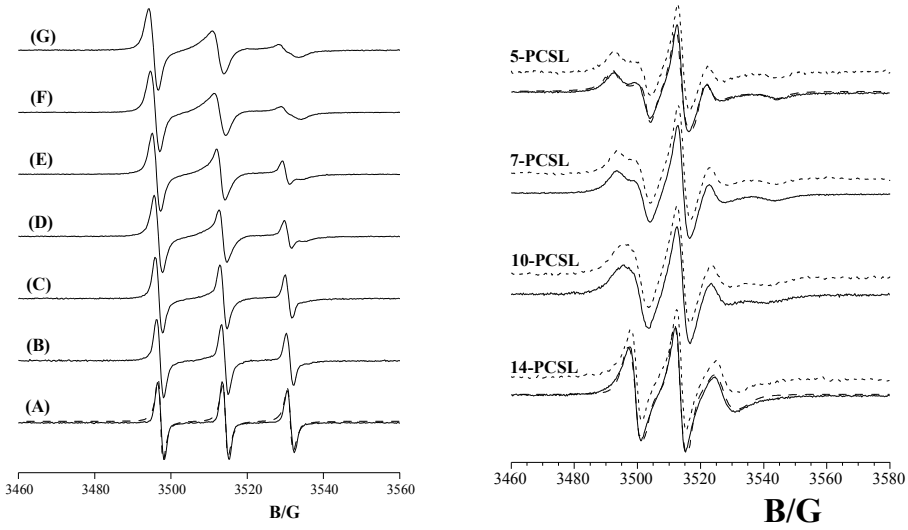
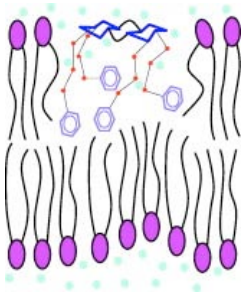


Fig. 3: ESR experimental spectra of spin-labeled CyPLOS (*on the left*) in: **(A)** buffer solution and **(B-G)** DOPC:DOPG bilayers at different CyPLOS-phospholipid ratios. ESR spectra of *n*-PCSL in DOPC:DOPG bilayers (*on the right*) in the absence (continuous lines) and in the presence (dotted lines) of spin-labeled CyPLOS. The dashed lines are exempla of simulated spectra.

The results point to a positioning of the cyclic saccharide backbone close to the lipid headgroups, largely exposed to the aqueous medium. The TEG chains, carrying a terminal benzyl group, are deeply inserted among the lipid acyl chains, showing high flexibility and relatively free motion. As a consequence, the order of the acyl chain packing is significantly reduced, and water penetration in the bilayer is enhanced. The resulting asymmetric perturbation of the bilayer leads to its local destabilization, thus facilitating, through a non-specific mechanism, the ion transport through the membrane.



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1B – Competitive protein adsorption from complex blood serum

N. Giamblanco, G. Marletta

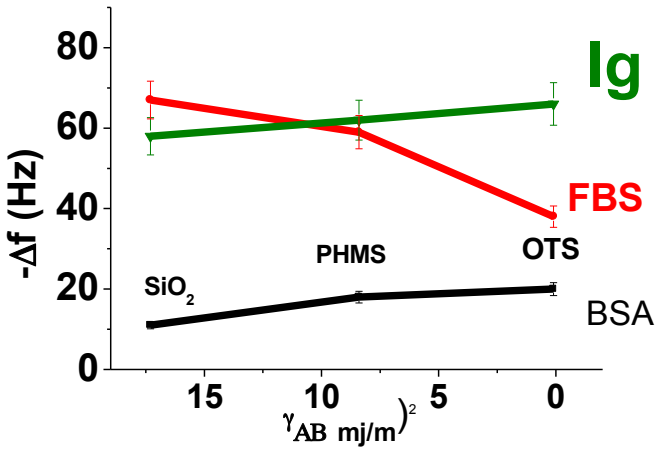
Aims

Competitive protein adsorption. Amount of adsorbed proteins, orientation and aggregation from single and complex blood serum.

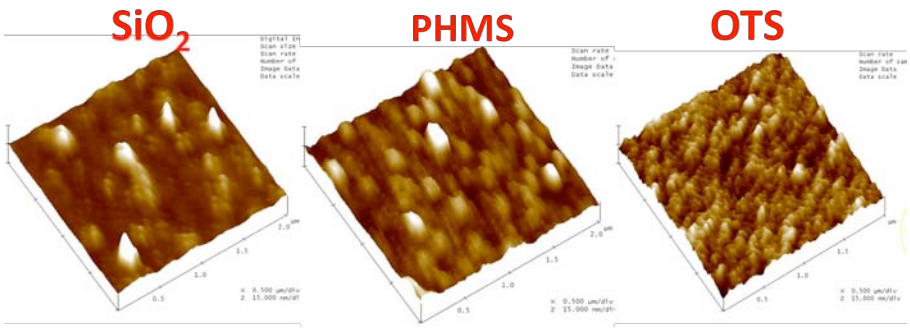
Results

We studied the influence of surface free energy of model silicon oxide, and poly(hydroxymethylsiloxane) (PHMS) and on octadecyltrichlorsilane (OTS) surfaces on the competitive protein adsorption, described in terms of amount, orientation and aggregation of adsorbed proteins, from single protein albumin and immunoglobulin solutions, and from complex blood serum.

We found that the adsorbed mass of FBS and Ig increases with the polar component (γ_{AB}) of SFE while that of BSA increase with the dispersive component (γ_{LW}) of surface free energy of the substrates.



Moreover, the amount of BSA adsorbed from fetal blood serum, detected by using the albumin antibody, resulted to be ten times more on hydrophobic PHMS and OTS surface than on SiO_2. Near Field Microscope (NFM) results showed that the different protein aggregates and multimeric assembly are surface-dependent as well



The results can be used as analytical methods able to differentiate the adsorbed species in complex mixture and understand the dependence of the competitive protein adsorption as a function of surface free energy by simply combining the single (HSA and Ig) and complex adsorption data performed on the same surfaces.

1B – Adsorption of protein on nanostructured surface

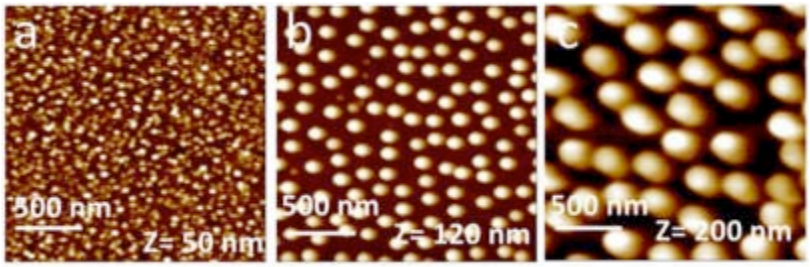
N. Giamblanco, E. Martines, G. Marletta

Aims

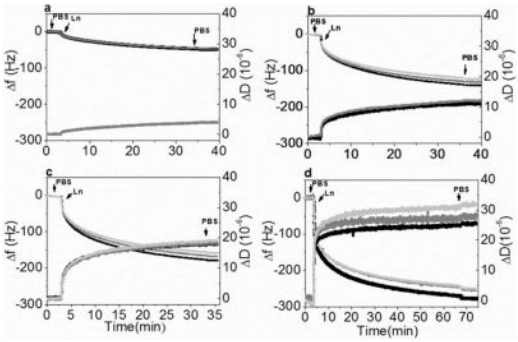
Influence of nanometric features of surfaces on the conformation and nanomorphology of adsorbed proteins.

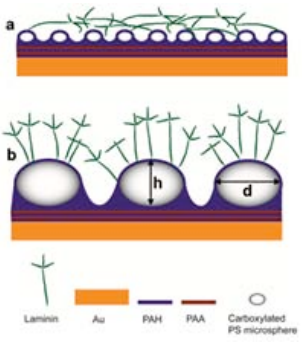
Results

We investigated the role of nanomorphology based on the use of chemically homogenous surfaces, with nanopatches having defined local surface curvature on protein adsorption. The local surface curvature, κ, was simply defined as a reciprocal of the nanopatches radius. Indeed, the adsorption of macromolecule is expected to depend on the matching of a structural parameter κ and a structural parameter describing the macromolecules, the radius of gyration, Rg. Chemically homogenous nanostructured surfaces of variable surface curvature were prepared by using colloidal lithography, based on casting of carboxylated polystyrene nanospheres with different dimension, coated with a polyelectrolyte polyallylamine.



The results are indicative of a much higher laminin mass adsorption and thickness on nanostructured surfaces, forming highly viscoelastic protein layers . The increase of overall mass adsorption observed for nanostructured surfaces cannot be simply explained in terms of the increase of the available area. Indeed, while the increase in active surface area were 54%, 46% and 44%, the corresponding increase in laminin adsorption were 65%, 74% and 83% so that the mass adsorption increased in a reverse trend with respect to the active area. Overall, it appears that the mass adsorption follow a trend inversely related to the curvature of nanostructures, increasing from the highest to the lower curvature. In other word, the increased number of molecules from nanostructured surfaces should correspond to different molecular orientation with respect to the one revealed on flat surfaces.





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1B – Quasi-2D-Surface Nanostructuring

G.M.L. Messina, G. Marletta

Aims

The aim of this work is to develop new techniques to achieve reproducible and cost-effective chemical and topographical patterns of polymeric and silicon substrates at nanometer scale for biological application. In particular, two-dimensional (2D) porous substrates are developed for a wide range of applications including chemical microcontainers, surface-plasmon resonance biosensors, catalytic supports and photonic crystals, including as nanocontainers, trapping sites, etc… Two main requirements were defined: flexibility in terms of lateral pattern dimension, which is indeed ranging from the micrometer to the sub-micrometer scale, and the compatibility with respect to preservation of biological activity of the adsorbed biomolecules.

Results

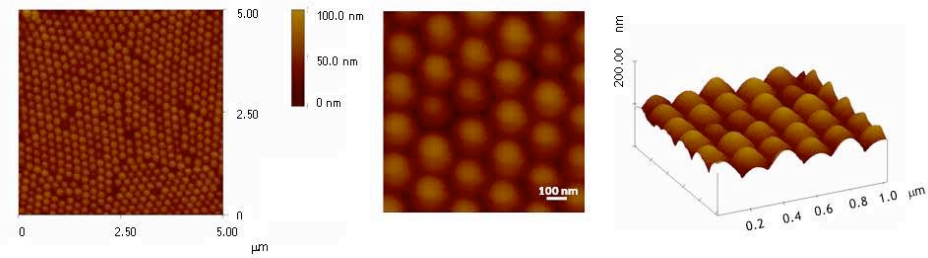
Today nanoscience is fed from a number of subdisciplines: nanoelectronics, nanomaterials, molecular nanotechnology, bionanotechnology and development of tools for analysis, especially scanning probe microscopies all contribute. The development of nanoelectronics and materials mostly relies on top-down methodology. Molecular and bionanotechnology have a more bottom-up approach.

A pure self-assembly approach towards spatial organization, to provide a complementary paradigm to the currently available top-down methodologies, including lithographic techniques, would in itself be a very desirable goal. Other parameters like cost and ease of fabrication only seem to be speaking more in favor of such an approach. Self-assembly, defined as the spontaneous, thermodynamically controlled, organization of individual molecules into a (meta) stable and (spatially) well-defined aggregate usually is a complicated and not very well understood phenomenon.

It critically relies on a delicate interplay of many interactions, often of different nature. It is exactly for this reason that self-assembly approaches have been put forward as an alternative to top-down methodology in nanotechnology. Self-assembly promises to be a cheap and potentially extremely easy methodology to decorate surfaces with all kinds of interesting templates. In general it would be highly desirable to be able to control interfacial properties, as interfaces play such a prominent role in many processes, e.g. in catalysis, molecular recognition, and as sites of nucleation, both in natural and synthetic systems.

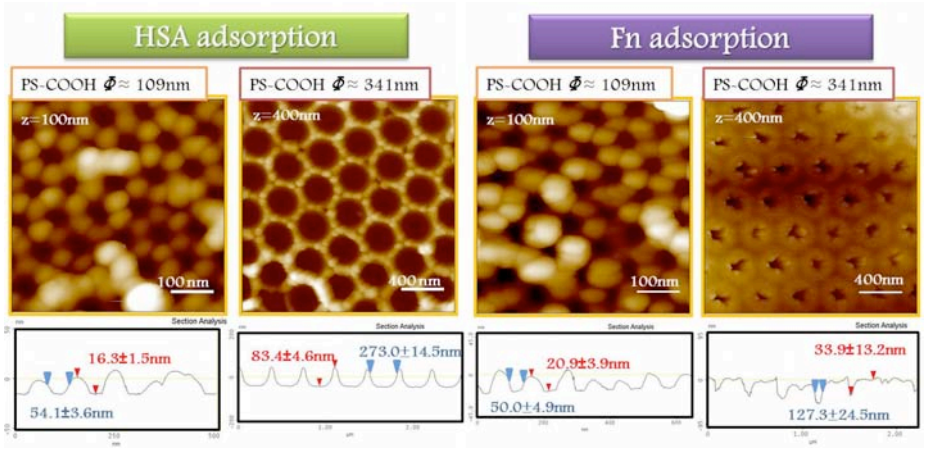
We present a versatile and simple approach for rapidly fabricating nanopatterned surfaces on micrometer scale, having different surface free energy. Monodisperse polystyrene nanoparticles were spin-coated onto hydrophilic PHMS (Poly-hydroxymethylsiloxane) thin film deposited on silicon wafer.

Nanoparticles, with an average diameter (D) of 109 and 341 nm, self-organised in the classical bidimensional hexagonal lattice structure. The produced arrays are in general not perfect, as intrinsic point and line defects appear in the resulting structure. Typically, defect-free domains have size in the 10-50 μm^2 range.



AFM image of 2D and 3D hexagonal silica spheres on gold substrate.

A second hydrophobic polymer layer of PHMS is then deposited on samples, embedding the nanoparticle distribution. Finally, the selective removal of the nanospheres leads to the formation of nanostructured micron-sized area. The nanopatterned surfaces consisted of 2D nanopore arrays, having internal area of hydrophilic polymer surface surrounded by hydrophobic polymeric matrix.
The preferential adsorption of proteins, e.g., Human Serum Albumin (HSA) and Fibronectin from human plasma (Fn), having different physico-chemical properties, was investigated onto the nanostructured surfaces.
The adsorption was studied as a function of the pore geometrical features, including volume, aspect ratio and diameter, as well as the chemical contrast. The driving chemical factors were identified in terms of surface free energy gradients and chemical termination of the pore bottom and walls.



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1B – Schottky barrier height of Au-p Si Schottky devices by polymer/metal nanograins hybrid multilayers

V. Torrisi, F. Ruffino, G. Isgrò, I. Crupi, G. Li Destri, M.G. Grimaldi, G. Marletta

Aims

The modification of the interfacial potential barrier for Au/p-Si diodes, by means of a favored transport of majority carriers at polymer/metal interface.

Results

Insulating, polymetilmethacrylate (PMMA), and semiconducting, poly-3-hesylthiophene (P3HT), polymers and copolymers/Au nanograins based hybrid multilayers (HyMLs) were fabricated on p-Si single-crystal substrate by an iterative method that involves, respectively, Langmuir-Blodgett and spin-coating techniques (for the deposition of organic film) and sputtering technique (for the deposition of metal nanograins) to prepare Au/HyMLs/p-Si Schottky device. The electrical properties of the Au/HyMLs/p-Si Schottky device were investigated by current-voltage (I–V) measurements in the thickness range of 1-5 bilayers (BL).

At different number of layers, current-voltage (I–V) measurements were performed. Results showed a rectifying behavior. Junction parameters, such as barrier height (BH), from the I–V measurements for example for the PMMA based Au/HyMLs/p-Si structure were obtained as 0.67±0.02 eV at 5BL and 0.75±0.02eV at 1BL. It was observed that the BH value of 0.67 eV calculated for the Au/HyMLs/p-Si structure was lower than the value of 0.71 eV of conventional Au/p-Si Schottky diodes. Thus, modification of the interfacial potential barrier for Au/p-Si diodes has been achieved using a thin MLs of different polymers based HyMls semiconductor, due to a favored transport of majority carriers at polymer/metal interface. Furthermore, the conduction of minority carriers (electrons) is promoted because of tunneling transport caused by interfaces electronic states produced in the organic layer by the defects originated by the sputtering deposition process.

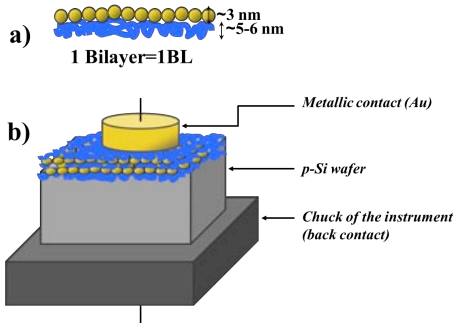

Fig. 1: a) schematic representation of polymer/metal bilayer; b) cross-sectional view of Au/Hybrid MLs/p-Si Schottky device for electrical characterization.

The modification of annealed and as deposited Barrier Heght (BH) of the hybrid multilayers was correlated with the morphology and the nanometric thicknesses of the layers that compose the hybrid system.

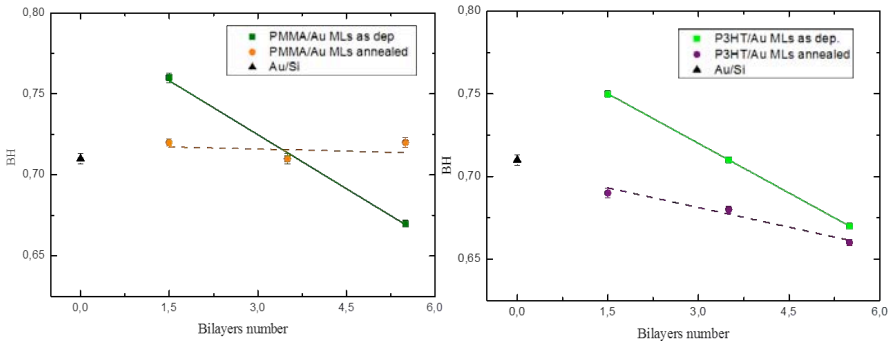

Fig. 2: Graphic of Barrier height vs number of hybrid bilayers

Thickness of Au film (nm)	1BL	3BL	5BL
	2.4±1.2	2.7±1.4	2.6±1.4
Thickness of PMMA film (nm)	1BL	3BL	5BL
	13.0±1.1	12.9±1.1	13.2±1.0

Tab. 1: Table of Au and PMMA thicknesses obtained by Xray reflectivity.

Thickness of Au film (nm)	1BL	3BL	5BL
	2.0±0.9	2.1±0.9	2.1±0.8
Thickness of P3HT film (nm)	1BL	3BL	5BL
	6.0±1.1	4.9±2.7	4.6±3.5

Tab. 2: Table of Au and P3HT thicknesses obtained by Xray reflectivity.

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1B – Thermoresponsive polymeric micelles as efficient tool for controlled drug delivery

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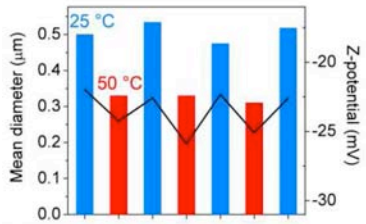
Aims

Design of thermoresponsive polymeric micelle for encapsulation and targeted release of drugs through laser-induced temperature jump.

Results

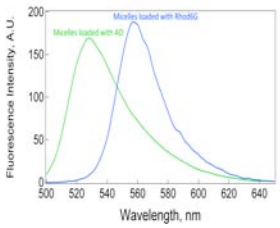
Recent research efforts on drug release strategies focus, besides liposomes and nanoparticles, on polymeric micellar systems that, thanks to their structural properties, are able to effectively encapsulate and release controlled and localized quantities of drugs in response to external stimuli. According to recent evidences of the importance of polymerosomes for targeted therapies, we studied self-assembled micelles obtained from triblock copolymers of PCL-PEO-PCL with the twofold aim of efficient storage of drug molecules and of sustaining thermodependent processes allowing chemical release on demand.

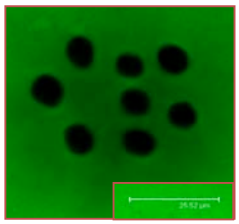


The thermoresponsive behaviour of drug-free micelles was assessed by means of Dynamic Light Scattering measurements run on PCL-PEO-PCL micelles as a function of temperature and aging time. Zeta-potential measurements for the same samples enabled the determination of the surface charge density of the polymeric micelles.

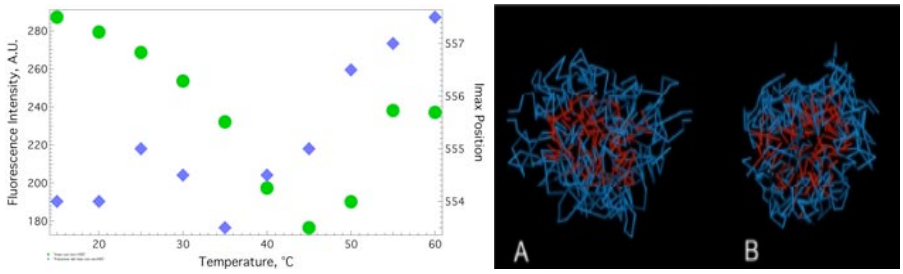
Measurements along the temperature cycles evidenced a micellar phase transition, centred around 40 °C, characterized by decrease of the micellar size at higher temperature paralleled by an increase of the absolute value of zeta-potential. The transition was shown to be reversible for at least 5 temperature cycles in terms of size, distribution and surface charge density of the micellar aggregates.

Two different fluorescent hydrophobic compounds, i.e. Acridine Orange and Rhodamine 6G, were inserted in the polymeric system to mimic the stimulated release of a potential drug upon thermal triggering. Insertion of the probes was demonstrated by fluorescence emission of the micellar solution and further confirmed by spatially resolved emission spectra acquired by means of Confocal Laser Scanning Microscopy once the micelles were immobilized in a planar porous biopolymer scaffold.

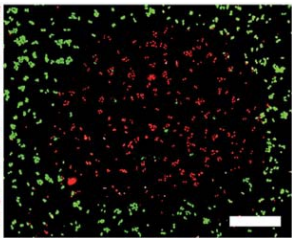




Fluorescence measurements performed on the dye-loaded micelles were recorded in the 15-60 °C temperature range, the results showed that the variation in intensity and position of the emission bands with temperature exhibit a clear-cut discontinuity at 40 °C. These findings were ascribed to a change of the probe microenvironment and to a variation of the aggregation state of the probes prompted by the migration of the fluorescent molecules from the interior of the micelle towards the water phase. Interestingly, this process superimposes with the shrinkage of the micellar aggregates at the transition temperature.



The study of the inclusion behaviour in thermoresponsive polymeric micelles was extended to drugs involved in pathologies that span from cancer therapy to neurodegenerative diseases and chemical suture strategies. The micelles have been immobilized on a biocompatible device in the form of a light-activatable sponge-like nanocomposite scaffold. The sponges consist of a Chitosan porous biopolymer containing a dispersion of gold nanorods, which acts as an absorber of the incoming laser light, and of thermosensitive micelles.



Fluorescence images showing viable (in green) and dead (in red) HeLa cells treated with the hydrophobic Doxyrubicin drug (Dox) released from overlying sponges subjected to laser irradiation. Dox-induced cell death is confined to those cells in close proximity with the irradiated portion of the sponge. (bar = 500 μm).

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1B – Complexing a small interfering RNA with divalent cationic surfactants

S. Falsini, M. In, L. Ciani, E. Di Cola, A. Arcangeli, S. Ristori

Aims

Insight in the structure and kinetics of siRNA complexation with micelles of divalent cationic surfactants.

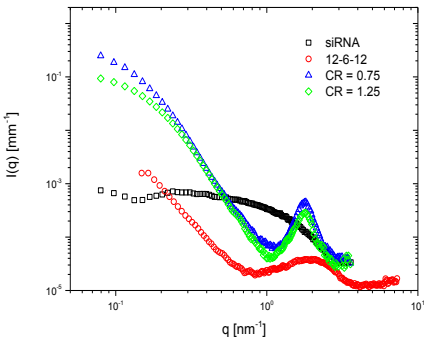
Results

small interfering RNAs (siRNAs) mediate the selective knock-down of genes in human cells, thus offering a powerful tool to modulate gene expression for therapeutic purposes. The main drawbacks in this approach are the transport of siRNAs *in vivo* and their protection against nucleases in the blood stream. To date, the requirement of new vectors necessary to complex and transport oligonucleotides has become increasingly urgent. Extensive physico-chemical characterization can provide the necessary knowledge of vectors and complexes to improve transfection efficacy.

In this work we studied the mechanism of siRNA complexation by micelles of two types of divalent cationic surfactants, i.e. three Gemini bis (quaternary ammonium) bromides with 12 carbon atom chains and variable spacer length (12-3-12, 12-6-12, 12-12-12), and one weak electrolyte surfactant bearing a triazine polar head and a 14C tail (SH14). Time resolved Small Angle X-Ray Scattering performed at the European Synchrotron Radiation Facility (Grenoble, France) was the chosen investigation tool.

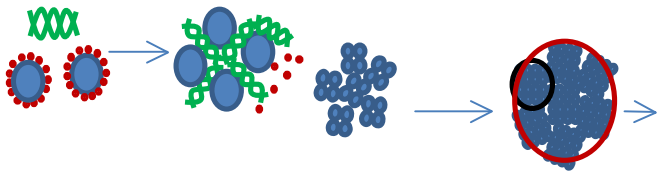
All systems contained a fixed amount of surfactant, which at the mixing instant was 2.5 10^{-3}M or 1.25 10^{-3}M, and different concentration of siRNA to obtain the desired charge ratio (CR = -/+).

Immediately after mixing (t < 0.05 s), new large aggregates were formed in solution and the scattering intensity at low q increased. The background signal of the micelle curves was lower than the background of complexes by 3-5 10^{-5} mm^{-1}, in agreement with the expected contribution of Br^- counterions which are transferred from the micelle surface to the bulk solvent upon complex formation. Concomitantly, the appearance of a quasi-Bragg peak at larger q values indicated core structuring within the complexes.



As an example for the siRNA/12-6-12 system, the peak maximum was located at ~ 1.7 nm^{-1}. This value is slightly shifted with respect to the maximum found in the micelle SAXS diagram, suggesting that siRNAs are internalized among micelles in the complex. From the peak shape analysis we hypothesized that siRNA and micelles are alternately arranged

into “sandwiches” and form coherence domain made by a compact array of 4-8 units.
The time evolution of the peak maximum and FWHM showed that after forming complexes underwent a reorganization process which followed a first-order kinetics and was completed in about 400-800s.
Aggregates containing Geminis were compact globular structures whose gyration radius R_g depended on the spacer length and was in the order of 7-27 nm. Complexes containing SH14 had larger R_g (14-16 nm) and were less ordered internally.
The whole complexation process could be schematized as follows:



Since the transient states of complexes might be as relevant as the final state for their efficiency, we were able to devise a time interval of 10-15 after mixing that can be used to perform transfection with complexes of a few nm size, that is significantly smaller than the size of conventional complexes formed by cationic liposomes or polymeric micelles.
The obtained data are encouraging evidence in the perspective of using these systems *in vivo* and *in vitro* after preparation by simple mixing a micelle solution of the cationic surfactant and a siRNA solution, both of which are obtained without passing through irreversible steps, such as sonication or extrusion.

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1B – Application of MOMD model on ESR spin labeling studies in the interaction between proteins and lipid bilayers

E. Busi, G. D'Errico, R. Basosi

Aims

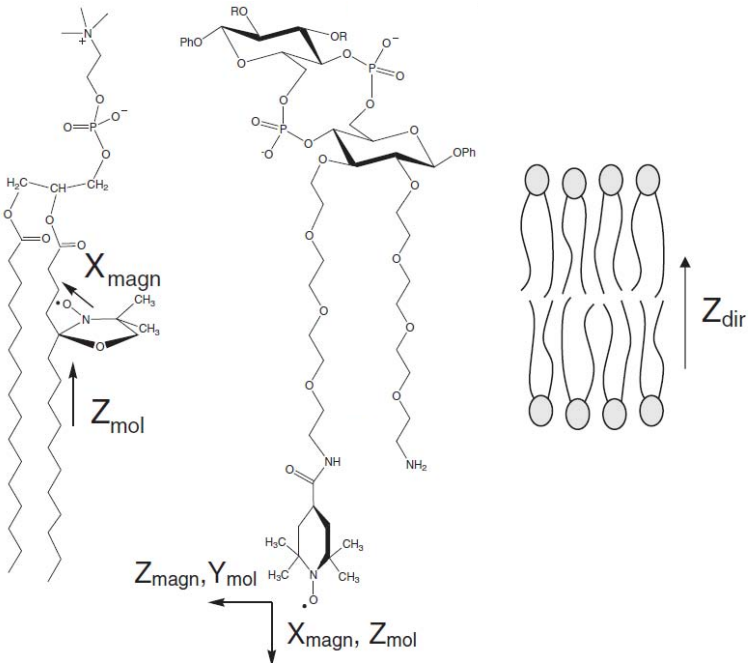
Study of the mechanisms of interaction between peptides/proteins (such as virus glycoprotein, carriers, ionophores) and lipid bilayers.

Results

Anisotropic fluids differs from anisotropic liquids in that there is a mean ordering potential in the former case. It leads to preferred spatial orientation being imposed on the constituent molecules. ESR spin labelling has been employed to elucidate ordering characteristic in liquid crystalline phases, in particular to investigate interaction between phospholipids bilayer and proteins. In the case of vesicle-associated spin-labeled molecules (either the spin-labeled protein or spin-labeled lipids), one has to consider that they are preferentially oriented by the local structure of the bilayer. In multi lamellar vesicles dispersions, lipid bilayer domains are overall distributed randomly. Consequently, the ESR spectrum can be regarded as a superposition of the spectra from all the domains. In these cases we applied the Microscopic Order Macroscopic Disorder (MOMD)model in the simulations. From the computational analysis, two sets of parameters were obtained: the best-fit parallel and perpendicular correlation times ($\tau_\perp$, $\tau_\parallel$), and the order parameters (S_0, S_2).

Nitrogen hyperfine coupling tensor components (A_{xx}, A_{yy}, A_{zz}) were set to the values obtained from simulations of the spectra obtained at 120 K. The local orientational ordering of the labeled molecule is characterized by the time-averaged order parameters S_0 and S_2, defined with respect to a unique axis Z_{dir} (the director normal to the bilayer plane) along which the reorienting potential acts. S_0 and S_2 can be calculated via the best-fitting potential energy parameters for a probe in a liquid crystalline solvent. S_0 is a measure of the extent of alignment of Z_{mol} with respect to Z_{dir}, while S_2 measures the extent to which there is a preferential alignment of X_{mol} vs. Y_{mol}. Thus, S_2 represents the deviation from cylindrical symmetry of the molecular alignment relative to Z_{dir}. The choice of the simulations which reproduce better the spectra was based on low $\chi 2$ values and good agreement between the details of the final simulated and experimental lineshapes. A series of computer simulation tools were used for these studies.

In the figure an example of the chemical structure of a phospholipid interacting with a ionophore, and their related frames is reported.



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1B – Peptide-Lipid interactions: implications on health and diseases

R. Pogni, A. Bonucci, E. Balducci

Aims

The aims of this work is to characterize the interaction of bioactive peptides with phospholipids membranes combining several spectroscopic techniques (i.e. Circular Dichroism, Fluorescence Emission, Site Directed Spin Labeling – Electron Paramagnetic Resonance) in order to clarify various features that regulates the mechanism of this interaction.

Results

Antimicrobial peptides (AMPs) are an essential part of innate immune defence system against microbial infection. Naturally occurring AMPs are basic peptides composed of 12-50 aminoacids that are ubiquitously distributed throughout all kingdoms of life. AMPs display a broad spectrum of antimicrobial activity against both Gram-negative and positive bacteria, fungi and enveloped viruses. Importantly, they retain activity against antibiotic-resistant strains and do not readily elicit resistance. AMPs base their capability to kill pathogens on the perturbation and the disruption of membrane cell wall.

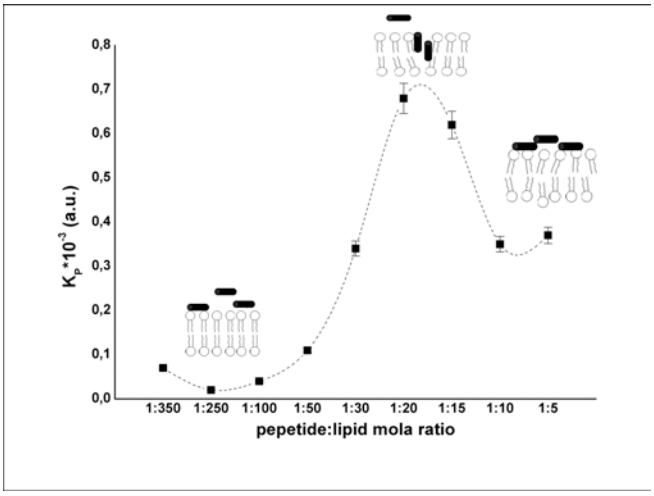

Fig. 1: Partition coefficients profile for HNP-1 at different peptide:lipid molar ratios. Experiments are performed using tryptophan emission fluorescence spectroscopy. The 1:20 ratio represents the threshold concentration for peptide insertion into phospholipid bilayer.

We investigated in details the mechanism of peptide-lipid interaction and the relative factors that influence the partition into lipid bilayer of two human antimicrobial peptides, human neutrophil peptide 1 (HNP-1) and cathelicidin LL-37, which exhibit a synergistic action against various pathogens *in vivo*.
We find that the defensin HNP-1 interacts with phospholipids mimicking Gram-negative inner membrane adopting a "spanning-mode" into a lipid bilayer only

reaching a specific threshold concentration represented by the 1:20 peptide:lipid molar ratio (Fig.1). The residue Arg-14 plays a fundamental role on the HNP-1 partition: in fact, replacing this residue with less cationic aminoacids altering the penetration of peptide into model membrane. Another limiting factor for HNP-1 activity is represented by cysteines connectivity. The reduction of disulphide bonds does not compromise the partition of peptide into model bacteria membrane expanding the applicability of HNP-1 on therapeutic treatment of infections. In addition, an analysis on the interaction of this peptide with model mammalian membrane provided that HNP-1 does not posses a relevant toxicity against eukaryotic lipid bilayer.

Another study is based on the individuation of mechanism of action of human AMP LL-37 against model bacteria membranes. The cathelicidin displays a "detergent-like" mode of action beyond the 1:50 peptide:lipid molar ratios in presence of negatively charged membranes. This effect is not confirmed in presence of model mammalian membrane: LL-37 deposits on the outer leaflet without altering the lipid packing of lipid bilayer resembling eukaryotic cell wall. Contrary to the results obtained for HNP-1, this peptide still maintain a disrupting action against phospholipid membranes in presence of high level of salt. Undoubtedly, the absence of rigid constrains and high net cationic charge conferred by arginine and lysine are important features that regulates the LL-37/lipids interaction.

Our studies provide new insights on the mechanisms of interaction with phospholipids membranes for defensin HNP-1 and cathelicidin LL-37. Principally, we expand the knowledge on AMPs, supporting the applications of these biologic compounds as possible substitutes of common antibiotics on therapies for the treatment of infections. Since both HNP-1 and LL-37 peptides are related to specific diseases, such as cystic fibrosis, our analysis supply information to understand and solve the processes that leads to the inception of these pathologies.

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Fig. 1: Cartoon of different PLN oligomeric states and PLN-SERCA interaction.
Fig. 3 Schematic representation of planar lipid bilayers (BLMs).

1B – Structure-function relation of Phospholamban: modulation of channel activity as a potential regulator of SERCA activity

S. Smeazzetto, M.R. Moncelli (University of Florence, Department of Chemistry)

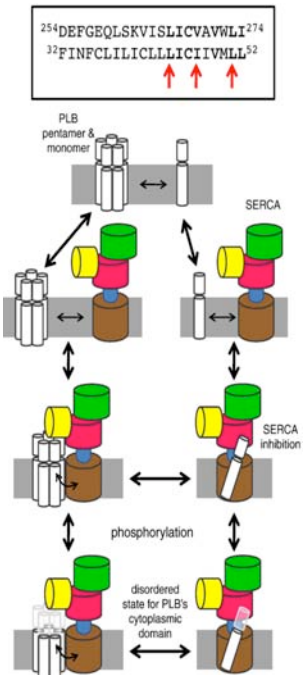
Aims

Investigation of Phospholamban (PLN) structure-function relation with the ultimate goal to modulate the sarco/endoplasmic Ca-ATPase (SERCA) activity.

Results

PLN is a small integral membrane protein, which is involved in the contractility of cardiac muscle by regulating SERCA. The activity of SERCA is inhibited by unphosphorylated PLN whereas phosphorylated PLN releases SERCA inhibition and allows pumping of Ca^{2+}. PLN occurs in equilibrium between a monomeric (6KDa) and a pentameric form (30KDa). While it is clear that the monomeric PLN is sufficient for SERCA inhibition, the functional relevance of the pentameric state is not yet fully understood (Fig.1).

In our laboratory, we have recently introduced an experimental setup (Fig. 2) to carry out single channel measurements in planar lipid bilayers (BLMs) (Fig3).



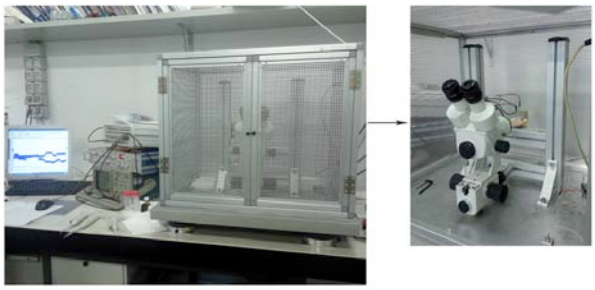
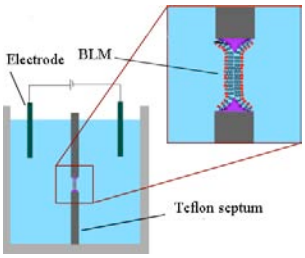


Fig. 2: Picture of experimental setup for single channel measurements in planar lipid.



Using our experimental setup and in collaboration with Prof. G. Thiel (FB Biologie, Technische Universitat, Darmstadt, Germany) we have shown that PLN, when reconstituted in BLMs, exhibits ion channel activity with a low unitary conductance, a long open/closed dwell times (Fig.4) and a moderate selectivity between monovalent cations and not perceivable Ca^{2+} permeability [1].
On the basis of experiments which allow an estimation of the pore size (radius between 2.2 and 6.6A°) we support the hypothesis that the conducting channel is generated by PLN in its pentameric form.
In collaboration with Prof. Thiel and Prof. Howard S. Young, Department of Biochemistry, University of Alberta, Edmonton, Canada, we studied phosphorylated PLN and some PLN mutants, which either stabilize (K27A and R9C) or destabilize (I47A) the PLN pentamer. Mutants and phosphorylated PLN still generate the same unitary conductance of the wt/non-phosphorylated PLN. However, the open probability of the phosphorylated PLN and of the R9C mutant is significantly lower than that of the respective wt/non-phosphorylated control. In the context of data on PLN/SERCA interaction and on Ca^{2+} accumulation in the sarcoplasmic reticulum the present results are consistent with the view that PLN channel activity could participate in the balancing of charge during Ca^{2+} uptake [2].

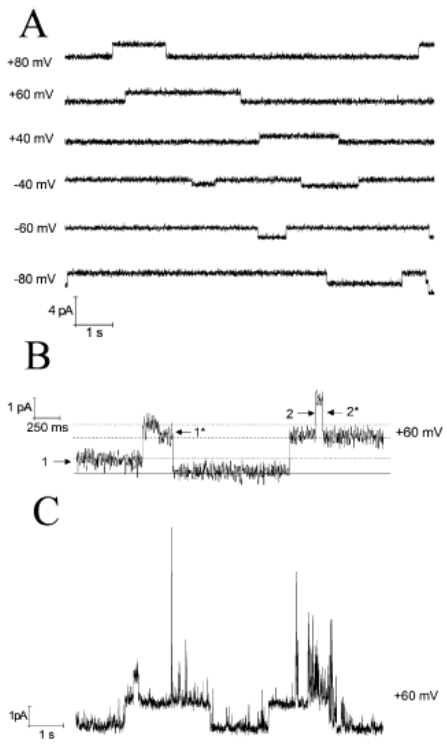


Fig. 4: PLN generates single channel fluctuations in planar bilayer. (A) Unitary current traces were recorded at various holding potentials, from – 80 mV to + 80 mV in symmetrical solution with 500 mM KCl in 10 mM MOPS (pH=7) buffer. (B) Example of concomitant opening/closing of large conductance and small conductance. The numbers at the trace denote opening/ closing of small conductance (1) and of large conductance (2). The two events are additive meaning that the low conductance is not a sub-conductance of the large one. (C) Example of flickering behaviours. Single channel trace at +60 mV.

References

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1B – Ion channels as selective drug targets

R. Gualdani, M.R. Moncelli (University of Florence, Department of Chemistry)

Aims

Study of TRP channel as target for new painkiller drugs and proarrhythmic activity of hERG potassium channels blockers.

Results

Ion channels are responsible for transport of ions across cell membranes, and are crucial for all physiological processes. A number of human diseases are caused by defects in the function of ion channels. The large number of physiological processes regulated by ion channels make ion channels highly interesting as target for new drugs. However, many new molecules (potential drugs) can induce arrhythmia and the reduction of this risk is considered a major hurdle in the development of new drugs. For this reason the investigation of hERG channel blockage represents a fundamental step along the drug discovery process. The most common problem is the acquired long QT syndrome, that is caused by drugs that block the human ether-a-go-go related gene (hERG) protein, a K^+ channel that regulates the heart's beating. Efforts to predict the cardiotoxicity of new drugs have been focused on assays testing hERG channel activities, since the blockage of hERG is considered an indicator of potential pro-arrhythmic risk. In our laboratory, using the patch-clamp technique, we are studying new molecules which modulate the activity of ion channels such as Nav1.6 (Sodium channel, voltage gated, type VIII, alpha subunit), TRPA1 (Transient Receptor Potential cation channel, subfamily A, member 1), TRPV1 (TRP cation channel, subfamily V, member 1) and TRPM8 (TRP cation channel, subfamily M, member 8).
Recently, in collaboration with Prof. Campiani (NatSynDrugs, Siena University) we tested the cardiotoxicity of two antimalarian drugs (‘6b’ and ‘6c’) [1]. Compound ‘6b’ was a potent inhibitor of the rat hERG K^+ channel and was comparable in its inhibitory activity to the antimalarial halofantrine. By contrast, ‘6c’ did not affect the function of the rat hERG K^+ channel, even when tested at 10 μM (Fig. 1).

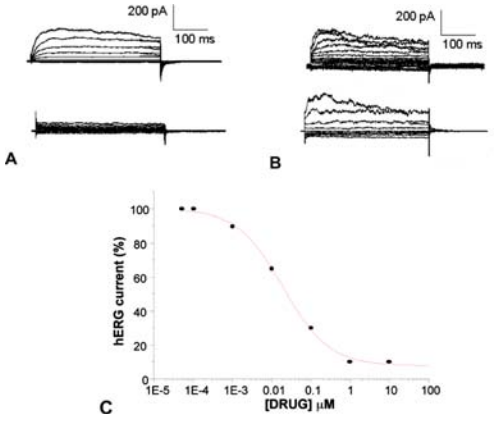


Fig. 1. Current traces activated by depolarizing voltage pulse in 20 mV steps from a holding potential of –80 mV in the absence (top) or presence (bottom) of 100 nM of compound 6b (A) and in the absence (top) or presence (bottom) of 100 nM of compound 6c (B). (C) Concentration-dependent blockade of the rat hERG K^+ channel by 6b. The IC50 value derived from the data is 22 ± 4 nM, and the nH value (Hill coefficient) is 0.64 ± 0.07 (n = 3).

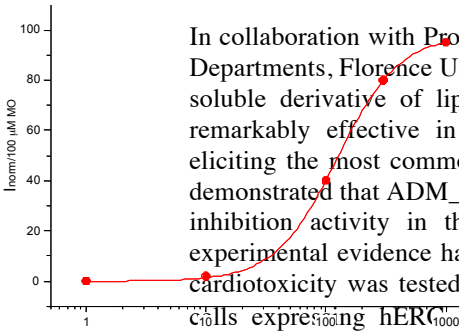


Fig. 3: Dose-response curves of Parthenolide on the activation of TRPA1. The EC50 ("half maximal effective concentration") value is 124 ± 1 µM.

In collaboration with Prof. Nativi and Prof. Ghelardini (Pharmacology and Chemistry Departments, Florence University) we have carried out a study on the effect of a water soluble derivative of lipoic acid, named ADM_09. This compound proved to be remarkably effective in the treatment of oxaliplatin-induced neuropathy without eliciting the most common negative side-effects. Whole-cell patch clamp recordings demonstrated that ADM_09 is an effective antagonist of the TRPA1 receptor, showing inhibition activity in the low micromolar range; a mode of action fitting the experimental evidence has been proposed for the observed blocking activity [2]. The cardiotoxicity was tested *in vitro* by recording whole-cell currents through HEK293 cells expressing hERG channels. In presence of 30 µM ADM_09, the measured outward current was reduced by 14.7 ± 5.4% with respect to the pure vehicle (Fig. IC_{50}>30 µM). According to a general system for ranking the inhibitory potency toward the hERG channel, compounds showing IC_{50} values larger than 10 µM are considered non-cardiotoxic. Thus, the hERG assay demonstrated that ADM_09 was largely above the toxicity threshold.

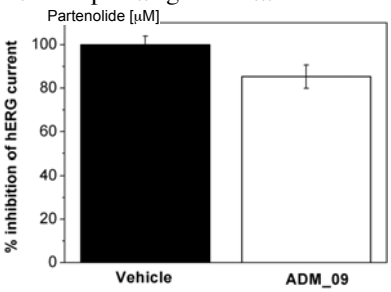
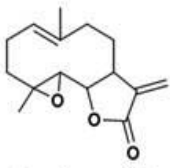


Fig. 2: Effect of 30 µM ADM_09 on hERG channels expressed in HEK293 cells.

In collaboration with Prof. Geppetti (Head of the Headache Center and Clinical Pharmacology Unit, Florence University) we studied Partenolide (PTL), a new TRPA1 modulator [3]. PTL is a sesquiterpene lactone (Fig. 3) derived from the leaves of the traditional herbal medicine feverfew (*Tanacetum parthenium*).



PTL has been traditionally used in Europe to treat inflammatory diseases. The biological activity of PTL is thought to be mediated through the α-methylene-γ-lactone moiety and the epoxide in its structure. However, the mechanism by which this occurs and the molecular targets of PTL are unclear. Electrophysiology and fluorescence experiments showed that PTL selectively activates, in a concentration-dependent manner, human or mouse recombinant TRPA1 channel, expressed in HEK293 cells (Fig. 3).

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1B – Spectroscopic measurements on P-type ATPases for functional characterization and inhibition studies

G. Bartolommei, M.R. Moncelli, F. Tadini-Buoninsegni
(University of Florence, Department of Chemistry)

Aims

Biochemical measurements of ATPase hydrolytic activity. Investigation of the ion transport mechanism in P-type ATPases. Characterization of inhibitory effects of compounds that interfere with enzyme functionality.

Results

P-type ATPases belong to the class of phosphatases, which are enzymes able to remove a phosphate group from their substrate by hydrolytic cleavage. P-type ATPases couple ATP hydrolysis to the transport of ions against their electrochemical potential gradient across cell membranes. ATPase hydrolytic activity is measured to evaluate enzyme functionality, as well as to provide useful information on possible inhibitory effects of compounds that interfere with the hydrolytic process.

We have optimized a molybdenum-based colorimetric method that makes use of potassium antimony (III) oxide tartrate (originally employed for phosphate detection in environmental analysis) to allow its use with phosphatase enzymes [1]. Under carefully controlled experimental conditions, an antimony-phosphomolybdate complex is formed when phosphorus is present as inorganic (orto)phosphate ion. This complex is blue-colored and therefore adsorbs light in the visible range, allowing its use in quantitative determination of phosphate released during the ATPase reaction cycle. The method was successfully applied to native and recombinant ATPases, i.e. Na,K-ATPase and sarcoplasmic reticulum Ca-ATPase, to demonstrate its reliability, validity, sensitivity and versatility (Fig. 1).

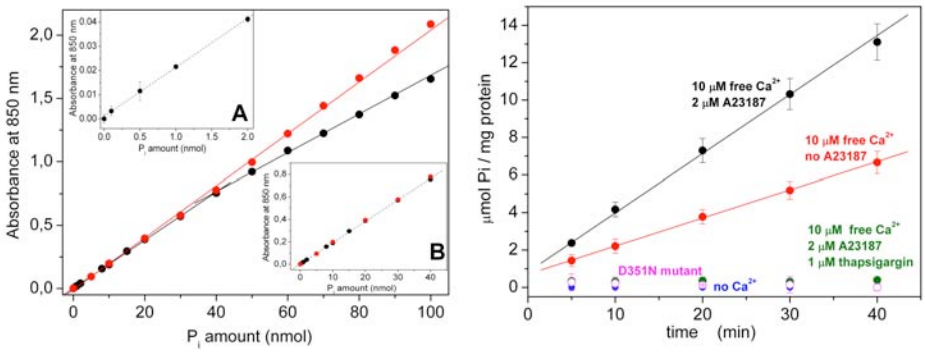

Fig. 1: *Left panel:* the range of linearity for the new method is 0.1–40 or 0.1–100 nmol Pi, **with** or **without** citrate, respectively. *Right panel:* application of the method to recombinant (wild type and D351N mutant) SERCA.

Our method introduces significant improvements to well-established experimental assays, which are currently employed for ATPase activity measurements. Therefore, it may be valuable in biochemical and biomedical investigations of ATPase enzymes, in combination with more specific tests, as well as in high throughput drug screening.

In our laboratory, the ion transport mechanism of P-type ATPases has also been investigated by a fluorescence technique that makes use of electrochromic styryl dyes. These dyes are organic molecules that can be incorporated into lipid bilayers with a very high lipid/water partition coefficient, and may sense local changes of electric field strength resulting from charge movement within the protein, thereby changing their fluorescence emission level. The fluorescence technique is useful to identify electrogenic steps in the ion pump cycle, as well as to analyze the effects of various inhibitors on the ATPase reaction kinetics [2].
Recently, we have employed steady-state fluorescence spectroscopy to investigate the molecular mechanism underlining Na,K-ATPase inhibition by Pb^{2+} ions [3]. Fluorescence measurements were performed using the electrochromic styryl dye RH421. We demonstrated that Pb^{2+} ions can bind reversibly to the protein and do not affect the Na^+ and K^+ binding affinities in the two main conformations of the enzyme, i.e. E_1 and phosphorylated E_2 state. This result indicates that Pb^{2+} binding to the protein does not block the access pathway to the ion binding sites. Interestingly, our measurements indicate that Pb^{2+} bound to the enzyme stabilizes an E_2-type conformation. In particular, under conditions that promote enzyme phosphorylation, Pb^{2+} ions are able to confine the Na,K-ATPase into a phosphorylated E_2 state, thereby interfering with hydrolytic cleavage of the phosphoenzyme intermediate (Fig. 2).

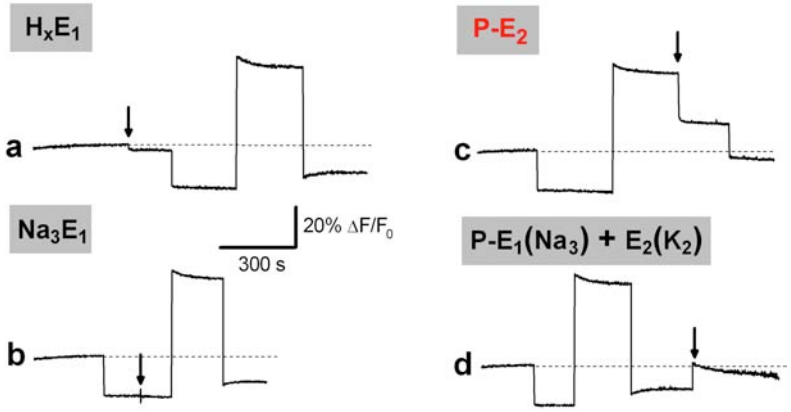

Fig. 2: Representative series of standard experiments showing the traces obtained by adding 10 μM Pb^{2+} in correspondence of the various steady-state fluorescence levels. The preferentially adopted conformation when Pb^{2+} is added is highlighted in grey. Lead(II) ions are added where indicated by the arrows. It is evident that a greater effect is obtained when Pb^{2+} is added to P-E_2 conformation (trace c).

We are now interested to extend the fluorescence method to recombinant ATPases, since it is mainly employed with native proteins that are usually present in higher concentration.

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1B – Wormlike micelles: relation between molecular interactions and bulk rheological properties

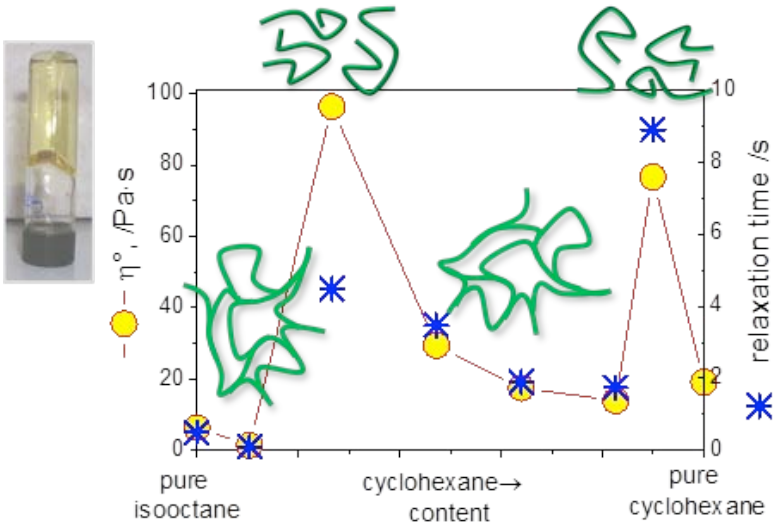
G. Palazzo, R. Angelico, G. Colafemmina, S. Murgia

Aims

In solution, surfactant molecules self-assemble into micelles of various shapes. Among these, very long cylindrical and flexible micelles have gained considerable interest because their remarkable visco-elastic properties are exploited in numerous technological fields. Deviations (defects) from the predominant cylindrical shape such as spherical end-caps and branched junction points do influence the rheological behaviour of these complex solutions.

Results

The effect of inter-micellar connection (branches) on the rheology of wormlike micelles was investigated in detail. The system chosen is made of lecithin, minute amounts of water and organic solvents. Lecithin and water self-assemble into wormlike reverse micelles that can be branched or unbranched depending on the oil composition (and on the water content). In this respect, cyclohexane favours disconnected reverse micelles while isooctane promotes the formation of branches. By using mixtures of cyclohexane and isooctane as oil phase and different water/lecithin ratios, the branch density of the system can be finely tuned. PGSE-NMR experiments allow to distinguish between branches free (unbranched) and branched systems and the response of the very same samples to mechanical stress has been measured by rheology. This allows, for the first time, an experimental correlation between rheological properties and the presence of branches. It turned out that the presence of few inter-micellar connections sensibly decreases the zero-shear viscosity measured in steady state flow curves. Comparison with oscillatory rheology experiments indicates that the main effect of branches is to shorten the terminal relaxation time by speeding-up the reptation.



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1C – Ion Specific Effects Part 1. How salt concentration and the type of buffer affects Hofmeister series reversal for lysozyme

A. Salis, F. Cugia, B.W. Ninham, D.F. Parsons, M.Boström, M. Monduzzi

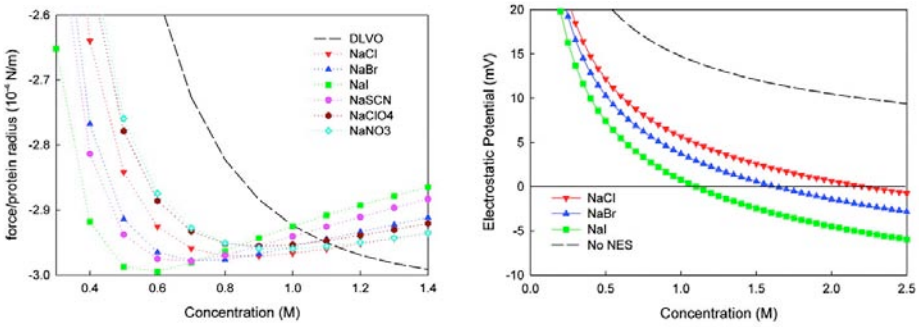
Aims

Ion Specific Effects on protein systems. pH Buffers. Intermolecular Forces. Theoretical Modelling. Electrophoretic Light Scattering.

Results

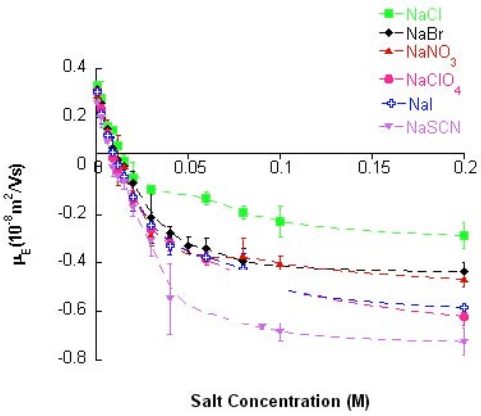
Protein solubility studies below the isoelectric point exhibit a direct Hofmeister series at high salt and an inverse Hofmeister series at low salt concentrations. The efficiencies of different anions measured by salt concentrations needed to effect precipitation at fixed cation are the usual Hofmeister series ($Cl^- > NO_3^- > Br^- > ClO_4^- > I^- > SCN^-$). The sequence is reversed at low concentrations. This has been known for over a century. Reversal of the Hofmeister series is not peculiar to proteins. Its origin poses a key test for any theoretical model. Such specific ion effects in the cloud points of lysozyme suspensions have been recently been revisited. Here, a model for lysozyme is considered that takes into account forces acting on ions that are missing from classical theory. It is shown that both direct and reverse Hofmeister effects can be predicted quantitatively.

The attractive/repulsive force between two protein molecules was calculated (A). To do this a modification of Poisson-Boltzmann theory is used that accounts for the effects of ion polarizabilities and ion sizes obtained from ab-initio calculations. At low salt concentrations adsorption of the more polarizable anions is enhanced by ion-surface dispersion interactions. The increased adsorption screens the protein surface charge, so reducing the surface forces to give an inverse Hofmeister series. At high concentrations enhanced adsorption of the more polarizable counter-ions (anions) leads to an effective reversal in surface charge (B).

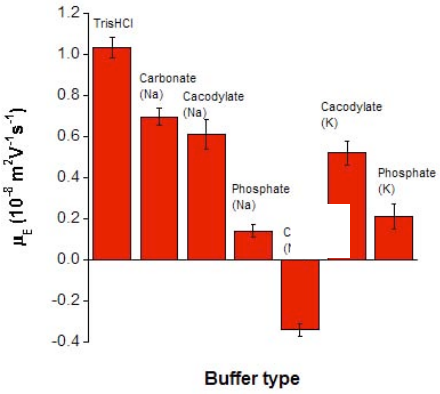


Consequently an increase in co-ion (cations) adsorption occurs, resulting in an increase in the surface forces. It is demonstrated that among the different contributions

determining the predicted specific ion effect, the entropic term due to anions is the main responsible for the Hofmeister sequence at low salt concentrations. Conversely, the entropic term due to cations determines the Hofmeister sequence at high salt concentrations. This behavior is a remarkable example of the charge reversal phenomenon.



The occurrence of charge reversal was then demonstrated by means of Electrophoretic Light Scattering (ELS) measurements. Lysozyme dispersions in the presence of different sodium salts were carried out at pH < pI (C). These were used to compare with protein-protein energy estimates. To do this electrophoretic mobilities were first used to calculate the zeta potentials (not shown) of dispersed lysozyme particles. The change in the sign of the mobilities ("charge reversal") observed confirmed theoretical predictions. The calculated values of lysozyme zeta potential were then used to calculate the repulsive interaction energy between model spherical particles having the same size of lysozyme. Thanks to such data we have then been able to reproduce a trend comparable with that observed for the cloud point temperatures of lysozyme. Similar experiments were carried out in the presence of different buffers at the same nominal pH (D). The observed electrophoretic mobility is due an interplay among ion specificity, pH and buffers. The role of buffers is not just to regulate bulk pH only. As well as strong electrolytes, also buffer species specifically interact with protein surface. This affects the effective charge of the protein (and hence, its electrophoretic mobility). All these results are not surprising in the new theoretical framework which properly includes dispersion forces.



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A

1C – Ion Specific Effects Part 2. Influence of ionic strength and specific ion binding on surface charge of BSA protein

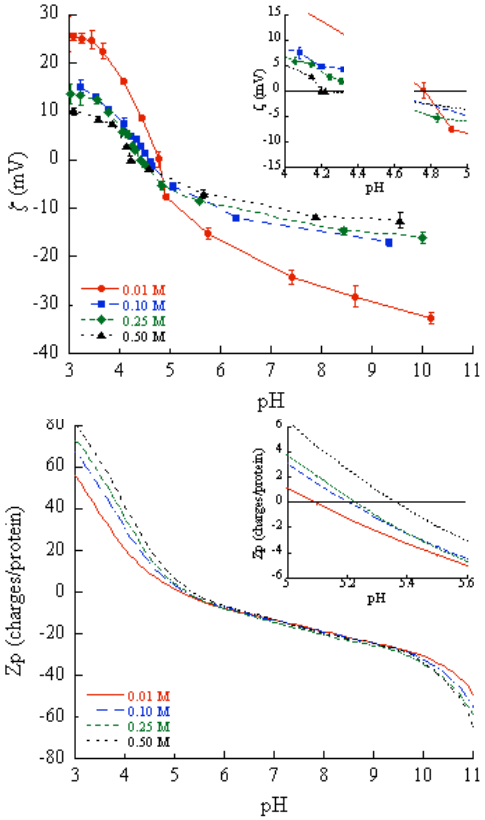
A. Salis, L. Medda, F. Cugia, B. Barse, B.W. Ninham, D.F. Parsons, M. Boström, M. Monduzzi

Aims

Ion Specific Effects on Protein systems. Intermolecular Forces. Determination of surface charge through potentiometric titrations and Electrophoretic Light Scattering.

Results

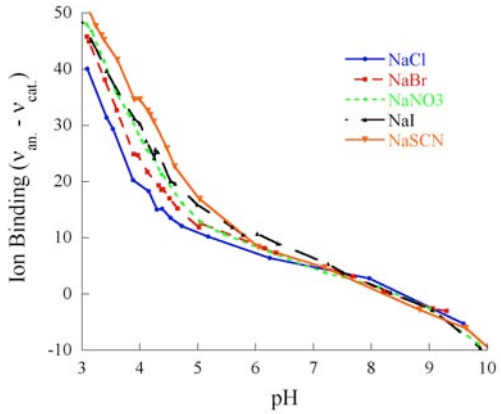
The points of zero charge/potential of proteins depend not only on pH but also on how they are measured. They depend also on background salt solution type and concentration. The protein isoelectric point (IEP) is determined by electrokinetical measurements (A), whereas the isoionic point (IIP) is determined by potentiometric titrations (B). We used potentiometric titration (PT) and electrophoretic light scattering (ELS) measurements at different NaCl concentrations to study systematically the effect of ionic strength on IEP and IIP of Bovine Serum Albumin (BSA) aqueous solutions. It is found that high ionic strengths produce a shift of both points towards lower (IEP) and higher (IIP) pH values.



This result was already reported more than 60 years ago. At that time the only available theory was the purely electrostatic Debye-Hückel theory. It was not able to predict the opposite trends of IIP and IEP with ionic strength increase. Here, we extend that theory to admit both electrostatic and nonelectrostatic (NES) dispersion interactions. The use of a modified Poisson-Boltzmann equation for a simple model system (a charge regulated spherical colloidal particle in NaCl salt solutions), that includes these ion specific interactions, allows us to explain the opposite trends observed for isoelectric point (zero zeta potential) and isoionic point (zero protein charge) of BSA. At higher concentrations an excess of the anion (with stronger NES interactions than the cation)

is adsorbed at the surface due to an attractive ionic NES potential. This makes the potential relatively more negative. Consequently the IEP is pushed towards lower pH. But the charge regulation condition means that the surface charge becomes relatively more positive as the surface potential becomes more negative. Consequently the IIP (measuring charge) shifts toward higher pH as concentration increases, in the opposite direction to the IEP (measuring potential).

The same techniques, PT and ELS, were then used to investigate BSA surface charge (Z_p) versus pH curves. It is found that they depend on anion specific effects. The effect is appreciable at a physiological concentration of 0.1 M. Despite the fact that protein titrations were extensively studied by Tanford and coworkers, as well as by many other authors before and after him, a study of specific ion effects has, surprisingly, not been reported previously. But the result is per se not really surprising. Z_p /pH curves are ion specific both below and above the isoionic point according to a Hofmeister series: $Cl^- < Br^- < NO_3^- < I^- < SCN^-$. At first sight the ion specific effects might be more easily rationalized only if the effect of salt concentration is better understood. The effect of different anions, at the same concentration (0.1 M), is to mimic the concentration effect. The more polarizable anions (SCN^-) behaving as do higher concentrations of less polarizable anions (Cl^-).



The combined use of PT and ELS allowed us to quantify ion binding, as the difference between bound anions and cations, in the range of pH investigated (C). We found that anions bind to the protein surface at acidic pH ($Z_p>0$) according to a Hofmeister series, as well as at the isoionic point ($Z_p=0$). This appears to be consistent with the higher polarizability of anions compared with that of cations. Indeed, the number of bound cations exceed that of anions (i.e. $\nu_{anion}-\nu_{cation} < 0$) only at pH > 8.5.

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1C – Effect of the shape on the evaluation of the passive electrical properties of the cell membranes

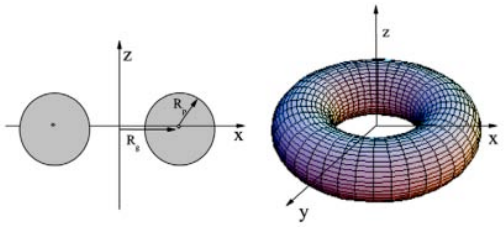
A. Di Biasio, L. Ambrosone, C. Cametti

Aims

The project aims to determine how the cell shape influences the dielectric and conductometric properties of cell suspensions.

Results

The passive behavior of a biological cell membrane under the influence of an external electric field is characterized by two parameter, i.e. the permittivity and the electrical conductivity, which take into account both the dynamical ionic transport process and the structural ionic and polar group arrangements of the cell membrane phase. The study of passive electric properties of the cell membrane is an area of active interest, yielding a lot of information about the structure and physiology of cells and different cell compartments. Radio wave dielectric spectroscopy measurements have been proved to be a method suitable to furnish quantitative data, direct to determination of significant properties of these biological systems. Since the cell membrane is a site of a high field amplification and the effective membrane parameters might strongly depend on the cell geometry, it is in principle uncertain the cell shape can affect the accuracy of the prediction in the electrical behavior and, therefore, it can be understood that the analysis of the experimental data of non-spheroidal cell to the spherical or spheroidal model could yield inconsistent values for the dielectric properties of the components (cytosol and plasmatic membrane). We find that the cell shape induces a higher electric conductivity of both the cytosol (of about 10%) and the membrane (of about 15%). The difference is larger in the case of different elongated particle shape or particle covered by shell non-uniform and/or non-negligible thickness.



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1C – Climate change impacts on Mediterranean coastal lakes and lagoons

S. Loiselle, L. Bracchini, A.M. Dattilo, A. Tognazzi, C. Rossi

Aims

The UNISI research unit is working closely with leading researchers in France, Italy and Morocco to develop long term monitoring and management approaches for coastal aquatic ecosystems. Major activities include the construction of a common database, scenario analysis workshops with local stakeholders in three ecosystems (Pontine Lakes (IT), Camargue (FR), Sidi Boughaba (MO), hydrodynamic and ecological modelling of key energy and matter fluxes in coastal ecosystem dynamics in relation to primary climate drivers, until 2050.

Coastal transitional aquatic ecosystems have a strategic role in meeting the needs and aspirations of current and future populations. Proper functioning of coastal lakes, wetlands, estuaries and lagoons is fundamental for water resources, food production and biodiversity. Yet, they have been witness to a progressive and occasionally irreversible degradation, in particular to their hydrological and biogeochemical cycles, which is further complicated by their sensitivity to climate change. To avoid further losses in resource availability and basic environmental services, an appropriate long term strategy must be developed.

Results

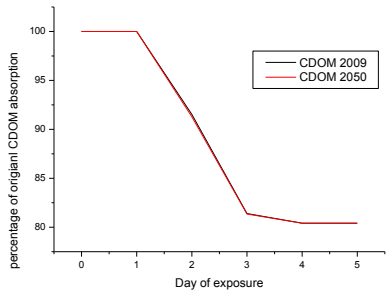
The Medcodyn database structure was completed in May 2009 and the database has been on line since, http://www.medcodyn.unisi.it/. The Medcodyn research team has been uploading data continuously and used the data to examine temporal trends in chemical, biological and physical parameters in the three coastal sites

Ecological and hydrological models were developed to study management options and potential impacts of climate change in coastal ecosystems. In Fogliano Lake, a dissolved oxygen model was developed to examine the impacts of changes in water temperature, sea/lake exchange, wind stress and organic matter load on oxygen concentrations in the water column and sediment, and in particular with respect to anoxia. An organic matter / photodegradation model was developed for each ecosystem considering estimated changes in cloudiness until 2050, with present day optical conditions measured in each ecosystem.

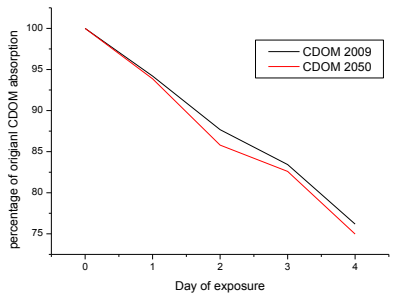
For Sidi Boughaba (Morocco), the lack of long term data made modeling and trends analysis difficult. An intensive baseline analysis of this ecosystem was made and used to set up a long term monitoring plan for local stakeholders and scientists to examine monthly trends in key ecological, hydrological and chemical characteristics of the lake.

Past and future trends in ecosystem dynamics, ecosystem services and climate were used to explore adaptation measures for the three coastal ecosystems studied. Through a process of consultation with stakeholders, indicator and model development,

different adaptation options were identified in relation to their potential success within the context of local and regional environmental change.



Change in absorption of chromophoric dissolved organic matter (CDOM) due to photodegradation by solar radiation in Fogliano Lake for the years 2009 and 2050.



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1C – Self Combustion of Cereals in Risk Assessment for Industrial Safety

G. Bufalo, M. Mosca, L. Ambrosone

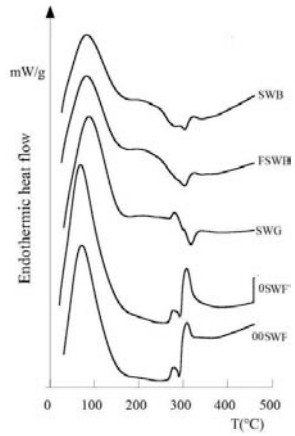
Aims

The project aims to evaluate the characteristics of self-combustion of cereal grains, ground them and to predict their effects on the trigger fires and explosions.

Results

The presence of air is considered to be an essential factor for the combustion of seeds and flour. However, the experiments carried out in our laboratories have shown that some types of seeds, or granules, may give spontaneous combustion even in the absence of air. The classic measure of fire prevention for the silos is the inerting by nitrogen or carbon dioxide, which, in the light of the experimental results, it should be re-thought. Indeed, in some cases, such measures may be completely ineffective and lead to an underestimation of the risk of abnormal temperature increases.

The thermal analysis of cereals, in various forms, shows that the presence of bran causes the formation of exothermic peaks that may trigger phenomena of self-combustion.



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1C – Energy Efficiency, Energy Growth and Complexity Leap

F.Ruzzenenti, F. Picciolo, R. Basosi

Aims

The aims of this project is to study the dynamic interplay between energy efficiency, energy growth and structural complexity of macroscopic thermodynamic systems – human made or biological, on an evolutionary time-scale.

The research project aims at studying the energy-evolutionary pattern of complex systems by means of network theory and information theory. Network theory is an evolution of graph theory and information theory extends statistical mechanics to non-experimental analysis. Information theory applied to network theory is commonly defined statistical mechanics of networks. Complex systems are therefore approached as complex networks and information theory -or to better say: statistical mechanics of networks, is employed to define a reference state whence the system can evolve (symmetry breaking).

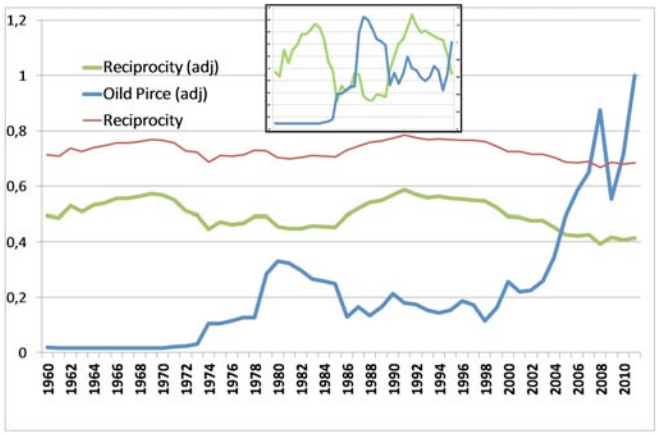

Fig. 1: Weighted reciprocity and adjusted reciprocity (null model: WDCM) in the world trade web compared to the trend in oil prices: the shock follows the symmetry

The research project develops two major lines:

1. investigating complexity leap as a result of symmetry breaking in the system' space that eventually affects the topological space of the network;
2. investigating the role of saturation in the symmetry breaking.

The first line assumes that symmetry breaking occurs in a underlying space of system's interacting components that would inevitably affects the topology of the describing network, whereby detection is possible. The second line investigates the occurrence of saturation in systems' growth stage and the hypothesis that saturation determines symmetry breaking.

Results

The analysis applied to the World Trade Web -here considered as the describing network, highlighted that a symmetry breaking in the topology of the network occurred between the late 1970's and the mid 1980's. According to our analysis the symmetry breaking actually occurred in the economic space of the productive structure and the transition reflected in the topological space of the WTW. A meaningful evidence of this hypothesis is given by the high correlation between oil price and a measure of network symmetry: weighted reciprocity (Squartini et al, 2013). Furthermore, it is noteworthy that the oil shock followed the symmetry breaking in reciprocal structure of the WTW (Fig 1). A dramatic energy efficiency change affected delivery costs of firms and the economic space changed thereafter. Symmetry breaking was thus firstly approached in terms of reciprocity of the binary network, and then in terms of euclidean embedding space and reciprocity of the weighted network. The study of the space embedding of the network shows that the system expanded because of the structural change (symmetry breaking), see Figure 2 (Ruzzenenti et al., 2012). It was thereby investigated the weighted structure of the network, as highlighted in Figure 1.

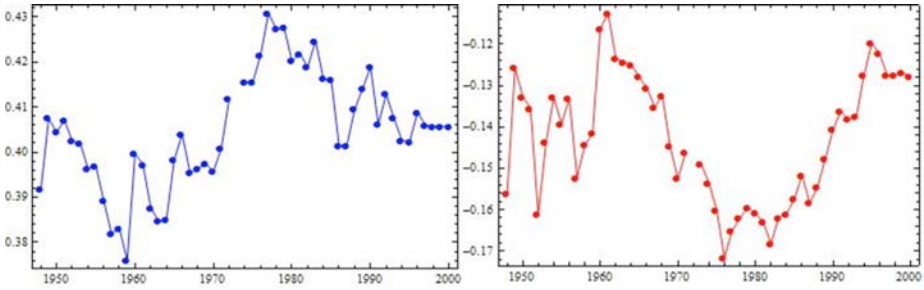

Fig. 2: Spatial filling of the WTW, normalized measure. In blue the spurious measure, in red, the measure discounts topological effect. The red line shows that if we wash out the topological evolution of the WTW, the system expanded after the 1980s.

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1C – Computational spectroscopy of protein radicals

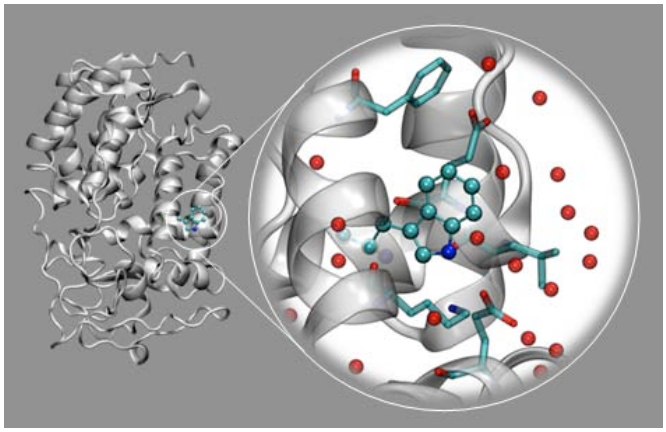
C. Bernini, R. Pogni, M. Olivucci, R. Basosi, A. Sinicropi

Aims

Redox-active amino acids form catalytically active, one-electron oxidized radicals that occur as key intermediates in many biological electron transfer reactions. State-of-the-art quantum-mechanics/molecular-mechanics (QM/MM) and dynamical QM/MM (QM/MM MD) methods are used to characterize the electronic, vibrational, and magnetic properties of these radicals in proteins and enzymes. The information obtained on these important reactive intermediates opens the way to a comprehensive understanding of amino acid radical-mediated electron transfer reactions.

Results

Hybrid quantum mechanics/molecular mechanics methods (QM/MM), in combination with methods of molecular dynamics (MD), have been used to characterize protein radicals, mainly tryptophan and tyrosine radicals, involved in long-range electron transfer pathways of several proteins/enzymes. In particular, we employed density functional theory and multiconfigurational perturbation methods to construct QM/MM models of i) versatile peroxidase (VP) from *Pleurotus eryngii* and its W164Y variant; ii) lignin peroxidase (LiP) from *Phanerochaete chrysosporium*, two engineered variants of LiP and C*oprinus cinereus* peroxidase (CiP); iii) two *Pseudomonas aeruginosa* azurin mutants (Az48W and ReAz108W); iv) cytochrome c peroxidase (CcP) from *Saccharomyces cerevisiae*. The models have been capable of reproducing specific features of their observed UV-Vis, resonance Raman, and electron paramagnetic resonance spectra.



The proper modeling of the environmental effects within the QM/MM protocol, in combination with the available experimental data, has made it possible the unambiguous assignment of the experimentally detected radical species and the clarification of the nature (neutral deprotonated or cationic protonated) of the intermediates. Furthermore, a mechanistic description of the proton-coupled electron transfer process leading to the radical formation has been obtained. Additional details on the role played by the nearby protein residues and solvent water molecules in affecting the spectral properties and the geometrical structure of the radical intermediates have also been provided. Indeed, the computational models are able to correctly replicate the spectral changes imposed by the eventually contrasting hydrophobic and hydrophilic environments in which the radicals are embedded. Most

importantly, the same models have proven useful to disentangle the molecular-level interactions responsible for such changes. The results obtained are expected to shed new light on the catalytic mechanism involving radical species and thus open the way to a comprehensive understanding of radical-mediated ET reactions.

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2A – Calcium and barium hydroxide nanoparticles for the consolidation of wall paintings

N. Toccafondi, G. Poggi, D. Chelazzi, Y. Jaidar, R. Giorgi, P. Baglioni

Aims

Consolidation of wall paintings with compatible inorganic materials.

Results

The consolidation and protection of immovable works of art, such as wall paintings, plaster and stone artworks can be successfully achieved by using dispersions of alkaline-earth metal hydroxide nanoparticles. Before the introduction of nanotechnology in the conservation field, synthetic organic materials were widely applied by conservators for consolidation purposes. Unfortunately, their presence on artistic substrates was shown to be detrimental due to the different physico-chemical properties of polymers with respect to the materials constituting the original artworks. On the other hand, alkaline-earth hydroxides exhibit high compatibility with many artistic and architectonic substrates and thus represent a valid alternative to the organic coatings. The nanosized structure of the applied crystalline phases, together with the dispersing medium, is a crucial factor for the efficacy of the consolidation: in fact, particle size influences their reactivity and penetration through porous matrices. Furthermore, particles polydispersity greatly affects their performance on substrates. For example, matrices to be consolidated often exhibit wide pores size distributions; in these cases the usage of suitable bimodal dispersions is advisable for the best consolidation.

It appears thus evident that the processes involved in the preparation of nanoparticles and their dispersion in carrier media, all play fundamental roles in determining the final effectiveness and applicability of these conservation tools. Synthetic pathways and peptization methods are both important to shape and finalize the particles down to the desired properties, so to meet the requirements of specific consolidation issues.

The same period during which the usage of polymeric coatings was very popular, saw the development of the first compatible consolidation method for wall paintings by Enzo Ferroni, who introduced several elegant solutions to solve the conservation issues following the disastrous flood of Florence, in 1966. In particular, the so-called Ferroni–Dini method, designed for the conservation of sulfate polluted wall paintings, consists in applying ammonium carbonate and barium hydroxide aqueous solution loaded on poultices, in a two-step procedure.

An improvement of this method is represented by the usage of a dispersion of barium (alone or in mixture with calcium) hydroxide nanoparticles, or, in other words, of a colloidal system instead of a solution. Recently, new formulations of barium hydroxide nanoparticles, alone or in combination with calcium hydroxide, have been successfully used for consolidation of degraded wall paintings, even in presence of large amount of salts.

These methodologies are currently used for the consolidation of wall paintings in Italy and other countries, including Mexico (for the conservation of mesoamerican paintings in Calakmul, Tlatelolco, Mayapan, Cacaxtla, Cholula and, more recently, Ixcaquixtla), Sweden, Israel, and Denmark.
CTS company (Italy) is now distributing in several countries this nanomaterial, whose trade name is "Nanorestore®", produced at the CSGI laboratory. Nanorestore is the first chemical product based on nanotechnology, made available specifically to the conservator community.

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2A – Nanotechnology for the deacidification of cellulose-based works of art

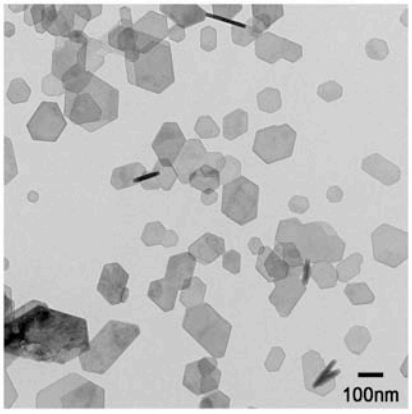
G. Poggi, N. Toccafondi, R. Giorgi, P. Baglioni

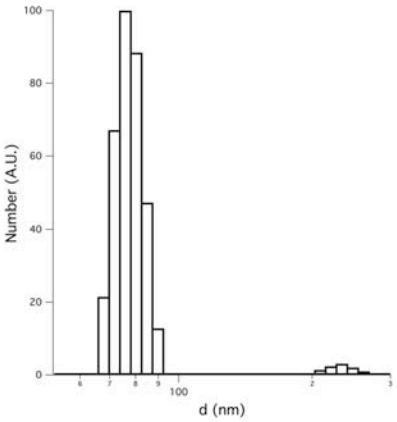
Aims

Deacidification of paper, manuscripts and wooden objects by means of alkaline earth metal hydroxide nanoparticles.

Results

Among the treatments used for the preservation and conservation of cellulose artistic substrates, deacidification represents the most diffused method, considering the primary role of acid-catalyzed hydrolysis in the degradation of cellulose-based works of art. In fact, almost every paper sheet produced in the past four centuries may be a carrier of potentially hazardous acid compounds that could initiate a degradation of the paper itself. For example, iron gall ink, obtained from the reaction between gallic acid and ferrous sulfate, leads to the formation of sulfuric acid. Moreover, "alum-rosin" sizing, introduced in the first decades of 1800 requires the usage of the two reagents, both extremely acidic, directly added to the stock before paper was formed. In the case of canvas, recent measurements made in the EU-PROPAINT project have shown that levels of trapped organic acids within a frame enclosure of easel paintings exceed recommended threshold levels of 1000μg/m3 and could cause long term damage. In addition to that, also archaeological wood can also be corroded by acid products, as in the case of the Swedish warship Vasa, whose preservation is probably





one of the most challenging tasks that conservators are facing these days.

Carbonates and hydroxides of alkaline earth elements, such as calcium and magnesium, are usually selected for the deacidification of cellulose-based artworks due to their high compatibility. Recently, the contribution of colloids and materials science to the conservation framework has lead to the development of innovative

solutions capable of overcoming the main issues of traditional methods. In particular, dispersions of alkaline nanoparticles, mainly calcium and magnesium hydroxide in non-aqueous solvents, have been proposed as efficient deacidifying treatments for cellulose-based works of art, such as paper, manuscripts and archaeological wood.
These nanoparticles, due to their high reactivity, provide a stable neutral environment by rapidly turning into mild alkaline species (carbonates). This will have the effect of hampering the β-alkoxy elimination, i.e., the alkali-catalyzed degradation of strongly oxidized paper that may be associated with the application of traditional deacidification methodologies, especially when aqueous methods are used. Moreover, low polar solvents (such as short chain alcohols usually used for the dispersing nanoparticles) offer good wetting properties without damaging cellulose fibers whilst ensuring a homogenous distribution of particles within the artworks supports.
Recently, a new method for obtaining calcium hydroxide nanoparticles has been developed, based on a solvothermal reaction at high pressure and temperature. The main advantage of the synthetic procedure relies in the possible future up-scale of the process, with great benefits in term of costs. For the production of these nanoparticles, calcium metal and short chain alcohols are mixed in order to obtain a calcium alkoxide, which turns to hydroxide after the addition of water to the reaction bulk. For deacidification purposes, two dispersions are usually prepared, starting from ethanol and n-propanol.
The effects of deacidification with calcium hydroxide nanoparticles, obtained via a solvothermal reaction and dispersed in alcohols, have been investigated. In particular, artificially acidified paper and canvas samples and wood from the warship Vasa have been deacidified by using calcium hydroxide nanoparticles, which homogenously penetrates into the substrates, increasing the resistance of cellulose to ageing.

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2A – Non-polar nanoparticles dispersions for the pH adjustment of parchment, leather and modern inks containing documents

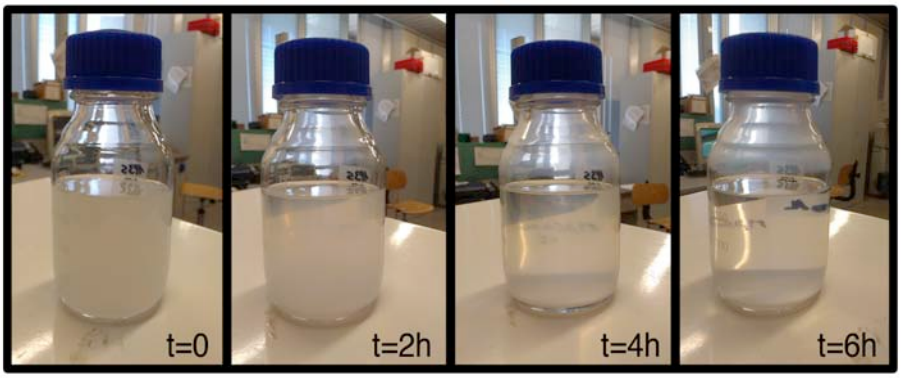
G. Poggi, D. Chelazzi, R. Giorgi, P. Baglioni

Aims

The preparation and synthesis of non-polar dispersions of alkaline-earth metal hydroxide and carbonates for the deacidification of parchment, leather and containing modern inks documents.

Results

The development of acidity as a consequence of natural ageing usually affects parchment and leather, as well as cellulosic materials. In the framework of a European project called Nanoforart, coordinated by the CSGI unit of Florence, the control and adjustment of pH of these materials is under study.
Considering the sensitivity of parchment and leather, as well as the one of modern inks and stamps present in paper documents and books, to water and to other low polar solvents, i.e. short chain alcohols, for deacidification purposes the usage of non-polar medium as dispersing agent for alkaline nanoparticles is advisable.
In this regard, several solvents are currently being tested on real samples, in order to select the best dispersing agent for the intervention on unique and historically valuable artworks. For example, in the Archivo Historico del Museo National de Antropologia (INAH) laboratories in Mexico City, official documents, containing several different types of modern inks, are being used as reference systems for compatibility tests. Benzyl alcohol, amyl acetate, ethyl acetate, xylene, methyl ethyl ketone, cyclohexane are some of the solvents selected and tested also in the Instituto del Patrimonio Cultural de España (IPCE) laboratories of Madrid. Both these institutions are working in the framework of the European project Nanoforart, among with other 13 partners.



For what concerns leather and parchment, other institutions are evaluating the compatibility of the same solvents with historical and modern samples.

From these preliminary tests, it seems that cyclohexane and heptane are suitable dispersing media that can be used on modern inks, as well as on parchment and leather, without altering the original characteristics of the materials.
Due to past experience on the synthesis of calcium and magnesium hydroxide nanoparticles for deacidification purposes, CSGI researchers are taking care of the preparation of non-polar nanoparticles dispersions.
Promising results, in terms of stability and nanoparticles size, have been recently obtained. Calcium hydroxide nanoparticles, synthesized via a solvothermal reaction at high temperature and pressure, can be stably dispersed in cyclohexane, leading to a system that can be safely used on water and polar solvents sensitive materials.
Other partners of the Nanoforart project, i.e. MBN Nanomaterialia and Zentrum für Bucherhaltung GmbH (ZFB), are working on the non-polar dispersions, focusing on the preparation of systems containing calcium and magnesium hydroxide carbonates, which may act as mild alkaline buffer on works of art.

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2A – Silica Gelatin composite for removal of chromate from water solutions

F. Lopez, A. Ceglie, F. Venditti (C.O.S.I.B. Termoli)

Aims

The main aim of this project is the removal of toxic ions from wastewater. For this purpose a new composite was fabricated characterized and utilized. A further aim of this project is to study the process of Cr(VI) removal by the new composite and determine whether chromate ions adsorption, could be affected by the presence of sulfate ions and a slightly acidic pH. Finally the possibility to use this matrix as reactor for the conversion of Cr(VI) to Cr(III) is evaluated.

Results

We focused our attention on the removal of chromates ions present in the environment. Several materials have been developed and tested, ranging from low cost waste material, such as moss peat, sawdust, zeolites, clay, hazelnut shell, to more sophisticated adsorbents, such as activated carbon, modified zeolite, modified clay, modified steel slag, nanoscale magnetic material, chitosan based composite.

We proposed a novel composite able to remove hexavalent chromium Cr(VI) from aqueous solutions obtained by adding the silica precursor tetraethoxysilane (TEOS) to the hexadecyltrimethylammonium bromide (CTAB) microemulsion-based gel [1-2]. SEM and NMR analysis showed that this material is made by an interconnected network of gelatin, silicate and surfactant molecules in which water molecules manifest a high mobility. Analyses of the elemental content in the CTAB-silica gelatin composite suggest that the adsorption of chromium takes also places in the internal areas.

Furthermore, we noticed that the composite containing the adsorbed hexavalent chromium left in water for 30 days undergoes a change in colour from yellow to green (Figure 1). This evidence is an indication of the reduction in situ of Cr(VI). X-ray Photoelectron Spectroscopy has been used to characterize the composite materials. Surface analyses performed at different times revealed chromium chemical speciation changes as a function of the pollutant-material interaction time (Figure 2) [3].

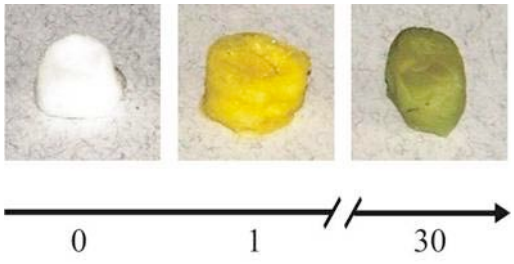
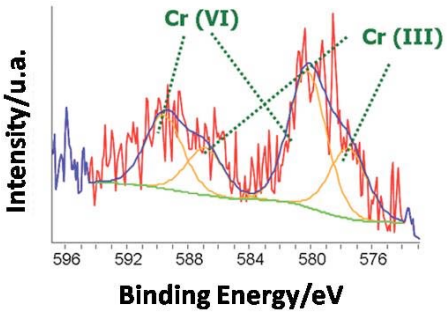
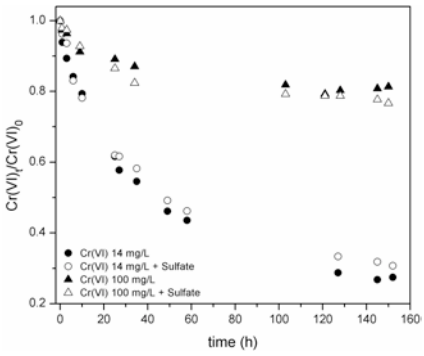


Fig. 1

Moreover, the removal of chromate was assessed also through evaluation of the adsorption kinetics of chromate ions on the composite under equilibrium conditions in the presence of sulfate ions and at a slightly acidic pH condition (pH 5.8) [4-5]. Adsorption competition tests in the presence of sulfate ions showed that Cr(VI) was still effectively adsorbed from aqueous solution regardless of the presence of the competing anions (Figure 3). The equilibrium adsorption data were fitted by Freundlich adsorption isotherms and confirmed that the adsorption efficiency of chromium on the CTAB–silica gelatin composite was unchanged in the presence of sulfate ions. These findings demonstrated a high specificity of the CTAB–silica gelatin composite for chromium, and highlight the possibility of using this matrix for





efficient removal of chromium from industrial wastewater without the need to eliminate contaminant sulfate ions.

Fig. 2 **Fig. 3**

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2A – Chemical gels for the cleaning of artifacts

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Aims

Removal of undesired materials from water-sensitive artifacts while avoiding solvents penetration.
Formulation of semi-IPN chemical hydrogels.

Results

Nowadays, cleaning procedures on artifacts are mainly based on the use of pure organic solvents. This approach presents some drawbacks for both the object and the operator: solvents can easily penetrate within the porous matrix of the artifact and swell or solubilize paint binders and pigments; a second issue is due to the fact that most of the commonly used solvents are toxic. To avoid these problems, recently conservators are using some confining tools. Most of them are physical gels, such as *solvent gels* or polysaccharide based hydrogels. The first class leave some substantial residues on the surface after the treatment while the second class is fragile and does not offer a suitable control in the release of the cleaning agent.
This project is focused on two main points: limit the use and volatility of free solvents and avoid any gel residues by substituting physical gels with chemical gels.
Chemical gels have strong gel cohesion due to covalent bonding between polymer chains and permit to load high amounts of liquid without undergoing gel solubilization. Chemical gels are versatile and can be functionalized to meet specific issues in conservation.
Cleaning water-sensitive artifacts (e.g. paper manuscripts, canvas paintings, etc.) is at present a problematic intervention in conservation, because the use of water and water-based systems (e.g. microemulsions) could interact strongly with the hydrophilic components of the artifact. Fiber swelling due to an excessive wetting of the fibers can cause mechanical stress or paint detachment. Chemical gels based on semi-interpenetrating polymer networks (semi-IPN) allow to obtain hydrogels that have suitable retention features for the cleaning of water-sensitive artifacts. Semi-IPNs are based on a polymer network that is formed in presence of an interpenetrating linear polymer. We have devised some formulations based on a poly(hydroxyethyl methacrylate) polymer network embedding linear chains of poly(vinylpyrrolidone).
The resulting p(HEMA)/PVP hydrogels are high hydrophilic, their equilibrium water content (EWC) for different hydrogel compositions ranges from 72% to 87%. Hydrogels are able to load water, o/w microemulsions and some pure solvents. By varying hydrogels composition the release/retention features can be tuned, making them suitable for different cleaning purposes.

Removal of grime from a *tempera magra* painting using a water-loaded semi-IPN p(HEMA)/PVP hydrogel.

An innovative approach based on the above-mentioned characteristics concerns the retention of aqueous solution of chelating agents for metal cleaning. These complexants (Rochelle salt, EDTA) can be embedded into the polymeric network thanks to the high hydrophilic capacity of these gels and then released on rough and irregular metallic surfaces to remove undesirable corrosion products. This method allows an extremely selective and controlled cleaning avoiding gels residues, increasing the interface contact area and optimizing the interaction time.

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2A – Peelable polyvinyl alcohol highly viscoelastic dispersions: a new class of cleaning tools for works of art

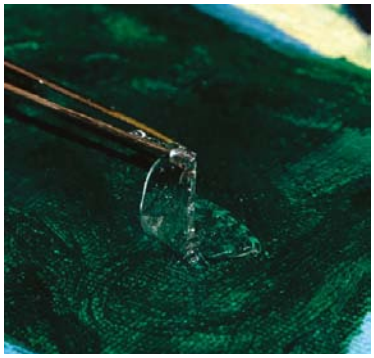
E. Carretti, L. Dei, P. Baglioni

Aims

The main objective of this project was to develop and characterize a new class of gel-like Polyvinyl alcohol highly viscoelastic dispersions (HVPD) cleaning tools for works of art that, even maintaining a good level of performance, minimize both the mechanical action usually needed to achieve the complete removal of traditional gels and the amount of residues left onto the cleaned surface. The ability of poly (vinyl alcohol) (PVA) aqueous dispersions cross-linked with borate ions to give highly viscoelastic systems, in the presence of some of the most largely used organic solvents and additives usually employed during the cleaning of many classes of works of art (metals, wall paintings, easel paintings, stone artifacts), has been largely explored.

Results

It has been observed that the PVA-borate systems do provide selective, surface-controlled cleaning action as well as facile and benign removal from a painting surface. Their very high elasticity allows them to be peeled from a surface without introducing a strong lateral force. By so doing, residues left on the painted surface from the patina and from the cleaning tool are expected to be minimized and the mechanical action and repeated washings usually necessary for the complete removal of traditional gels can be avoided. Moreover, this elasticity can be easily modulated by changing the ratio of PVA to borate or their total concentration.



Recently, it has been found that the weight fraction and range of organic liquids within the aqueous liquids of borate gels can be maximised (up to 50 w/w% for solvents like 2-propanol, acetone, N-Methylpyrrolidone and methyl acetate) by employing poly(vinyl alcohol-*co*vinyl acetate)s (Poly(VA-VAc)) as the cogellants. In particular, the attention has been focused on the Poly(VA-VAc) 80:20 because of the easiness of HVPDs preparation that can be achieved at room temperature.

In order to evaluate the behaviour of these new polymeric dispersions when they are in contact with the painted surfaces and during their removal once they have carried out their function, the rheological properties have been explored as a function of both the organic co-solvent concentration and chemical nature. Frequency sweep curves collected for samples containing different amount of organic co-solvents indicated the presence of a crossover between the G′ and the G″ curves meaning that, at least from the rheological point of view, these systems can be classified as high viscous polymeric dispersions rather than as true gels.
Furthermore, the possibility to load wide range of organic solvents into the cleaning agent increases their ability to swell or soften/solubilize several different forms of deteriorated coatings and varnishes (as well as other hydrophobic substances) as demonstrated in several cleaning tests performed onto artistic surfaces (Santo Stefano by Ludovico Cardi detto il Cigoli, *Incoronazione della Vergine* by Neri di Bicci and others). These systems require no after-washing to remove residues, their cleaning action is easily controlled, and they can be removed in one piece by peeling.

Recently, we have found that inside the HVPDs, apart organic solvents, it is possible to insert also other molecules like chelates that increase the range of possible applications and support that can be treated with these systems. In particular the study of the potentialities of these systems for the cleaning of metal artifacts and for the selective removal of sulphates from the surface of carbonatic stones is ongoing. The preliminary results are absolutely promising.

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2A – Amphiphile-based nanofluids for the cleaning of works of art

P. Baglioni, M. Baglioni, M. Raudino, Y. Jaidar, D. Berti, E. Carretti, L. Dei, R. Giorgi

Aims

Development of innovative, effective and safe systems for the cleaning of painted surfaces.
Combination of cleaning fluid with gels and thickening compounds in order to limit liquid spreading when the substrates to be cleaned are particularly sensitive to water or other solvents.
Comprehension of the cleaning process, in order to become capable of tailoring the formulations according to specific conservative issues.

Results

The removal of undesired material from the surface of a work of art has always been one of the most important and delicate operations in the conservation of cultural heritage. The availability of a great choice of pure organic solvents at first opened up new perspectives for cleaning operations. Nevertheless nowadays, most organic solvents are not the preferred option, in view of their poor-controlled action, their toxicity and the disposal and recycling concerns. Surfactant-based aqueous nanostructured fluids, such as micellar solutions and microemulsions, represent the most effective, safe and selective cleaning media currently available for cleaning operations in the conservation of cultural heritage. Due to their nature, these systems can be used to remove oily grime or hydrophobic substances from hydrophilic surfaces, as it is the case of polymer removal from wall paintings and stones. During last decade the effectiveness of microemulsions and micelles in removing polymers from painted surfaces was thoroughly demonstrated.
Since the removal of wax spots from fresco paintings by Masaccio, Lippi and Masolino (Brancacci Chapel, Basilica del Carmine, Florence), which represented the first example of microemulsion application to conservation of cultural heritage, several other representative case studies, addressing particularly challenging conservative issues, can be reported: the removal of a multilayered aged coating that was irreversibly damaging the pictorial layer of the Annunciation Basilica in Nazareth, the removal of vinyl/acrylic coatings from Mesoamerican wall paintings conserved in the archeological sites of Cholula and Mayapan (Mexico), or the cleaning of the mural paintings in the Conegliano Cathedral façade.
Recently the focus of this study was moved also to other polymers, such as Sokrat 2802A©, which has been widely used in some conservative contexts, such as Eastern Europe or Guatemala. Laboratory and *in situ* cleaning tests have been successfully performed with microemulsions specifically formulated for the removal of Sokrat© coatings.
Sometimes the surfactant can remain on the surface of cleaned works of art as a residue (which, nonetheless, can easily washed away by rinsing with water). Thus, using surfactants that spontaneously degrade to harmless volatile compounds would

be a major advancement of this methodology. Therefore, two nonionic surfactants (Berol OX 91-6© and Berol 266©), which possess interesting (bio)degradability properties, have been proposed to set up new cleaning media, together with water and 2-butanone. The excellent performances of the investigated nanofluids in the removal of organic polymers from wall paintings were assessed by laboratory tests on model systems. As an alternative, a ternary microemulsion containing diethyl carbonate as the oil phase and dodecyl dimethyl amine oxide (DDAO) as the surfactant was proposed. DDAO is a well known and widely used detergent and solubilizing agent, and its degradability and eco-compatibility properties make it particularly suitable for our purpose.

Furthermore, the production of advanced complex highly viscous cleaning tools, in which the main applicative technological advantages of the liquid nano-compartmented systems (i.e. microemulsions and micellar solutions) and the ones of HVPDs and gels are merged, is achieved by embedding the nanodroplets constituting the microemulsion and the micellar solutions in a gel or gel-like matrix.

Micelles, microemulsions, thickened complex fluids, and microemulsion-loaded gels constitute the new ‘‘cleaning palette’’ for modern conservators. The development of these smart nanostructured systems requires the comprehension of their behavior and interactions with other materials down to the nanoscale. Therefore, most recently a major effort has been spent in order to investigate the mechanism of polymer removal from porous artifacts using these nanofluids. The rules of classical detergency seem to not fully address the polymer removal mechanism, and a complete and satisfactory description of the process is still missing. SANS, DLS, NMR, QCM and AFM investigations are being combined in order to obtain a clear picture of the cleaning mechanism.

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2A – The controlling factors of productivity in African Great Lakes

S. Loiselle, A.M. Dattilo, L. Bracchini, A. Cozar, A. Tognazzi, C. Rossi

Aims

The UNISI research unit has been collaborating with 20 research institutions throughout Africa and Europe in the study of the African Great Lakes. These activities were funded by the UK ESPA programme and concluded in 2013. The significance of the East African Great Lakes lies in the ecosystem services that they provide to the local and regional communities (water supply, fisheries, waste disposal, transportation, recreation, tourism, energy, …). To address challenges occasioned by climate change and other regional drivers that compromise ecosystem functioning, researchers from CSGI-UNISI collaborated in the creation of the East African Great Lakes Observatory (EAGLO) to develop an inter-basin knowledge exchange and comparative analysis. The specific objectives of the most recent project were:
To create regionally based protocols for the long term monitoring of resource quality and ecosystem functioning
To improve access to shared data and information,
To develop future scenarios in ecosystem services and lake functioning.
The two PIs, Eric Odada and David Harper worked closely with the Co-PIs, Victor Langenberg, Frank Kansiime and Steven Loiselle together with a large number of scientists and policy makers from 13 East African countries, allowing the network to create a strong regional presence as well as opening up the project to international collaborations.

Results

An inter-lake dialogue and comparison of socio-economic and environmental drivers were made with respect to ecosystem functioning and services, in particular their links to sustainable development and poverty reduction. The workshop used participatory scenario-development methodology coupled with expert and stakeholder presentations. The network identified the need for a regional approach that reinforces and supports policy making and resource management. Specific recommendations were directed at key requirements for successful regional lakes management including: poverty alleviation, monitoring of ecosystems functioning and catchment's land use and fisheries management. Requirements for regional indicators and new communication approaches were developed after extensive discussion. An EAGLO scientific workshop concluded in the constitution of working groups (Regional Monitoring working group, Ecosystem scenario working group, Regional management and communication working group).
Members of each working group conducted specific analysis and developments. Exchange of ideas and progress between working groups occurred particularly on the inter-linkages between ecosystems services and trade-offs. The EAGLO project continued to acquire new participants and attract the attention of policy makers and decision makers throughout East Africa. New proposals and shared activities were

developed where methodological shortcomings and information gaps were identified. The results of these developments were presented at international conferences and published in the second year of the project.
Significant efforts were made to further develop and refine the EAGLO scenario/design approaches and ecosystem analysis tools. These approaches were validated and further refined in the second Scientific Meeting and Scenario Workshop, held in Nairobi (24-27 April, 2012) with the participation of nearly 30 scientists, stakeholders and policy makers from East Africa and beyond. During the workshop, an expert review of the best practices, scenario building, monitoring approaches and management approaches was made. The emerging scenarios were refined and communication products were generated targeting knowledge users. Project delivery strategy and post-project strategies were discussed. Prior to the workshop, consultations were conducted among the scientists and broad cross-section of other actors using an online survey, aimed at, through a Delphi technique, collating expert views of the EAGL ecosystems and poverty linked trends and trade-offs. From the best practices, key lessons were synthesized to inform ecosystem services provisioning, fisheries management and design of tools and methods. Results from the three working groups were integrated to explore the implications of trends of key ecosystem services of the East African Great Lakes region, and then modified (management and monitoring) to respond to optimum trade-offs. Knowledge sharing strategies were further developed, with specific attention on perceived key ecosystem services by regional and community level stakeholders.
Three new issues (co-management, climate change adaptation and ecosystems services valuation) emerged from the scenario activities as well as the findings of the working groups. EAGLO network members strived to integrate them in subsequent activities. Furthermore, to improve the regional comparison of lake ecosystem services, a subgroup of scientists and decision makers began work on a summary matrix of key ecosystem services for EAGLO lakes, based on primary inputs from the EAGLO network and analysis of secondary sources. Specific local case studies were made to explore, analyse and value suites of ES and their livelihood contributions, through empirical work by EAGLO team members (within the limits of the Framework programme).
New working groups (Co-management working group, Climate change adaptation working group and Ecosystem services valuation sub-working group) were formed and worked together to meet these information challenges. The existing working groups contributed with regional information and including the initial results of the new groups into their ongoing analysis.

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2A – Ar.Chi.Min. Archaeology and Chemistry for the ancient mining heritage: a multidisciplinary project for the study of the mining area of Colline Metallifere (Toscana, Italy)

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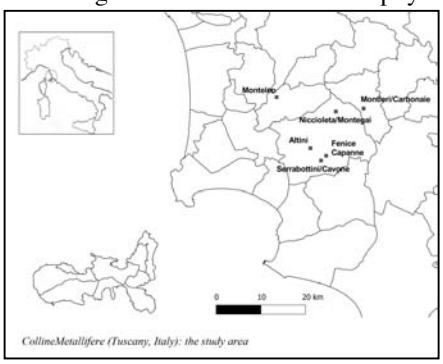
Aims

The aim of this work was the chemical investigation of archaeological settlements of Colline Metallifere with particular reference to archaeo-industrial and mining activities spanning from Etruscan to Medieval time.

Results

The "Colline Metallifere", a wide territory located in the south-west of Tuscany, is characterized by the presence of strong arsenic and heavy metals contamination probably associated to a relevant anthropic impact for the long-standing tradition of ore mining and processing. The great development of mining activity in this area was due to the presence of a large mineral deposit, mainly constituted by mixed sulfide ores that were exploited since Eneolithic age for the extraction of copper, silver, lead and iron. Beside this, considerable alunite deposits underwent to a systematic extraction activity recorded from Late Middle Age to early XIXth century. The area is of extreme relevance for the study of pre-industrial mining and smelting processed. Here, archeological research has been developed since '80 through excavations and surveys, covering a territory of more than 145 km^2, recording and describing over 2500 sites (about 50% of these were ancient mining and/or smelting sites) (1).

The Ar.Chi.Min. project derives from an established collaboration between archaeologists and chemists of the University of Siena (2). It implies the comprehensive study of ancient mining sites, combining classic historical and archaeological observations with physical-chemical measurements and statistical methods. Two main results were expected: i) to get a deeper understanding of the productive and technological horizons of every single site, that is mandatory for their conservation and valorization; ii) to obtain answers about the role played by ancient mining activities in soil contamination, which is crucial for the environment protection of that area. Several analysis campaigns were performed on selected key sites. High throughput analytical data were



CollineMetallifere (Tuscany, Italy): the study area

obtained by a portable XRF instrument.

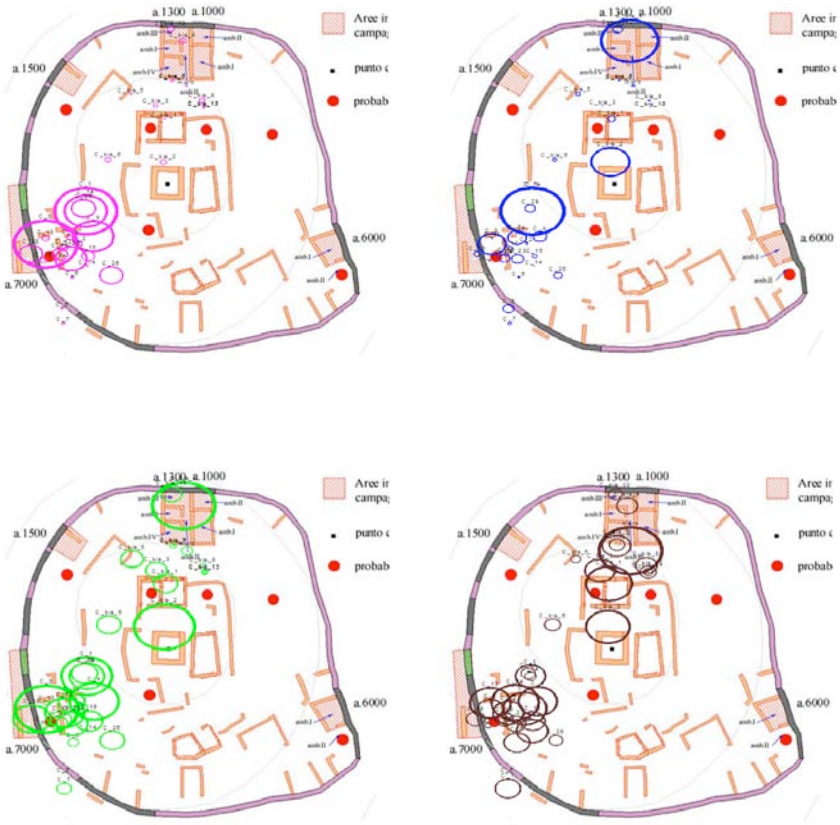


Fig. 1: Castello di Cugnano: an example of results obtained by the chemical analysis of productive mining site by XRF. Going from top left clockwise the distribution of Cu, Pb, Mn and Zn was reported.

Results were merged in a GIS application together with data collected in previous studies and with all the archaeological information, producing a comprehensive database which has high relevance both for environmental monitoring and for historical and technological issues. In particular, recent data revealed that mixed sulfide ores deposits, were exploited for various productive aims according to different historical periods and technological skills. Moreover important evidences emerged about the alum production cycles.

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2A – Impact of land use change and climate on the Biogeochemical cycles of freshwater bodies in China

S. Loiselle, A. Donati, C. Rossi

Aims

Continental aquatic ecosystems such as lakes and reservoirs are considered as large sources of CO_2 to the atmosphere on a global scale. Carbon dynamics are regulated by a combination of biotic and abiotic processes: catchment import and export, detritus dynamics, photosynthetic and respiratory processes in the water column and sediment. Even though these ecosystems occupy only a small fraction of the earth's surface, they play a quantitatively significant role in the global carbon cycle and hence in the climate system. However, this active role remains poorly understood, as carbon sources, carbon sinks and sedimentation in these complex ecosystems is highly sensitive to catchment conditions, climate and ecosystem management. Because climate change will modify catchment sources, local hydrology and degradation processes, significant modifications on carbon sequestration and emission to the atmosphere is expected in the coming decades.

In the project, funded by the Chinese Academy of Sciences, the European Space Agency and the Chinese Ministry of Science and Technology, CSGI researchers and their Chinese colleagues work in close collaboration to examine several key mechanisms in carbon sequestration and release through the development of new technologies to improve analysis and monitoring capacities.

Results

In the last year, the focus has been on the development of algorithms and modelling tools to examine carbon sequestration by phytoplankton dynamics and carbon emission by photo and bio degradation of organic carbon. The results of these activities will be used to estimate primary productivity, and more specifically algal biomass and algal bloom dynamics for the former, and CDOM, POC and DOC dynamics for the latter. The research has combined field work, laboratory studies, model development and algorithm development.

The results of the last year include the study of the spatial and temporal dynamics of chromophoric dissolved organic matter (CDOM) in optically complex inland waters. Semi-analytical and empirical modelling approaches were used to examine CDOM absorption in four shallow inland water bodies using the spectral bands and sensitivities of major satellite observational systems. Of the models examined, an empirical multiband model was found to provide the highest correlation with measured CDOM absorption. The spectral characteristics of the MERIS sensors yielded the best results with respect to the other available satellite sensors. High detritus load was observed to be a major impediment to estimating CDOM absorption while lakes with elevated phytoplankton biomass did not present similar problems.

Another major result was the study of the dynamics of particulate organic matter (POC) in eutrophic waters. A new algorithm was developed to estimate POC concentrations in complex optical environments (aph(620)-based algorithm) and compared to other POC estimation approaches that are based on backscattering or

reflectance ratios. The new optical algorithm was validated and applied to a one-year series of MERIS data in Taihu Lake. The analysis revealed peak concentrations in the spring over a limited geographical area of the lake and more homogeneous concentrations in the summer.

Another result was the study of phytoplankton dynamics, with a particular emphasis on algal blooms. We are presently exploring bloom estimation methods to better identify links to global and local drivers using MODIS, GOCI and MERIS data. Our preliminary results indicate that the use of a new Floating Algae Index (FAI) algorithm was successful in identifying algal blooms in the highly eutrophic Lake Taihu. MODIS 250-m resolution Level-0 data from 2000 to 2012 showed that the spatial extent of the algal blooms reached a maximum in 2006, 2007 and 2010. Temporal and spatial decomposition analyses are being performed to obtain an improved understanding of the blooms dynamics over the study period. Global and regional driver datasets are being explored to identify links to bloom dynamics.

In the coming year, this research will continue with a focus of bringing these results together to understand the links between these carbon pools and their sensitivity to major catchment based and global drivers.

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2A – Innovative and smart materials for the "Made In Italy" technological development: self-cleaning and flame retardant textiles

E. Busi, S. Jez, M.L. Parisi, C. Bernini, S. Maranghi, R. Basosi

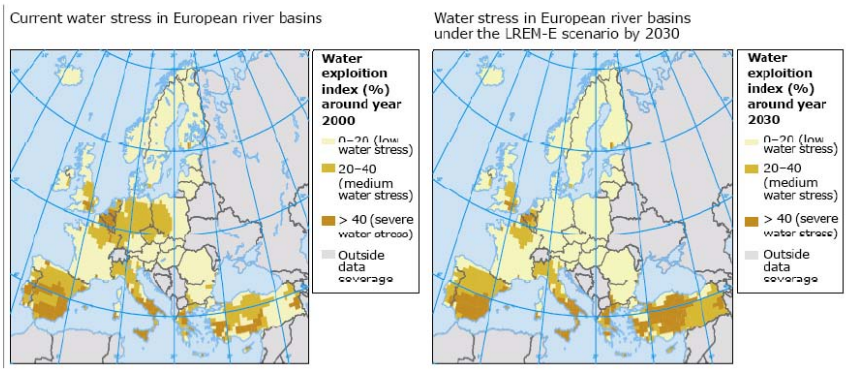
Aims

Life Cycle Assessment (LCA) study of a new generation textiles which are maintainable through simplified industrial washing cycle for work wear applications.

Results

The laundry sector becomes increasingly important in the globalized world, especially for corporate uniforms and particular attention has to be paid to the need for international regulations, sustainable solutions, modern machines, new care labels, energy efficiency and hygiene, as well as the demands on textile-service companies working in the hotel and hospital sectors.

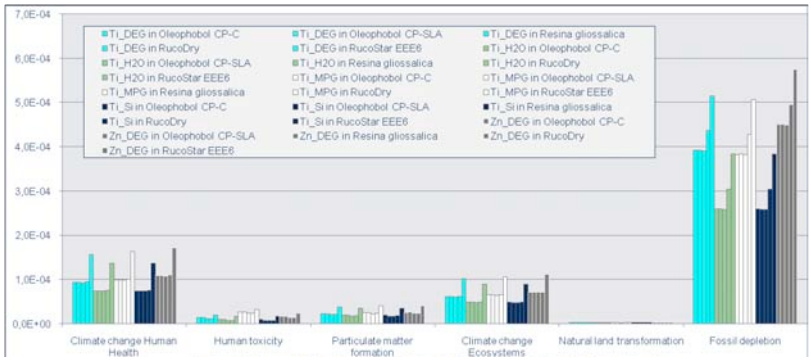
In Italy, laundry sector includes nearly 600 business (Unione Italiana Manutenzione dei Tessili) that just represent 1.6% of the textile industry in Italy: it demonstrates that innovative strategies must be pursued to avoid the production of wastes, over-consumption of water resources, and excessive energy utilization. The Environmental European Agency has predicted a significant reduction in fresh water exploitation (WEI) in the next 20 years and nine European countries, including Italy, can be considered water-stressed; according to the expected reduction in the fresh water exploitation (WEI) up to 40% water saving is one of the most critical issue for the Southern European countries.



The new textile product will allow to define a new washing procedure, characterised by the reduction of the environmental impact of the overall process. The most critical step in the design of the new washing procedure is the design of the functional textiles able to perform a self-cleaning reaction promoted by photo catalysis, to ensure either antibacterial and self-cleaning properties. Whenever these compounds are illuminated by light of energy higher than its band gap, electrons jump from the valence band to the conduction band, and the electron (e^-) and electric hole (h^+) form pairs on the

surface of the photo catalyst. The negative electrons and oxygen will combine to form O_2^-. radical ions, whereas the positive electric holes and water will generate hydroxyl radicals ·OH. Since both products are unstable chemical entities, when the organic compound i.e. dirt, pollutants, and micro organisms falls on the surface of the photo catalyst it will combine with O_2^- and OH^- and turn into carbon dioxide (CO_2) and water (H_2O). Once several photoactive compounds are introduced in the tissue (maintaining mechanical and aesthetic properties of the textiles) via different methods and preparation, another important step in the design of the new washing procedure is the set-up of an innovative washing machine.

In commercial laundries, a plurality of separate washing machines, each with its individual controls, operates on a separate load of laundry by subjecting the laundry to a predetermined sequence of laundering steps, including washing, rinsing, etc. Typically, the laundry is first washed in hot water containing soaps and other additives, and is thereafter rinsed using hot or warm, or sometimes cold, water. In many systems, fresh water is used for each bath and the water of the previous step wasted by being sent to a sewer. The use of a photo catalyst loaded textile will allow to substantially modify the laundry washing machine by installing an irradiation source, able to actively interact with the degradation of persistent soils and so to directly interact with the laundry load, saving water, detergents and heating energy. LCA methodology is used to gain information about environmental impacts and energetic consumptions related to conventional finishing processes both from the literature and available industrial data. In particular, it can be employed for the comparison of two or more different products, groups of products (as in the Figure, where are reported indicator impacts for a series of formulations, calculated by SimaPro 7.3.3 Recipe Method), activities or services thus allowing for weak points identification of the system and improving the environmental performances of products or processes.



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2A – LCA of integrated agro-industrial chains for energy and biochemicals production from renewable sources and for the land valorisation

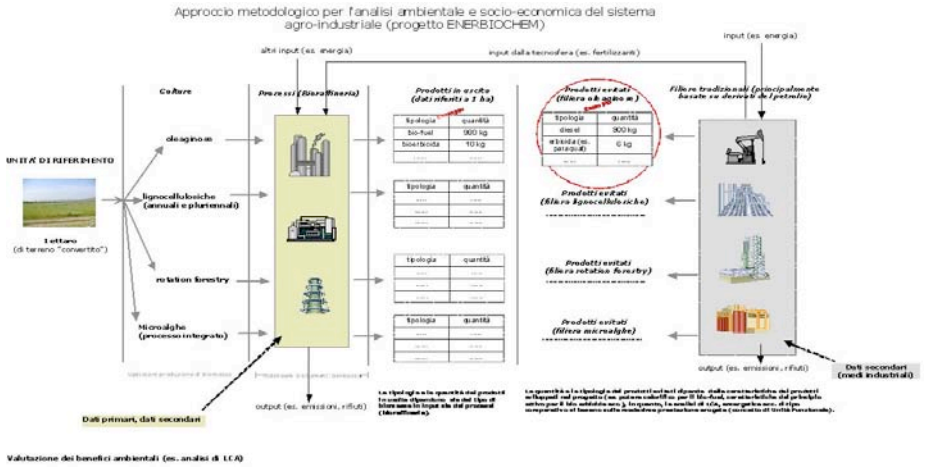
S. Jez, E. Busi, D. Spinelli, M.L. Parisi, R. Pogni, R. Basosi

Aims

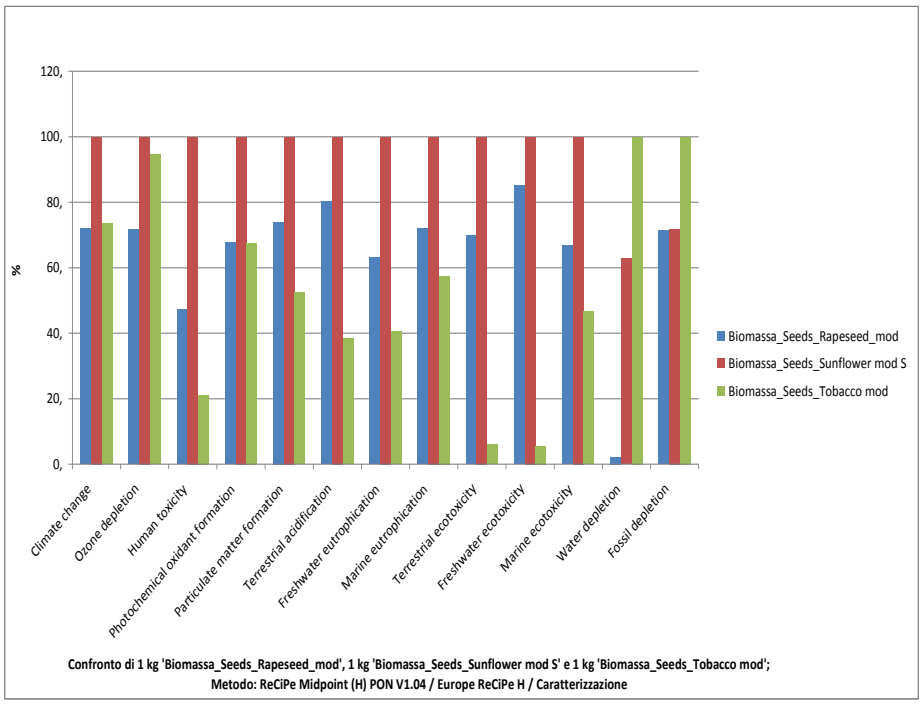
Environmental assessment trough LCA of Integrated agro-industrial chains with high energy efficiency for the development of eco-compatible processes of energy and biochemicals production from renewable sources and for the land valorisation, within a new model of less dissipative system economy.

Results

In the framework of the EnerbioChem project (PON "Ricerca e Competitività 2007-2013") two agro-industrial (from oleaginous and lignocellulosic biomasses) and aquatic biomass (from microalgae) chains are investigated with the aim of maximizing the energetic efficiency, both in the agricultural/production phase than in the industrial processes. Valorisation of residues and by-products through the production of new renewable products such as bio-humus fertilizers, composts, hydro-colloid bio-plastics, are investigate in order to improve the competitiveness of the entire production system. A variety of studies and investigations are carried out on agronomic aspects for production of agricultural biomasses and on other techniques of biomass production (autotrophic algae and yeast), on transformation processes of oleaginous and lignocellulosic biomasses, on optimization of end-products use and recycling of by-products. The analyses on energy efficiency and environmental impacts are carried out on the whole agro-industrial life cycle. Furthermore, the best available technologies (raceway pond and photo-bioreactors) for the microalgae cultivation are compared in order to evaluate the eco-profile of a large scale biomass production: using wastewater as nitrogen source, carbon dioxide from industrial flue gases and renewable energies.



Environmental Impact Indicators (Embodied Energy Analysis (EEA), Emergy Accounting (EA)) and LCA has been applied to oleaginous crops: sunflower, rapeseed and tobacco. The results, according with our previous studies, show that the major impacts and uses of resources of the three crops are due to the production of mineral nitrogen fertilizers and diesel fuel. The comparison of the environmental impact of the three crops (LCA conducted with SimaPro 7.3.3) show that sunflower has the highest impact on most of the impact categories, tobacco has the higher impact on water depletion and fossil depletion caused by irrigation and more intensive mechanization. Preliminary results for microalgae cultivation by photobioreactors show high impact of the reactor design and use of mineral fertilizers for all the environmental impact categories.
Therefore, LCA methodology can be used for the eco-profile evaluation of a biomass production chains in order to investigate the environmental burdens of each production step.



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2A – LCA and LCC for energy efficiency and waste management improvement in paper mill production chain

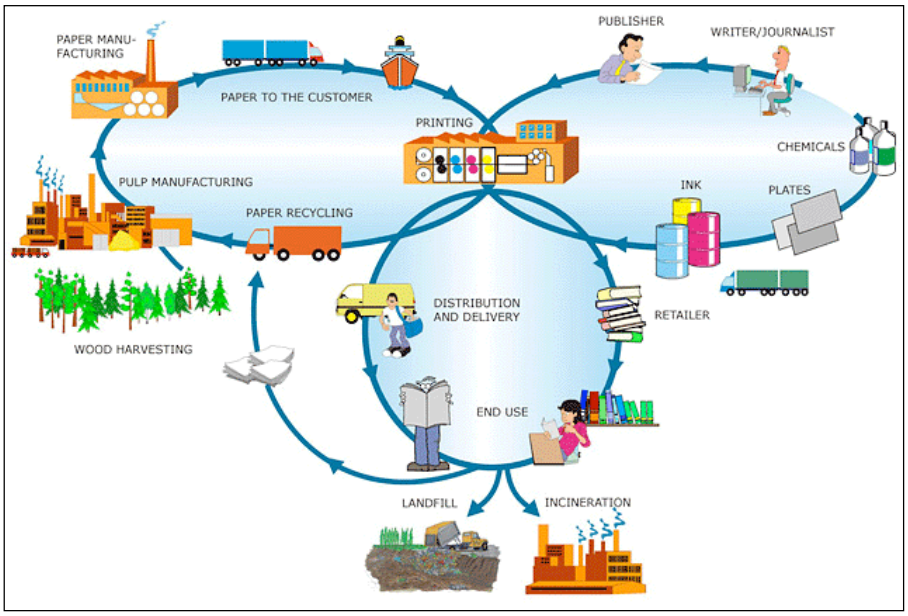
M.L. Parisi, S. Maranghi, R. Basosi

Aims

Environmental life cycle assessment (LCA) and life cycle cost analysis (LCC) of production processes in the Tuscan paper district for the critical review of applied technologies and manufacturing cycles and their improvement in terms of energy efficiency and waste management.

Results

Pulp and paper mills located in the Tuscan paper district, one of the largest in Europe, are facing tremendous challenges, which may necessitate major factory modernizations. An example is process modification to reduce dependency on purchased power, which is an expensive resource. Such modifications may have environmental implications at the mills'sites, on their product life cycle, and on other interconnected systems, and therefore, systematic tools such as life cycle assessment need to be applied.



This present project is focused on the improvement of the whole manufacturing process on the basis of primary data and information coming from three different paper mills located in the Lucca Province. The research is developed through the integration of methodological closely correlated analyses and specific activities on

three different areas: energy efficiency and recovery, reduction of water consumption, employment of new raw materials and optimized waste management. An in-depth life cycle analysis will assist the development of the project and it will be pivotal to highlight the hot spots of the existing production chain in terms of several environmental impact categories. This approach permits to "weight" in a comparative way the magnitude of each step on the sustainability of the whole process. Moreover, the development of an environmental life cycle cost analysis will integrate the economic issue in the study.

Thus the critic evaluation and validation of the results will allow to suggest technological alternatives, process modifications and system innovations for the improvement of the case studies and, more in general, to recommend options and solutions for the paper production chain.

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2A – Enzymes for green chemistry

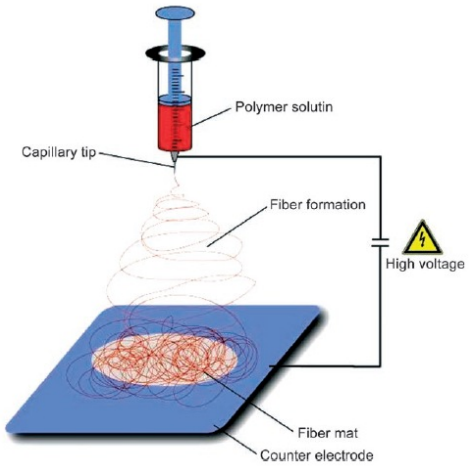
R. Pogni, D. Spinelli, E. Fatarella, M.C. Baratto, R. Basosi

Aims

The aim of this research is to address the catalytic properties of different enzymes for the bio-synthesis of new compounds for industrial applications.

Results

Immobilization of enzymes is advantageous for industrial application due to convenience in handling, ease of separation of enzymes from the reaction mixture and reuse, low product cost and a possible increase in thermal and pH stability. An important requirement for protein immobilization is that the matrix should provide a biocompatible and inert environment. Poor biocatalytic efficiency of immobilized enzymes, however, often limits the development of large-scale bioprocessing to compete with traditional chemical processes. The result of immobilization, including the performance of immobilized enzymes, strongly depend on the properties of supports. Improvements of biocatalytic efficiency can be achieved by manipulating the structure of carrier materials for enzyme immobilization. In recent decades, nanostructured materials have attracted much attention because of their unique properties and interesting applications. For example, electrospinning has emerged as a novel tool to prepare fibers and membranes with high surface area-to-volume ratio in a cheap, fast and simple way.

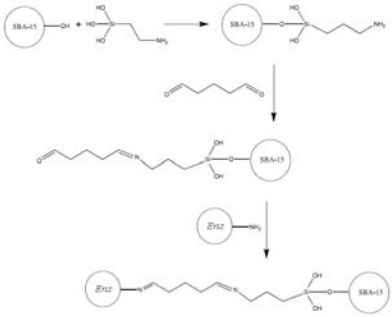


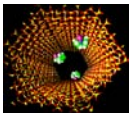
For the same reason, novel ordered mesoporous materials like Santa Barbara Amorphous (i.e. SBA-15) has been synthetized in order to verify the application as enzyme carriers. Furthermore, the surface of these materials can be modified accordingly to the functional groups present on the enzyme surface to enhance the amount of supported enzyme and increase its activity.

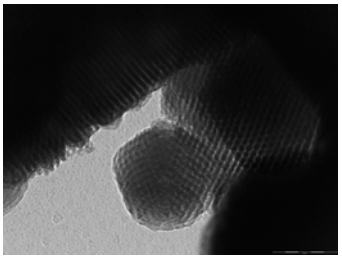
Prepared and synthetized carriers have been analyzed by Scanning Electron Microscope, Transmission Electron Microscopy and Infra-Red Spectroscopy.

In particular, our attention has been focused on the study of the catalytic mechanism of laccase from *Trametes versicolor* (oxidative enzyme) and lipase from *Candida rugosa* (esterase/hydrolase enzyme) covalent immobilized onto the above mentioned carriers by the use of crosslinker molecules like glutaraldehyde.

Moreover, their potential use in organic synthesis has been investigated in order to compete with conventional synthetic methods. Indeed, immobilized enzymes have been used in antibiotic production, drug metabolism, food industry and bioremediation.







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2A – PON Project 01_01377 "Polybioplast - Technologies and processes for the production of clothes functionalised with biopolymers from microbial conversion and biosurfactants"

Parco Scientifico e Tecnologico della Sicilia
Operating Unit: MVFA Laboratory, Dpt. of Biological and Environmental Science, University of Messina. Resp. Prof. S. Guglielmino

Aims

Setup of fermentative processes for simultaneous synthesis of polyhydroxyalcanoates (PHAs) and biosurfactants, to be used for production of biodegradable shoppers.

Results

Effective processes for production of microbial biomass containing PHA and biosurfactants by a single fermentative process.
In detail, the Operating Unit of Messina has achieved the following points:
identification and optimization of chemo-physical parameters influencing the production of microbial biomass;
identification and optimization of chemo-physical parameters influencing the production of PHA;
identification and optimization of chemo-physical parameters influencing the production of biosurfactants.
The experimental data were combined to set up an integrated fermentative process for simultaneous production of PHA-containing biomass and biosurfactants.
The combination of experimental data has been approached by predictive mathematical models, in order to understand which parameters were critical for the integrated process. Each block of the process was adjusted and the mathematical predictions were experimentally verified.
After optimization at laboratory scale level, the fermentative processes were tested in 15-30 liters bioreactors, in order to scale up the process for industrial production.

2B – New cathode materials for technological applications

V. Massarotti, D. Capsoni, M. Bini, S. Ferrari

Aims

Characterization and optimization of the physico-chemical properties of materials with technological applications to put into evidence the relationship among properties, synthesis method and doping.

Results

We investigated in detail a series of undoped and doped compounds that find application in the electrochemical devices; in particular, the main interest is devoted to cathode materials for lithium batteries. The investigation involves the structural and microstructural studies, and the physico-chemical characterization of pure and doped ceramic compounds and oxides solid solutions. Conventional and synchrotron X-Ray and neutron diffraction data are used to study the structure stability with temperature, the cations and doping ions distribution in the cell framework, and to quantify the possible impurity phases formed in the synthesis process. The obtained results are useful to explain the materials properties. Among the materials for electrochemical applications, the most recently investigated compounds belong to the Li-Ti-P-O, Li-Fe-P-O, Li-V-P-O and Li-Fe/Mn-Si-O systems. For the preparation of pure and substituted compounds, different synthesis routes were used, to optimize the material properties for its technological application.

In the case of the Li-Ti-P-O system, the $LiTi_2(PO_4)_3$ compound has been investigated: its NASICON-type structure and its high ionic conductivity make it really promising as intercalation cathode and as solid electrolyte for sensors. Our structural investigations, developed on both the undoped compound and on the Mn-doped and/or Li-rich one, put into evidence the close relationship among conductivity values and (i) the Mn content on Li site, (ii) the Li excess, whose position in the crystalline lattice has been determined by neutron powder diffraction data.

For what concerns the Li-Fe-P-O system, preliminary studies were devoted to investigate the structure, microstructure, and the influence of Mn doping and synthesis route on the material's properties. Then, a complete defect study based on the combined use of diffraction (synchrotron XRPD and Pair Distribution Function analysis) and spectroscopic (Mossbauer) data allowed us to unambiguously identify anti-site defects and the presence of a few amount of Fe^{3+}, that influence the electrochemical performances of the material.

For what concerns the Mn substituted $Li_3V_2(PO_4)_3$ cathode material, a solubility limit is reached for the Mn insertion ($x = 0.124$ in $Li_3V_{2-x}Mn_x(PO_4)_3$) in the NASICON type structure. This insertion plays a favourable role on the electrochemical performances of the material, as suggested by the improvement in the charge-discharge performances with respect to the undoped $Li_3V_2(PO_4)_3$ compound.

Recently, wide interest has been devoted to the potential application of the lithium transition metal ortho-silicates (chemical formula Li_2MSiO_4 and M = Co, Mn, Fe, Ni) as promising Li-ion batteries cathodes: the anionic framework is particularly stable

thanks to the strong Si-O chemical bonds, that promote a stabilization similar to that observed for the P-O bonds in $LiFePO_4$, but with the advantage of the possible extraction of two Li ions per formula-unit. Notwithstanding these promising peculiarities, the electrochemical performance needs optimization. The presence of different polymorphic forms, the defects formation, and the easy segregation of impurity phases during the synthesis are the main point to be investigated, because they directly influence the Li diffusion and its intercalation-deintecalation mechanism. In this frame, we compared different synthesis procedures, and we studied their influence on the obtained structures, defects formation and purity of Li_2FeSiO_4, Li_2MnSiO_4 e $Li_2Fe_{0.5}Mn_{0.5}SiO_4$. Polymorphs stability and Li-M (M = Fe, Mn) anti-site defect concentration have been investigated both at room and high temperature (up to 950°C), by in-situ X-Ray powder diffraction. Computational studies support the anti-site defect formation in the silicate structure.

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2B – New electrolyte and electrode materials for thin-film lithium microbatteries

M. Bini, I. Quinzeni, P. Mustarelli, D. Capsoni, S. Ferrari

Aims

Solid state synthesis of solid electrolyte: $Li_7La_3Zr_2O_{12}$. Synthesis of $LiFeSO_4F$ cathode material. Physico-chemical characterization of materials. Thin films deposition.

Results

This research is performed in the frame of the financed project CARIPLO 2011 "New electrolyte and electrode materials for thin-film lithium microbatteries" (M. Bini, Principal Investigator). The development of lithium thin films batteries as power sources for the last generation microdevices has been rapidly growing over these last years. Such microsystems show several advantages, above all their intrinsic lightness, low cost and better integration due to a possible miniaturization of size and dimensions. A wide area of applications is possible, which ranges from the microelectronics to the sensors in medical and military field, smart cards and micro-machines. New generation of electrolytes and electrodes for innovative lithium microbatteries is needed. We synthesized, by means of solid state reaction at high temperature, Li-garnet such as pure and Ta doped $Li_7La_3Zr_2O_{12}$ as solid electrolytes. The X-ray powder diffraction applied to the synthesized materials allowed us to verify the purity level and the presence and amount of possible impurity phases to choose the most appropriate times and temperatures for obtaining the cubic phase (2-4 hours at about 1220°C), which is the most interesting one for the application. On the prepared materials we determined the conductivity data by using the impedance spectroscopy. Values of about $8.6*10^{-5}$ S cm^{-1} were obtained at room temperature, close to those reported in the literature, but the synthesis and also the preparation of samples for conductivity still need optimization. The next step will be the deposition of the best materials as thin films on different substrates. Some trials were performed but the power, time and temperature of deposition still need optimization. Some depositions of $Li_2Fe_{0.5}Mn_{0.5}SiO_4$, a material that could substitute the lithium fluorosulphate as cathode material, were also made on gold covered stainless steel and nickel as substrates. The XRD patterns show an amorphous thin film that, even if treated at 700°C, does not present the crystallization of lithium silicate but phases obtained for reaction with the substrate. Work is in progress to clarify these last points.

2B – PON Project 02_00355_2964193 "Development of innovative Micro and Nano-Technologies and Advanced Systems for Healthcare (HIPPOCRATES)"

2) PON Hippocrates - Neurodegenerative Diseases
Operating Unit: M&Nbit Laboratory, Dpt. of Biological and Environmental Sciences, University of Messina. Resp. Prof. S. Guglielmino

Aims

The aim is to identify molecular probes for binding and concentration of markers to be used for early diagnosis of Alzheimer's Disease (AD).
The proteins beta-Amyloid and phosphorilated Tau have been selected as markers.

Results

The selection of AD specific molecular probes is in progress and both highly-specific monoclonal antibodies and genetically-modified bacteriophages are under investigation.
The lastly, the Operating Unit of Messina will be part of the validation phase of biosensors prepared, in comparison to the gold standard currently in use.

2B – Bioprocessing for Sustainable production of COLoured textiles (BISCOL Eco/256112)

R. Pogni, D. Spinelli, M.L. Parisi, M.C. Baratto, R. Basosi

Aims

BISCOL project has been focused on the dyeing industry proposing a new dyeing process as global alternative for the bioconversion of raw materials into competitive eco-viable final products.

Results

BISCOL is an European project in the framework of CIP Eco-innovation "First Application and market replication projects", led by the University of Siena (coordinator: prof. R. Pogni). Eco-innovation covers a wide range of green products, services and processes that can turn environmental challenges into business opportunities. The textile and clothing industry is one of the world most global industries and constitutes an important source of income and employment of many EU countries. In particular, the dyeing process represents an important step of the textile production chain and it is responsible for the environmental impact of the final products.

The objective of the European project BISCOL is to propose a new dyeing process as global alternative for the bioconversion of raw materials into competitive eco-viable final products has been performed through:

- textile plasma pre-treatments aiming to increase dyeability of textiles
- synthesis of bio-dyes using new safe and environmental friendly routes (enzymatic processes by the use of glass beads immobilized laccase from *Coriolopsis Polyzona*)
- synthesis of new auxiliaries at lower environmental impact
- optimisation of dyeing process reducing energy demand (e.g. lowering temperature and time of treatments).

The synthesis of new bio-dyes has been investigated starting from the previous results on the laccase-mediated synthesis of dyes like LAR-1 during the SOPHIED project (FP6-NMP2-CT-2004-505899) (Figure 1).

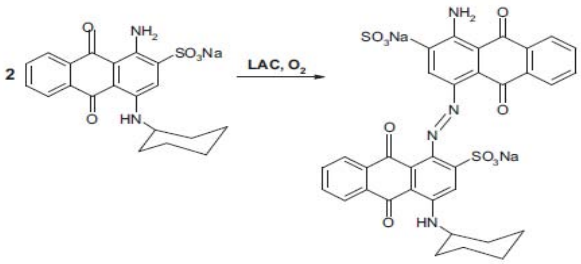


Fig. 1: Synthesis of azoanthraquinone dye LAR-1 (Enaud et al., 2010).

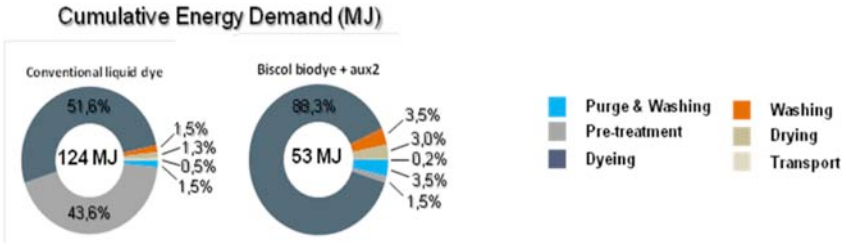
In the frame of Biscol project a tri-colour set (yellow, red and blue) of acid biodyes has been obtained and selected for woollen fabrics and their scale up has been conducted by the bioreactor system. The bio-dyes showed a better or comparable

toxicity and light fastness/washing properties comparable to the industrial ones. Then, the dyeing process using plasma pre-treated textiles, new auxiliaries and bio-dyes has been optimized.

Mn^{3+}

Fig. 2: Selected acid bio-dyes from the BISCOL project.

Furthermore, all steps has been assisted by Life Cycle Assessment (LCA) analysis in order to compare the conventional dyeing process and that proposed by BISCOL project. The functional unit has been defined 1 kg woollen fabric. The LCA on the whole dyeing process shows interesting results concerning the comparison between the conventional and BISCOL dyeing process.



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2C – Biomimetic/Bioinspired Oxidative Degradations Catalyzed by Redox-active Metalloporphines

P. Zucca, G.M. Cocco, E. Sanjust

Aims

Catalytic and operational behavior of redox-active metalloporphine immobilized on functionalized solid supports. Molecular mechanism(s) and application fields.

Results

We investigated in detail the immobilization procedures for some selected Fe- and Mn-porphines commercially available at reasonable prices. Among the immobilization supports, poly(vinylalcohol)-based and silica-based materials were chosen, all sharing imidazyl, pyridyl, or sulfhydryl tethers, capable of recognizing the central metal ion within the porphine ring, therefore leading to coordinative bonds. Such bonds to a certain extent are comparable to those found in hemoproteins, in particular the coordinative bonds between ferro- and ferri-heme and histidine or cysteine residues. The obtained preparations showed a distinctive peroxidase- and peroxygenase-like behavior, and are capable of oxidizing a very wide range of recalcitrant organic substrates, both by electron abstraction and/or oxygen insertion. In particular, several industrial dyes, belonging to different chemical classes, were efficiently bleached in the presence of the immobilized metalloporphine catalysts and hydrogen peroxide as the environmentally friendly oxidizing agent. Moreover, some methoxybenzenes and analogues were degraded under the same conditions, leading to more hydrophilic compounds. Further studies are in progress to find new supports, and to refine and extend the application fields of the obtained preparations.

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2C – Expression and purification of the diphtheria toxin variant CRM197 in *Escherichia coli*

A. Stefan, A. Hochkoeppler

Aims

This study describes a specific procedure for the production of the diphtheria toxin variant CRM197 (cross reacting material 197) using a prokaryotic system.

Results

The CRM197 protein is a variant of the diphtheria toxin (DTx, 58 kDa) characterized by a single mutation that reduces its toxicity, (i.e. a glycine-glutamic acid substitution in position 52). It is widely used in the preparation of conjugated vaccines and its production is, at the moment, performed using lysogenic cultures of *Corynebacterium diphtheriae* in a fermentation process. Studies on the use of alternative bacterial hosts have been limited. In *Escherichia coli* it has been possible to express only truncated forms of CRM197. The protein comprises two domains, A (catalytic) and B, bonded together by a disulphide bridge. These fragments, often produced as fusion proteins, have been expressed with low yield (from 0,4 to 10 mg/mL) due to solubility problems followed by protein degradation.

This study concerns about a new process for the over-expression of CRM197 in *E. coli* using an artificial polynucleotide sequence associated with a tag of 6 histidines. Moreover, it is also proposed a method for the isolation and purification of the recombinant fusion protein.

This artificial gene was cloned into the pET9a vector (Novagen), under the T7 promoter and the resulting construct was introduced into BL21AI and BL21(DE3) *Escherichia coli* strain by electroporation. The expression of recombinant CRM197his was induced for different times by adding arabinose 13 mM or IPTG 1 mM to the culture medium (LB). The target protein was always expressed and visible as a discrete band on denaturing gels (Figure 1) and the expression yield reached up to more than 40-50 % of total cell proteins, indicating *E. coli* as a suitable host for the industrial-scale production.

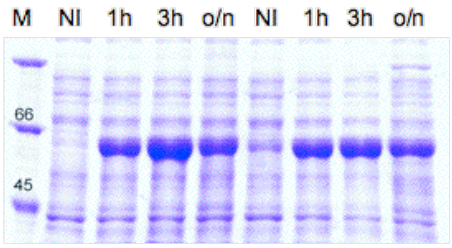

Fig. 1: SDS-PAGE (10%) of total protein extracts.

Further analysis indicated that the over-expressed CRM197his accumulates inside the insoluble fraction. Different solutions and conditions were assayed (combination of

denaturing agents, temperature, agitation) in order to solubilize CRM197his from the insoluble aggregates. The solubilization procedure was experimentally optimized: insoluble pellets were resuspended in a solution containing 50 mM Tris-HCl pH 8, 150 mM NaCl, 1% Triton X-100, 6 M urea under shaking conditions at 30 °C for 2 h.
The solubilized inactive sample was then loaded into a metal chelating affinity column (HiTrap Chelating, GE Healthcare). This procedure allows removing the denaturant during the first step of purification. Our purification procedure includes three following stages: 1) removal of the detergent Triton X-100; 2) removal of the urea by a two-step inverse gradient; 3) elution with an imidazole gradient (0-500 mM). The presence of CRM197his and its purity in each eluted fraction was then evaluated by SDS-PAGE gel stained with Comassie brilliant blue (Figure 2).

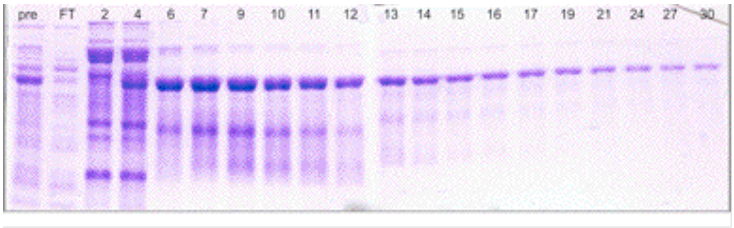

Fig. 2: SDS-PAGE of the fractions purified by affinity chromatography.

Those fractions containing most of the recombinant protein were pooled, concentrated by ultrafiltration (Amicon cell with a YM-30 membrane, Millipore, USA) and frozen. With this procedure, we can estimate a recovery of about 40-50 %. The second purification step can be performed by ion-exchange chromatography using an anionic matrix at alkaline pH or, alternatively, by gel-filtration chromatography.
This production process represents a promising alternative to the conventional method based on *C. diphtheria*.

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2C – pGOOD: new plasmid for the co-expression of proteins in *Escherichia coli*

E. Conte, G. Landolfi, G. Vincelli, A. Stefan, A. Hochkoeppler

Aims

This study describes the construction of a new expression vector, called pGOOD, suitable for *Escherichia coli*.

Results

In Escherichia coli the co-expression of native proteins is limited by the compatibility of the plasmid origins of replication. In recent years, some vectors were constructed and described, the usefulness of which is their compatibility with the most commonly used expression plasmids for *Escherichia coli*, containing a ColE1-type origin of replication (ori). An ideal co-expression system should featuring two properties: i) the easy shuttling of clones between low- and high-copy number expression vectors sharing the same MCS; ii) the coexpression of two proteins, one in excess of the other, and vice-versa.

To take advantage of these features, we have constructed the pGOOD expression vector, featuring the p15A ori, the tetracycline-resistance cassette, the lac repressor-promoter-operator regulatory elements, and the MCS from pTrcHisB. This MCS is identical to the one present in the pBADHis series, making the entry of two clones into pBADHis and into pGOOD easily revertible (Figure 1). Moreover, the stability of pGOOD is remarkable: no significant loss of plasmid was observed after *E. coli* was grown for 30 generations in non-selective medium.

The performance of pGOOD was tested by co-transforming *E. coli* TOP10 with: i) the pBAD-α1160 plasmid, which contains an insert coding for the α (polymerase) subunit of *E. coli* DNA polymerase III (DNA Pol-III); ii) the pGOOD vector bearing the gene coding for the ε (proofreading) subunit of DNA Pol-III.

Co-transformants were grown in the presence of both ampicillin and tetracycline, and induced for overexpression of α or ε by addition to the culture medium of arabinose or IPTG, respectively (Figure 2). As clearly visible on the gel, when arabinose was used alone, overexpression of the DNA Pol-III α subunit was observed. On the contrary, when only IPTG was added to the medium, overexpression of the DNA Pol-III ε subunit was detected. Lane 4 indicates that both α and ε subunits were expressed if the growth medium was supplemented with arabinose and IPTG.

This result implies that the pBAD-pGOOD vector couple can be efficiently used to co-express proteins in *E. coli*. Moreover, adding one inducer before the second one could modulate the levels of expressed proteins.

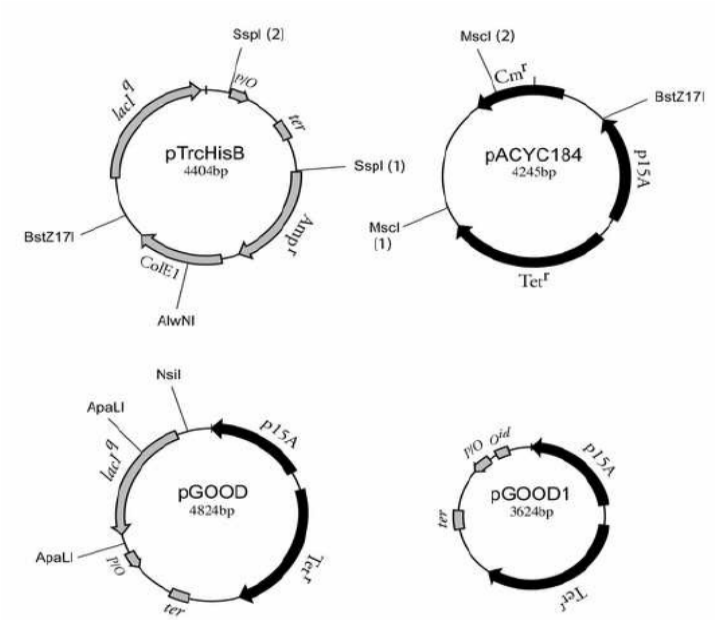

Fig. 1: Construction of pGOODs. The pTrcHisB plasmid was digested at completion with BstZ17I and AlwNI enzymes; the reaction products were further subjected to partial digestion with the SspI enzyme, and the BstZ17I-SspI(1) fragment was recovered. The pACYC184 vector was totally digested with MscI and BstZ17I enzymes, and the BstZ17I-MscI(1) fragment was recovered. Ligation of the BstZ17I-SspI(1) and BstZ17I-MscI(1) yielded pGOOD, the map of which is indicated according to the orientation determined by restriction analysis. pGOOD was then digested with ApaLI and NsiI enzymes, and the ApaLI(1)-NsiI fragment was recovered.

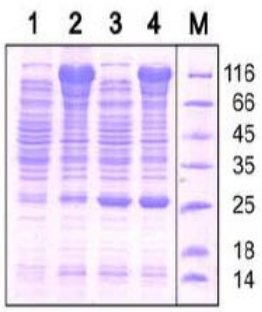

Fig. 2: SDS-PAGE of total proteins extracted from *E. coli* TOP10 / pBAD-α1160 /pGOOD-ε243 grown in the absence of inducers, in the presence of arabinose only, of IPTG only, or in medium supplemented with both arabinose and IPTG (lanes 1-4, respectively).

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2C – Continuous enzyme-coupled assay of phosphate- or pyrophosphate-releasing enzymes

A.S. Guillen Suarez, A. Stefan, S. Lemma, E. Conte, A. Hochkoeppler

Aims

The study describes a continuous enzyme-coupled assay able to monitor the kinetics of reactions catalyzed by phosphate- or pyrophosphate-releasing enzymes.

Results

Different enzymatic methods have been proposed for the detection of inorganic phosphates or pyrophosphates. In addition, chemosensors for phosphates were recently designed, synthesized, and tested. Nevertheless, these procedures are discontinuous, rendering rather cumbersome the kinetic evaluation of reactions involving phosphates.

A continuous enzyme-coupled assay of phosphate- or pyrophosphate-releasing enzymes (PREs) is presented here. In particular, the PPase-PNPase-XOD (PPX) system was investigated in detail to: (i) identify the concentration of each auxiliary enzyme necessary to correctly detect the kinetics of reactions catalyzed by PREs; (ii) define the pH interval where the activity of PREs can be determined; (iii) compare the PPX assay with a well known reference method based on the Malachite green reagent. To determine the appropriate amount of each enzyme to be used in the coupled assay, we first determined the relevant catalytic constants of XOD and PNPase at pH 7.8 (100 mM Tris-HCl). First, we assayed XOD activity, as a function of hypoxanthine concentration, in the presence of 25 mU/mL of enzyme. Under these conditions, we estimated Km and Vmax equal to 52.7 ± 5.7 μM and 33.5 ± 1.5 nM/s, respectively (Fig. 1).

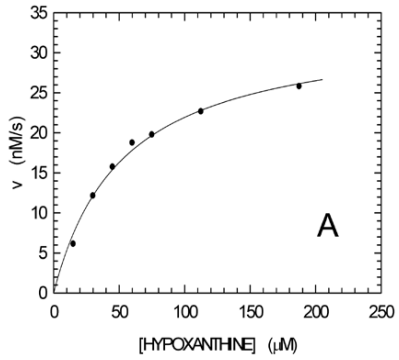

Fig. 1: Initial velocities of hypoxanthine oxidation by XOD as a function of substrate concentration. The assays were carried out at pH 7.8 (100 mM Tris-HCl) in the presence of 25 mU/mL of enzyme

Next, we assayed PNPase activity, as a function of phosphate concentration, in the presence of 5 mM $MgCl_2$, 0.25 mM inosine, 500 mU/mL of XOD and 10 mU/mL of PNPase. Under these conditions, K_m and V_{max} were estimated equal to 170 ± 8 μM and 285 ± 3 nM/s, respectively (Fig. 2).

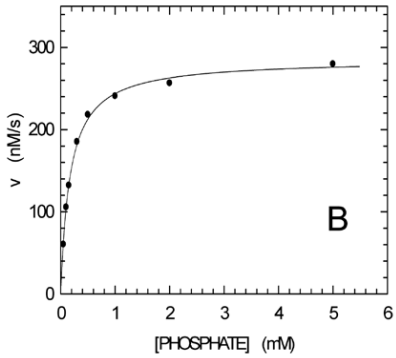

Fig. 2: Initial velocities, at pH 7.8, of inosine phosphorolysis by PNPase as a function of phosphate concentration. The assay mixtures contained 5 mM $MgCl_2$, 0.25 mM inosine, 500 mU/mL of XOD and 10 mU/mL of PNPase.

We decided to test PPase activity in the presence of 50 and 500 mU/mL of PNPase and XOD, respectively. As Figure 3 shows, a linear dependence of pyrophosphatase activity as a function of PPase concentration was observed in the range 2–20 mU/mL of PPase. According to this observation, we propose that, to detect a pyrophosphate-liberating enzyme (such as a DNA polymerase), 2–10, 50, and 500 mU/mL of PPase, PNPase, and XOD can be conveniently used, respectively.

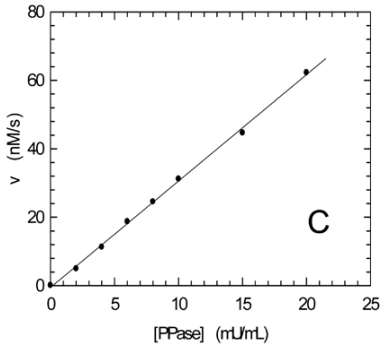

Fig. 3: Initial velocities, at pH 7.8, of pyrophosphate hydrolysis by PPase in the presence of 50 and 500 mU/mL of PNPase and XOD, respectively.

In conclusion, the PPX enzyme coupled assay represents a robust and sensitive method to perform activity assays of phosphate- or pyrophosphate-releasing enzymes. Using this coupled assay, enzyme activities can indeed be determined continuously, quantitatively, and over a wide pH range. Moreover, the assay can be performed in microplates to determine the activity of partially purified enzyme preparations.

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2C – Physico-Chemical Properties of Pharmaceutical Systems

G. Bruni, V. Berbenni, C. Milanese, M. Maietta, A. Girella, A. Marini

Aims

The research activity in the pharmaceutical field proposes developing methods for the resolution of problems related to the preformulation phase of active principles. The topics of interest are: polymorphism and stability of drugs in the solid state, host-guest systems, drug-excipient compatibility, crystallinity degree and phase diagrams characterization. In particular, in the years 2011-2013 the efforts have been directed towards the preparation and the characterization of salts and co-crystals with improved pharmaceutical behaviour.

Results

We prepared two new salts of perphenazine and fumaric acid in molar ratios 2:1 and 1:2. Their physico-chemical properties were thoroughly characterized by differential scanning calorimetry (DSC), powder X-ray diffraction (XRPD), Fourier infrared spectroscopy (FT-IR) and scanning electron microscopy coupled with the energy dispersive X-ray spectrometry (SEM-EDS). In addition, the crystal structure of the 2:1 salt was determined by single-crystal X-ray diffraction (SCXRD). The pharmaceutical characterization included solubility and dissolution studies in comparison with the commercial product Trilafon®. Perphenazine solubility is strongly pH-dependent: the binary systems show improved solubility and intrinsic dissolution rate compared with perphenazine, but only the capsule formulation containing the 1:2 dihydrate sample shows a quick and complete dissolution behaviour at neutral pH. This sample could represent an interesting perphenazine formulation to improve drug bioavailability and perhaps reduce in vivo variability even when the gastric fluid pH is increased by the presence of food.

A new salt of domperidone with succinic acid in molar ratio 1:1 was prepared and characterized. The crystal structures of the pure domperidone and domperidone: succinc acid salt were solved by SCXRD. The new salt shows enhanced solubility and dissolution rate in water and could improve the drug availability in vivo regardless of the pH. Succinic acid offers many advantages over the maleic acid present in commercial preparation: a lower toxicity, preventing chronic health effects caused by repeated administration, a good solubility and a very fast dissolution rate at both neutral and acidic pHs. This new salt could improve domperidone bioavailability, particularly in fed state, and may reduce inter-patient variability.

Carprofen co-crystals with selected co-formers were prepared by solvent evaporation and wet/dry grinding. Their effective formation was investigated by thermal analysis, FT-IR, SCXRD, XRPD and SEM-EDS. This last technique, to date never applied to the study of co-crystals, gives an important contribution to confirm or discard the co-crystals formation. Among the investigated co-formers, only 4,4’ dipyridyl allowed to obtain co-crystals. Two different crystal structures were identified with the 2:1 and 1:1.5 molar ratio carprofen : 4,4’ dipyridyl, a triclinic cell and a monoclinic one respectively. At the solid state, several hydrogen-bond supramolecular synthons can be identified. For both the 2:1 and 1:1.5 co-crystals, the main hydrogen-bond

interaction involves the COOH group of carprofen, as H-donor, and the nitrogen of 4,4' dipyridyl molecule, as H-acceptor, defining the O-H---N heterosynthon.
We synthesized a hydrogen-bonded supramolecular compound between loperamide hydrochloride (a topical analgesic for the gastro intestinal tract) and glutaric acid through solvent evaporation. Whereas the formation of the co-crystal was inferred by comparing the DSC curves and the NMR/FT-IR spectra of the starting materials with those of the final product, a deeper understanding of the chemical/physical interactions between the component molecules was obtained by the combined use of spectroscopic and modelling approaches. Here, the combination of spectroscopic techniques (FT-IR, SS-NMR) and DFT calculations allowed us to obtain a clear insight on the complex hydrogen bonding motifs which are at the basis of the co-crystal formation. The new solid phase shows six fold increased solubility in water compared to loperamide HCl and a faster dissolution rate, when formulated in tablets, in comparison with three reference commercial products, when tested at neutral pHs. This product could improve drug disposition for in vivo local effect through the different environmental pHs of the gastro-intestinal tract.

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2C – Viscoelastic solutions for fluorescence imaging of aqueous humor outflow structures

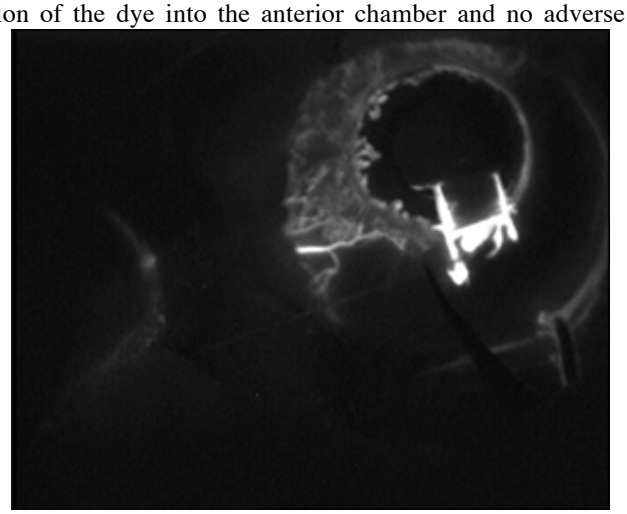
L. Ambrosone, L. Zeppa, C. Costagliola

Aims

The project aims to formulate solutions of ”vital dyes” to visible in vivo outflow pathways

Results

A wide range of imaging techniques have been used to elucidate the normal structure of the aqueous humor (AH) outflow pathway, and among these, optical coherence tomography is the most promising modality. However, it does not allow to evaluate all the structures involved in the AH outflow structures due to the intrinsic limitations of the methodology. Applying a micro-catheter into the Schlemm’s Canal (SC) and injecting 1.25 µg of indocyanine green diluted in 1 ml of viscoelastic solution both SC and outflow pathways are clearly recognized. The obtained infrared images may be video-recorded (Figure). The image allows a direct examination of the complete AH circulation, from the SC up to the ophthalmic veins. This is probably because infrared signal passes through the sclera. Furthermore the signal is enhanced by the presence of ICG-stained hyaluronan, which binds to specific receptors on endothelial cells. There was no diffusion of the dye into the anterior chamber and no adverse effects were



encountered while performing the procedure.

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2C – Effects of verbascoside-based functional extracts on the oxidative state of plasma and ocular tissues of rabbits and hares after oral and topical administration

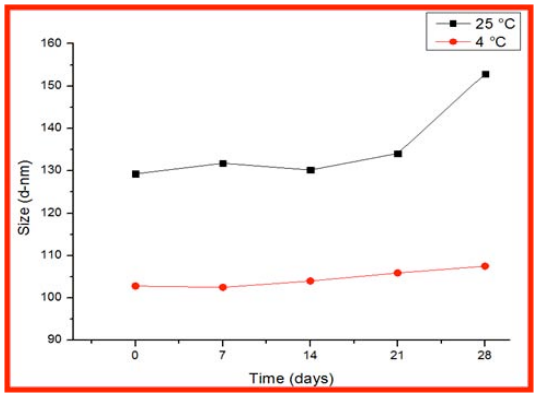
M. Mosca, C. Costagliola, L. Ambrosone

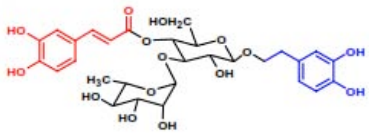
Aims

Increased natural flavonoids consumption is associated with a decreased incidence of cardiovascular diseases, cancer and other chronic diseases. This project deals with the study of the effect of verbascoside on the oxidative state of plasma and ocular tissues of animals after oral and topical administration of verbascoside based formulations.

Results

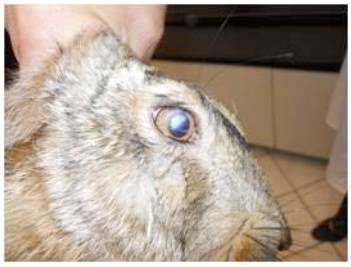
As topical formulations to test verbascoside effectiveness, liposomes were prepared with soy lecithin and cholesterol as main ingredients. Liposomes including the functional extract were characterized by Dynamic Light Scattering, Z-Potential, in order to study their stability as a function of temperature, storage time and presence of verbascoside extract. Moreover, experiments of Spectrophotometry UV-Vis and Fluorimetry allowed us to determine the percentage capture, the antioxidant capacity of formulations by ORAC test (Oxygen Radical Absorption Capacity) and the oxidative behavior of different liposomal formulations. In conclusion, the results show that some preparations are stable for 1 month at 4°C and they are able to encapsulate from 36 to 63 % of verbascoside in the functional extract, depending on the lipid composition. For their stability and their complete biocompatibility, these formulations have been tested as novel pharmaceutical preparations for topic and ophthalmic use.





Verbascoside

As oral formulation to test the effect of verbascoside on plasma oxidative state of rabbits, a food supplement containing verbascoside was administered to the animals.
The results indicate that verbascoside effects can be grouped into two classes. The first class collects the effects that show a monotonic change of the average rate, when the daily dose is varied. The other class identifies those effects that reach a saturation value. Among all properties investigated in this study, bilirubin and vitamin A belong to the first group. This mean there are metabolic processes, involving verbascoside or more generally polyphenols, which are very fast and reach steady state in short time, i.e. for low dose.



The influence of a prolonged diet supplemented with the powerful antioxidant verbascoside on the oxidative state of 20 healthy hares eye fluids and tissues has been studied. Verbascoside was dosed at 2, 3, 4 mg/die and the impact on the oxidative state of ocular tissues and fluids was tested by TBARS (thio barbituric acid reactive substances) and TEAC (Trolox Equivalent Antioxidant Capacity) assays. The percentage of change in antioxidant activity increased largely in retina and lenses at a daily verbascoside dose of 3 mg, whereas for optic nerve and vitreous humor the higher antioxidant capacity was measured at 4 mg/die verbascoside-dose.
The present findings demonstrate that verbascoside supplementation is able to protect ocular tissue and fluids from naturally occurring oxidation and that its protective effect depends on the daily dose, being maximum up to 3 mg/die.

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2C – Heat-induced precipitation process of sodium caseinate

F. Lopez, F. Cuomo, A. Ceglie

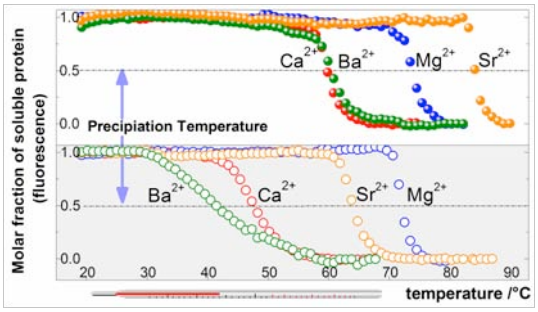
Aims

Caseins are defined as native unfolded proteins characterised by an increase in their structural complexity in response to extreme environmental changes, such as high temperature or extreme pH. Hence, the effects induced by exposure of caseins and caseinates to temperature treatments have been under intensive investigation for many years. On this basis, the study of temperature induced changes, in the presence of ions, in the physicochemical properties of these proteins can elucidate the general mechanisms responsible for the structural stability and functionality of peptides.

Results

The intrinsic fluorescence of casein was used to detect the precipitation of caseinate solution upon exposure to interactions with divalent ions. The specific precipitation temperatures (TPs) were calculated by following the molar fractions of the soluble protein.

The TPs of caseinate obtained for the sets of experiments performed in the solvent H_2O lead to the following binding capacities: $Ba^{2+} \geq Ca^{2+} > Mg^{2+} > Sr^{2+}$, regardless of salt concentration. At low salt concentrations, binding is driven by the ion hydration level; the less hydrated the ion, the higher is its ability to induce precipitation. The role of the protein in response to the temperature increase and thus the additional binding interactions occurring in certain experimental conditions are demonstrated by the experiments performed in D_2O. The trend of the binding capacities for this solvent was $Ba^{2+} > Ca^{2+} > Sr^{2+} > Mg^{2+}$. We propose that while for calcium, strontium and barium at low salt concentrations, competition between the solvent and the casein molecules occurs, magnesium maintains the same behaviour in both solvents in terms of binding affinity. In particular these results provide an example of how salts, temperature and solvents can interact and thus stabilize or destabilize proteins through mechanisms of solubilisation and precipitation.



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2C – The role of the interface and antioxidant dispersions in the radical induced oxidation of food emulsions

M. Mosca, L. Ambrosone, A Ceglie

Aims

Lipid oxidation in emulsions is largely affected by the properties of the interfacial layer surrounding the oil droplets. In this project, the effect of the emulsifier layer structure, presence of both hydrophilic and lipophilic antioxidants and radical initiators on the development of lipid oxidation in olive oil-in-water and water-in-oil emulsions was investigated.

Results

Water-in-olive-oil emulsion stability was studied as a function of the composition of the water dispersed phase. In particular, different polyphenolic extracts from natural sources were dispersed in the olive oil and their impact on emulsion kinetic stability and susceptibility to oxidation was evaluated. As natural sources, extra virgin olive oil, olive mill waste and green tea leaves were chosen. To test their impact on emulsion properties, the emulsions were prepared with fixed aqueous phase content. As emulsifiers, a fixed percentage of a mixture Span 80 (sorbitan monoleate)/Tween 80 (polysorbate 80) was used. The effect of the antioxidant dispersion on emulsion oxidation was studied by triggering the oxidation reaction in the oil phase with the lipophilic radical initiator AMVN (2,2-azobis(2,4-dimethylvaleronitrile). Then, the oxidation reaction was followed by using diphenyl-1-pyrenylphosphine, which becomes fluorescent when it is oxidized by hydroperoxides. The impact of antioxidant dispersions on emulsion kinetic stability was studied by UV–Vis turbiditymeasurements. The oxidation results were correlated to antioxidant extracts oxygen radical adsorption capacity (ORAC) and to emulsion kinetic stability. On the whole, antioxidants dispersions delayed the oxidation reaction to different extents in dependence on their ORAC values and their components amphiphilicity. Remarkably, among the antioxidants tested, the aqueous polyphenol extract from virgin olive oil was the most effective because it protected emulsions both from oxidation and from phase separation. Additionally, from this set of experiments, the primary role of the interfacial properties of olive oil polyphenols was highlighted.

The role of the interfacial layer was studied in olive oil-in-water emulsions when both the antioxidants and the radical initiators came from the two different emulsion compartments. Emulsions were prepared by using food grade emulsifiers of the Tween series (polyoxyethylene sorbitan esters) in the water phase and Span 80 (sorbitan monoleate) in the oil phase. The properties of the interfacial layer were changed by using Tween 20, Tween 60, Tween 80, which have different hydrophobic tails. These systems were oxidized by means of both hydrophilic (AAPH (2,2'-azobis,2-methyl-propanimidamide dihydrochloride), AIPH (2,2'-azobis[2-(2-imidazolin-2-yl) propane] dihydrochloride) and lipophilic (AMVN (2,2'-azobis(2,4-dimethylvaleronitrile)) radical initiators at 40 °C. A continuous fluorescent method based on the front face technique allowed us to follow directly the development of oxidation in the whole

emulsion. The combination Tween 80/Span 80 produced an interfacial layer more resistant to radical attack. Moreover, a polar paradox was verified also for radical initiators, while the results suggest that the best way to protect emulsions is to use a combination of antioxidants in both phases, to promote a synergy and the regeneration of antioxidants mediated by the interfacial layer.

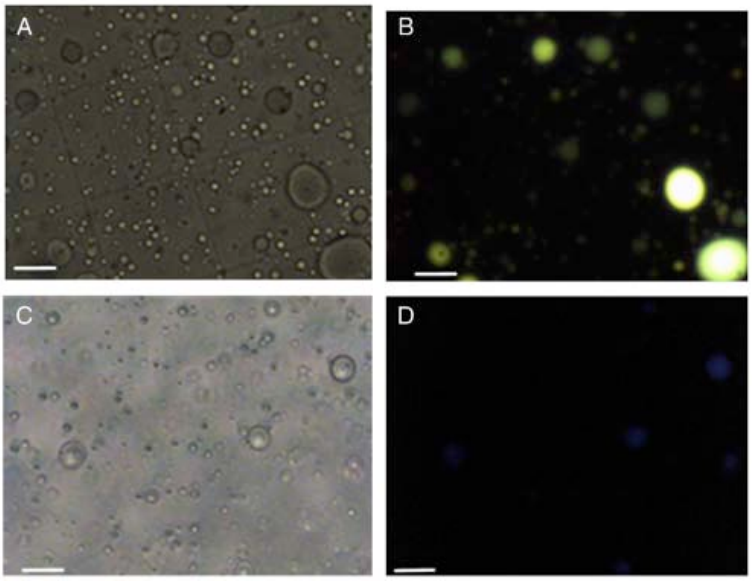

Fig. 1: Olive oil-in-Water emulsion: oil droplets with an oxidation fluorescent indicator inside. A and B emulsions without ascorbic acid. C and D, emulsions with ascorbic acid. Bar = 10 μm

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2C – Physico-chemical modification of vegetable fats: enzymatic activity in olive oil and polymorphic behavior of palm oil.

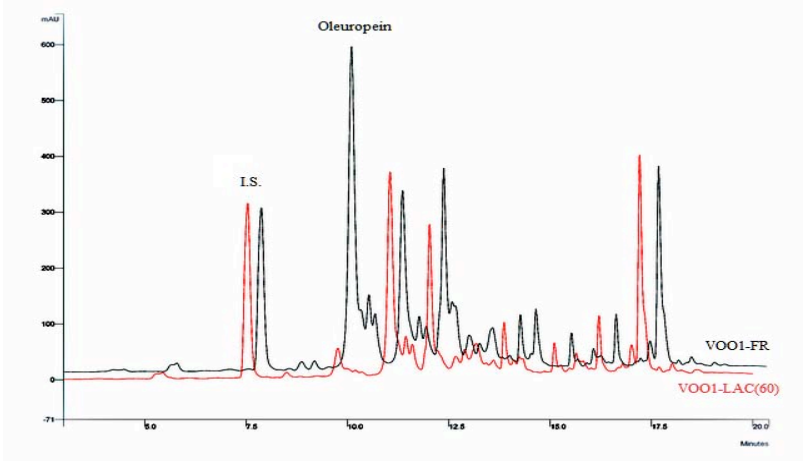
R. Angelico, A. Ceglie, S. Lampis, M. Monduzzi, V. Macciola, A. De Leonardis (Dip. A.A.A., Università del Molise)

Aims

In this project we investigate several physico-chemical processes occurring in both liquid and solid fat matrices.

Results

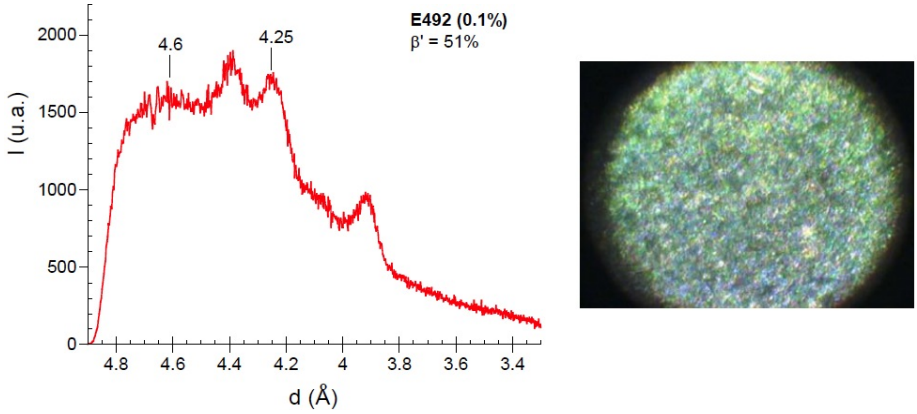
Activity of laccase from Trametes versicolor was assayed directly in virgin olive oil (VOO) samples. Laccase-treated oils led to the formation of insoluble precipitate and to significant qualitative and quantitative changes of their polyphenol composition. At the extreme condition of oil/laccase incubation (60 °C for 1 h) depletion of oleuropein and o-diphenols was estimated up to 90% and 77%, respectively. Results of Rancimat test (130 °C and 20 L h^{-1}) and oven-test (60 °C) evidenced controversial effects on the VOO oxidative stability. At high temperature, induction time of laccase-treated oils was found to be similar or even lower than the one recorded in the chemically-dephenolized oils; therefore, enzyme treatment induced a pro-oxidant effect. Conversely, during the storage at 60 °C, all the laccase-treated oils showed an improvement on their oxidative stability compared to the fresh oil counterparts. Experimental data suggest that polyphenol enzymatic-oxidation generated oil by-products able to manifest higher radical scavenging or conversely pro-oxidant property, depending on the treatment temperature and storage conditions of the oils.



Evolution of phenolic profile of virgin olive oil due to laccase activity. HPLC (black) chromatogram at 280 nm of fresh (VOO1-FR) compared to analogous profile (red)

recorded for laccase-treated oil (VOO1-LAC(60)). Time and amplitude axes are offset by 5%. Internal standard (I.S.) is 4-methyl catechol.

Palm oil is used as cooking oil, to make margarine and is component of many processed foods. To obtain a given texture, this oil can be crystallized: it appears that crystal size can be considered as a key of flow properties with a direct influence on sensory perception. For some case, the rate of crystallization of fat is very important, this is the case of chocolates and confectionary coatings, dairy products such as butter and cream and vegetable spreads. Today, two different crystallization methods are used in the industry: scraped surface heat exchanger (SSHE) plants and chilling drum plants. We investigated the fat crystallization behaviours in refined palm oil by testing an alternative experimental procedure for the plasticization of palm oil having more than 40% of crystal fats in β' form. This type of crystals are the most desirable since they are relatively small and can incorporate a larger amount of liquid oil in the crystal network. Moreover β' crystals result in a glossy surface and a smooth texture. The proposed process transforms palm oil (35-40°C) emulsified with less than 1% wt/wt of food-grade surfactants into its crystalline state by a discontinuous cooling process with cryogenic fluids. The extents to which additives may be used as well as the maximum dosages have been tested to maximise the relative percentage of β' crystals as judged by optical microscopy of sample textures and measured SAXS-WAXS patterns.



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2C – Rapid analysis of pesticides in complex matrices by new ultrasound dispersive liquid–liquid micro-extraction coupled with gas chromatography-flame ionization detector

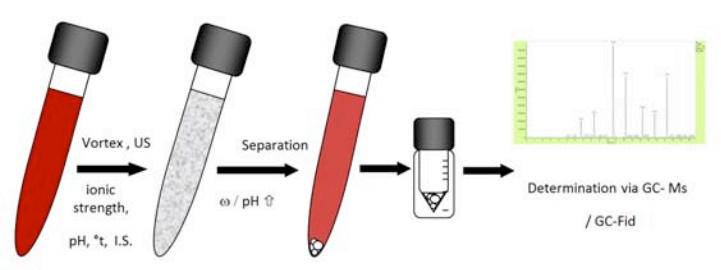
G. Cinelli, I. Notardonato, P. Avino, M.V. Russo

Aims

The focal objective of this research is to develop and apply a new dispersive liquid-liquid micro-extraction coupled with GC technics to determine pesticides at trace and ultra-trace levels. The studied pesticides are those considered in the European and/or Italian normative and those so-called "conventional" because not present in the legislation but they are significant in human health.

Results

The results obtained using the analytical procedure based on a new Ultrasound - Assisted Dispersive Liquid–Liquid Micro Extraction and GC-FID or GC-IT/MS analysis, allow investigating phthalates esters, Triazine, and organophosporus pesticides in food and environmental matrices. The analytical procedure investigated combines the DLLME procedure with a vortex step allowing analyzing all kind of matrices. This last step enhances the recoveries; on the other hand, LODs and LOQs are adequate for determining such compounds at trace and ultra-trace levels in wine samples. The whole procedure has been tested on different samples demonstrating to be rapid, simple and cheaper. Furthermore, strength of this study regards the possibility of use GC-IT/MS or GC-FID instrument: this last equipment can be found worldwide, also in no-specialized laboratories.



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2C – In-vitro activity of liposomial resveratrol against *Helicobacter pylori*

C. Bonechi, S. Martini, N. Figura (Dept. of Internal Medicine, Univ. of Siena, Italy), C. Rossi

Aims

Helicobacter pylori is an infection that affects millions of people worldwide, being the main cause of gastritis, gastroduodenal ulcer and gastric cancer. Strains, which possess the chromosomal insertion c*ag*, are endowed with increased inflammatory potential. Some phytochemicals in grapes have antimicrobial properties and it has been suggested that an antibacterial agent in wine, the polyphenol, resveratrol, produced during fermentation. The efficacy of resveratrol could thus be improved by formulations which protects the active molecular against chemical degradation and delivers the active in solubilized form to enhance oral absorption.

Results

To assess the bacterial effect of liposomes loaded with resveratrol against *Helicobacter pylori* formulations recently designed and characterize were selected. These contain the zwitterionic lipid DPPC and the neutral lipid cholesterol (CHOL) or the cationic DC-CHOL lipid.

Figure 1 reports the MBC values of liposomial samples after 24 hours of exposure. Plain zwitterionic liposomes did not exert any appreciable bactericidal activity against *Helicobacter pylori*, whereas cationic liposomes showed antibacterial properties, especially the formulation DPPC/DC-CHOL with 75:25 molar ratio.

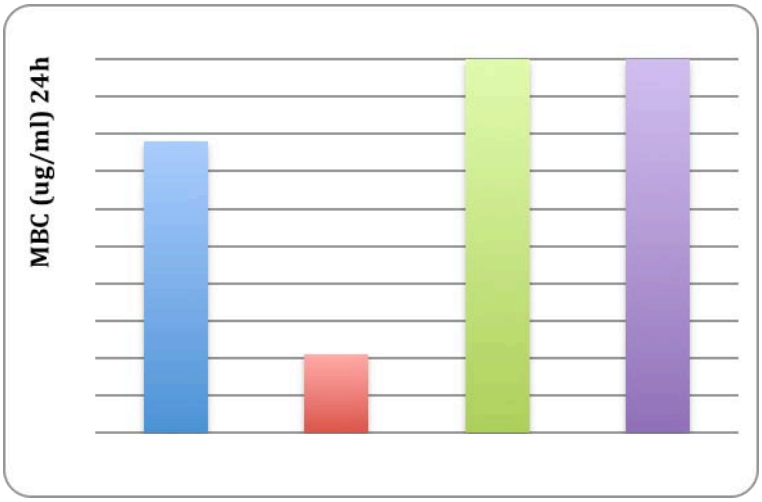

Fig. 1: Bactericidal activity (MBC) of plain liposomes versus Helicobacter pylori.

This result is in agreement with findings that cationic lipid possesses antimicrobial activity.

Figure 2 compares the MBCs of different control liposome formulation with those of the corresponding resveratrol containing systems.

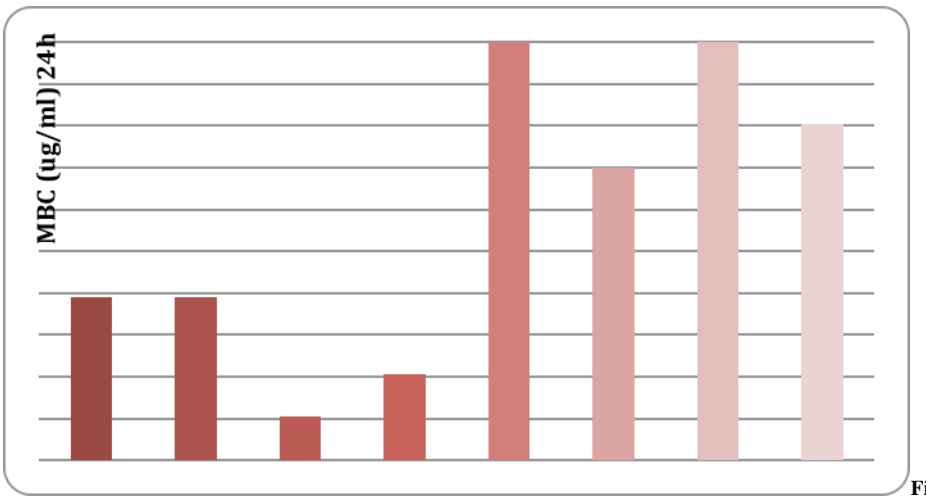

Fig. 2: comparison of MBCs of liposomes with and without resveratrol against Helicobacter pylori

The obtained data show that the presence of resveratrol into liposomes caused different effects depending on the formulation and on the relative concentrations of lipids. For the zwitterionic formulation appreciable bactericidal activity was enhanced by the presence of resveratrol, whereas for cationic liposomes the bactericidal activity was reduced by the presence of resveratrol in the liposomes. This rather surprising result may be explained by a different association of resveratrol with the bilayer, i.e. deeply inserted among the lipid chains in zwitterionic liposomes and adsorbed on the surface in the cationic liposomes.

The above results showed that in vitro antimicrobial activity of resveratrol against Helicobacter pylori can be enhanced by using liposomial carriers comprising DPPC/CHOL. Liposomes comprising DPPC/DC-CHOL showed on their own an antimicrobial affect and the presence of resveratrol in these liposomes decreased their antimicrobial effect.

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2C – Liposomes as Carriers for Plant Derived Polyphenols

C. Bonechi, S. Martini, A. Donati, S. Ristori, C. Rossi

Aims

Resveratrol (3,5,49-trihydroxy-trans-stilbene) is a polyphenol found in various plants, especially in the skin of red grapes. The effect of resveratrol on human health is the topic of numerous studies. In fact this molecule has shown anti-cancer, antiinflammatory, blood-sugar-lowering ability and beneficial cardiovascular effects. However, for many polyphenol compounds of natural origin bioavailability is limited by low solubility in biological fluids, as well as by rapid metabolization in vivo.
Therefore, appropriate carriers are required to obtain efficient therapeutics along with low administration doses. Liposomes are excellent candidates for drug delivery purposes, due to their biocompatibility, wide choice of physico-chemical properties and easy preparation. In this work liposome formulations made by a saturated phosphatidyl-choline (DPPC) and cholesterol (or its positively charged derivative DC-CHOL) were chosen to optimize the loading of a rigid hydrophobic molecule such as resveratrol. Plain and resveratrol loaded liposomes were characterized for size, surface charge and structural details by complementary techniques, i.e. Dynamic Light Scattering (DLS), Zeta potential and Small Angle X-ray Scattering (SAXS). Nuclear and Electron Spin magnetic resonances (NMR and ESR, respectively) were also used to gain information at the molecular scale.

Results

In this work we studied the association of trans-Resveratrol with different formulations of zwitterionic and cationic liposomes, which were designed ad hoc to optimize RESV loading.
Rigid bilayers made by DPPC were chosen to obtain good compatibility with substantially rigid guest molecules. Cholesterol and its positively charged derivative DC-CHOL were included in the formulation to improve cell delivery by enhancing the interaction with plasma membranes. The obtained results allowed to give an account of loaded liposomes in which resveratrol interacted with the bilayer, being more deeply inserted in cationic liposomes than in zwitterionic liposomes. Relevant properties such as the mean size and the presence of oligolamellar structures were influenced by the loading of RESV guest molecules.
Extensive physico-chemical characterization allowed to draw a model in which size, surface charge, lamellarity and resveratrol location were assessed. In particular, the analysis and comparison of DLS, SAXS, NMR and ESR results pointed out marked differences in RESV location within the bilayer of zwitterionic and cationic liposomes, as it is shown in Figures 1a and 1b, respectively.

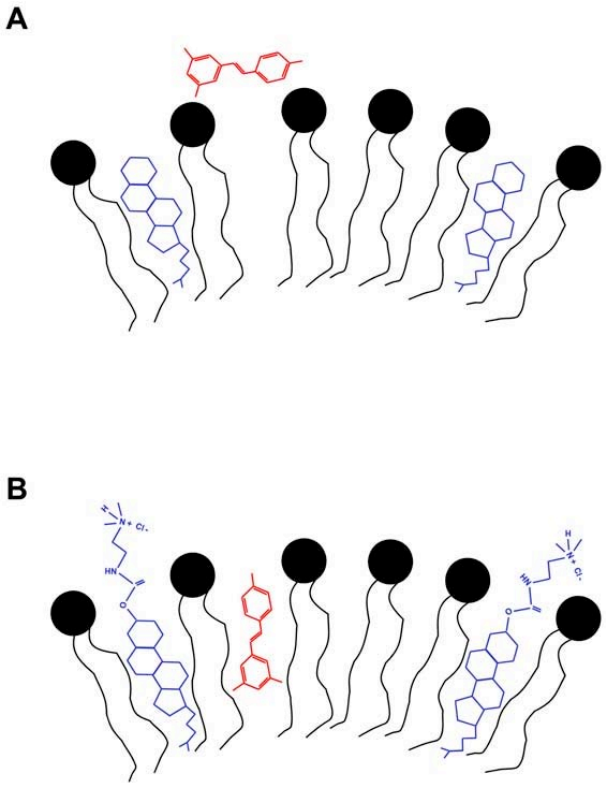

Fig. 1: Sketch of RESV insertion in the bilayer of DPPC/CHOL (a) and DPPC/DC-CHOL(b) liposomes.

Finally, as a first step towards biological trials, the innocuous nature of all the investigated systems was checked by administration to NIH3T3 (mouse fibroblast) and U373-MG (human astrocytes) stabilized cell lines.

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2C – Discrimination of human semen specimens by NMR data, sperm parameters and PCA

C. Bonechi, S. Martini, A. Donati, C. Rossi

Aims

In this study 83 human seminal plasma samples were analyzed using a combined Nuclear Magnetic Resonance Spectroscopy and Principal Component Analysis approach as a challenge to discriminate patients in relation to semen characteristics and/or conditions affecting the fertility status. In the first step of the statistical analysis, patients with testicular cancer, necrozoospermia, azoospermia and fertile men came out as outliers. This methodology was able to identify patients with leukocytospermia and with the concomitant presence of varicocele/ex varicocele and leukocytospermia, as well as to discriminate among seminal specimens in relation to semen quality.

Results

We developed a methodology by including important biological data in the set of the variables used in the PCA analysis that enabled the identification of two clusters of patients. The metabolites playing the most important role in the detection of differences among samples were glycerophosphocholine, a group of metabolites (choline, phenylalanine, citrate, lactate and histidine), uridine together with seminal parameters (concentration, motility and morphology).

Within cluster 1, citrate was the only variable which did not show any linear correlation with the other variables. In fact, citrate is the unique prostatic metabolite in seminal plasma investigated by high resolution NMR analysis as a marker to diagnose prostatic cancer. None of these conditions were detected in our patients population. In cluster 2 no correlations were found for uridine and citrate. (Figure 1)

In PC1 and PC2 scatter plot of data was evident that six patients such as fertile men, azoospermic individuals, a case of testicular cancer and a case of necrozoospermia were not included in the clusters.

The importance of the applied method resides in the ability to discriminate among seminal specimens of unselected patients between cluster 1 that showed a better semen quality then cluster 2.

In our population cluster 2 was characterized by a decreased semen quality and by the presence of all the cases with leukocytospermia only or associated with the other conditions. It is known that leukocytospermia has a negative impact on semen quality due to the production of the reactive oxygen species that are able to decrease sperm motility. We can hypothesize that in cluster 2 leukocytospermia may cause a reduction in sperm motility, altering the ability of the spermatozoa to utilize substrates involved in ATP production and subsequently fertility. In this cluster, ATP showed several linear dependences with aminoacidic residues such as histidine, tyrosine, choline, lysine, glycine, isoleucine and leucine.

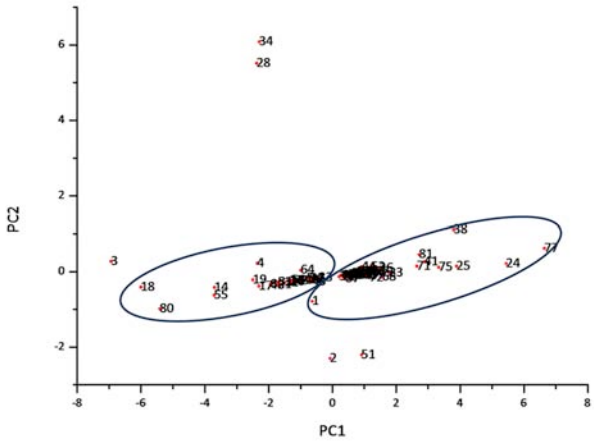

Fig. 3: PC1 and PC2 scatter plot of all data collected without the sample n. 54. The cluster ellipses were determined according to a cluster analysis. Cluster on the left has been indicated by number 1 while the other one with number 2.

The presence of patients with varicocele or with a past history of varicocele was almost equally distributed in cluster 1 and 2, since this pathology may have different impact on the quality of seminal fluids related to considered metabolites.

In conclusion, Nuclear Magnetic Resonance Spectroscopy coupled to statistical analysis was applied to an unselected group of patients with the aim of developing a statistical method to investigate complex biological samples. In first step of the statistical analysis, patients with testicular cancer, necrozoospermia, azoospermia and fertile men came out as outliers. After ignoring these samples, the method enabled to identify two populations of men with different semen quality. In addition all patients with leukocytospermia were located in a specific cluster.

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2C – An in vivo statistical total correlation NMR spectroscopy approach in-vitro

M. Ricci, C. Bonechi, S. Martini, A. Donati, C. Rossi

Aims

In vivo NMR spectroscopy, together with selectively ^{13}C-labelled substrates and 'statistical total correlation spectroscopy' analysis (STOCSY), are valuable tools to collect and interpret the metabolic responses of a living organism to external stimuli. In this study, we applied this approach to evaluate the effects of increasing concentration of exogenous ethanol on the *Saccharomyces cerevisiae* fermentative metabolism. We show that the STOCSY analysis correctly identifies the different types of correlations among the enriched metabolites involved in the fermentation, and that these correlations are quite stable even in presence of a stressing factor such as the exogenous ethanol.

Results

In this study we adopted a STOCSY analysis in combination with *in vivo* ^{13}C NMR to investigate the effects induced by the exogenous ethanol on the *Saccharomyces cerevisiae* fermentative process. The presence of exogenous ethanol reduced the yeast metabolic activity leading to a lowering in the total fermentation rate.

STOCSY analysis was carried out on three sets of *in vivo* ^{13}C NMR experiments of yeast fermentation performed at increasing concentrations of exogenous ethanol (0, 20 and 50 g/L respectively).

According to the ^{13}C-enriched substrates used in this study, the correlation matrices we obtained from the STOCSY analysis correctly identify the pattern of the structural and temporal correlation peaks arising from the NMR signals of the molecules involved in the fermentation.

The comparison of the STOCSY matrices obtained from experiments at different exogenous ethanol concentrations highlights the same intensities and displacement pattern of the correlation peaks.

Thus, our study demonstrated that, in contrast to the effects on the fermentation rate, the exogenous ethanol leaves the pattern of the correlations between the enriched metabolites involved in the yeast fermentation unchanged.

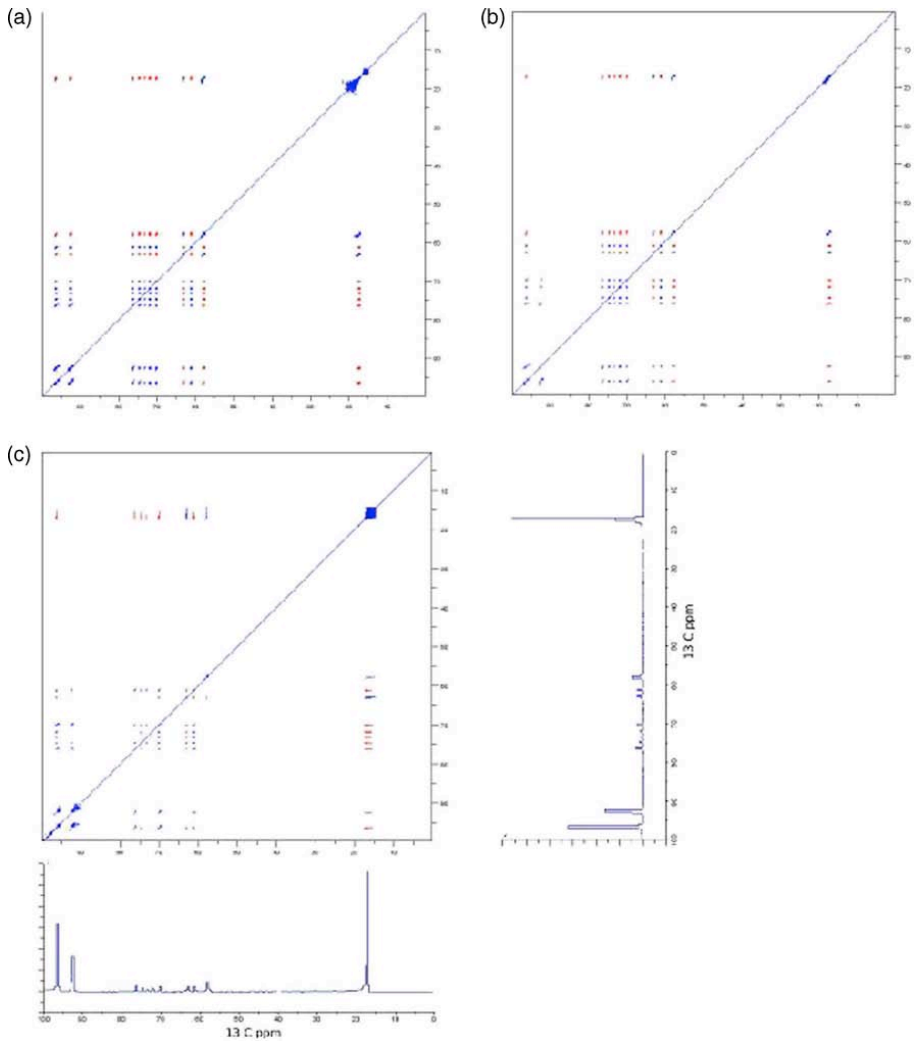

Fig. 1: The correlation matrices obtained from the three sets of ^{13}C in vivo NMR experiments: (a) in the absence of exogenous ethanol, (b–c) in the presence of 20 g/L and 50 g/L of exogenous ethanol, respectively. The pattern showed by the three correlation matrices reveals which metabolites have positive (blue) or negative (red) Pearson correlation coefficient (r). The analysis correctly identifies the negative correlation between glucose and ethanol; glucose and glycerol; and the positive correlation between glycerol and ethanol.

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2C – Structure/Activity Relationships of Metal Complexes with Ligands of Biological Interest

M.C. Baratto, R. Basosi (Department of Biotechnology, Chemistry and Pharmacy, University of Siena)

Aims

The aim of this project is a spectroscopic characterization through EPR technique aided by computer simulations to investigate Cu(II)-complexes with biological applications in solution, in order to determine a structural/activity relationship.

Results

This research project is focused on the study of structural information of Cu(II)-complexes in solution, to determine their stability and dynamics using a multifrequency EPR approach aided by computer simulations. On this regards, the research concerned the investigation of different systems.

In [1] Cu(II) coordination to peptide fragments encompassing residues 45–55 of alpha synuclein (aS) has been exhaustively characterized, including systems containing the inherited mutations E46K and A53T, as model peptides of the His-50 site. Through potentiometric titrations all the speciation profiles have been determined and the stability constants have been used to estimate the dissociation constants of complexes corresponding to the binding modes at pH 6.5 and 7.5. Spectroscopic analyses allowed determination of (i) the copper coordination sphere, (ii) its geometry and (iii) the constraints where from the 3D structural models of the copper complexes could be obtained.

In [2] Interpenetration of wood samples of pine sapwood (Pinus sylvestris L.) with hybrid inorganic–organic silica xerogels bearing amine functions able to coordinate copper(II) cations has been successfully carried out. These materials have been prepared by sol–gel processing TEOS/APTES mixtures inside the wood. Solid state 29Si NMR data provide evidence that the interpenetrated xerogel material has the same degree of condensation of the corresponding xerogel formed outside the wood. Copper(II) is effectively vehiculated inside the wood by coordination linkages with two ammine functions well evidenced by ESR measurements. SEM/EDX investigations show that the chlorine/copper atomic ratio inside the wood is lower than that of the starting salt CuCl2, suggesting an exchange reaction with silanol groups with the formation of Si–O–Cu linkages and HCl. This reaction could be promoted by the excess of amine functions with formation of ammonium chloride species which remain onto the surface of the wood and in the mother solution owing to a higher degree of condensation. Sodium silicate was tested in place of TEOS in order to have a cheaper and ethanol-free formulation. However, gel penetration results significantly lower than that of the corresponding formulation containing TEOS and preservation performance are lower than that of TEOS formulation against brown-rot fungal decay.

In [3] the copper complexes [Cu(Pyimpy)(H2O)](ClO4)2 (1), [Cu(Pyimpy)2](ClO4)2 (2), [Cu(Pyimpy)(Cl)2]_2H2O (3_2H2O), [Cu(Pyimpy)(N3)(ClO4)]2 (4) and [Cu(Pyimpy)(SCN)(ClO4)]2 (5) were synthesized and characterized by spectroscopic techniques, crystal structures and electrochemical studies (Pyimpy: (2-((2-phenyl-2-

(pyridin-2-l)hydrazono)methyl)pyridine)). The superoxide scavenging activity of the two water soluble complexes 1 and 3 was examined. DNA interaction studies by UV–Vis absorption spectral changes during a titration experiment indicated the generation of new species. These small molecule SOD mimics exhibited excellent DNA cleavage activity in the presence of H2O2 as well as 2-mercaptoethanol. Complexes 1–5 exhibited better cytotoxicity compared to CuCl2_2H2O and the ligand Pyimpy, and showed more potency than cisplatin for MCF-7, PC-3 and HEK-293 cells. Complex 3 exhibited the highest potency for MCF-7, PC-3 and HEK-293 cells compared to the other complexes.

In [4] changes in speciation of copper(II) in reactions with epigallocatechin gallate (EGCG) and gallic acid (GA) as a function of pH have been investigated by multifrequency (X- and S-band) EPR spectroscopy in the fluid and frozen states. The EPR spectra show the formation of three distinct mononuclear species with each of the polyphenols, and these are interpreted in terms of one mono- and two bis-complexes. However, di- or polymeric complexes dominate the Cu(II) speciation in the pH range 4–8, and it is only at alkaline pH values that these mononuclear complexes make appreciable contributions to the metal speciation. Each mononuclear complex displays linewidth anisotropy in fluid solution as a consequence of incomplete averaging of the spin Hamiltonian parameters through molecular motion. Rotational correlation times for the individual complexes have been estimated by analysing the lineshape anisotropy of the fluid solution spectra using parameters determined by simulation of the rigid limit spectra. These show that the molecular masses increase with increasing pH, indicating either coordination of increasing numbers of polyphenol molecules as ligands to the copper or the increasing involvement of polyphenol dimers as ligands in the copper coordination sphere.

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2C – Multifrequency EPR characterization of radical intermediates formed in the biocatalytic processes mediated by laccase

A. Martorana, M. Ayala Aceves, R. Vazquez-Duhalt, R. Basosi, M.C. Baratto

Aims

The aim of this project is a multifrequency EPR analysis and characterization of the radical intermediate species formed during the catalytic mechanism mediated by laccase, in order to get a better insight into the oxidation process.

Results

Enzymatic reactions are becoming increasingly important for many industrial applications owing to the environmental safety of this approach. Several enzymes are currently used in industrial processes, and among them the oxidoreductases family, such as laccases that uses dioxygen (O_2) as final acceptor of electrons, have found large applications. Laccases (benzenediol oxygen oxidoreductases) belong to the multicopper oxidases containing four copper ions in their catalytic site that catalyze the monoelectronic oxidation of substrates without releasing any toxic by-product. These enzymes are able to oxidize a broad range of organic compounds such as phenols, aminophenols, polyphenols, polyamines, lignins, aryl diamines, and their oxidation is coupled to the reduction of molecular oxygen to water. However, the low redox potentials of laccases (0.5 to 0.8V) only allow the direct degradation of low redox potential substrates and not the oxidation of the most recalcitrant aromatic compounds. Moreover, in several cases, the substrate inaccessibility to the enzyme active-site does not allow the direct oxidation, as in the case of lignin degradation. These difficulties can be overcome by using low molecular weight compounds acting as redox mediators.

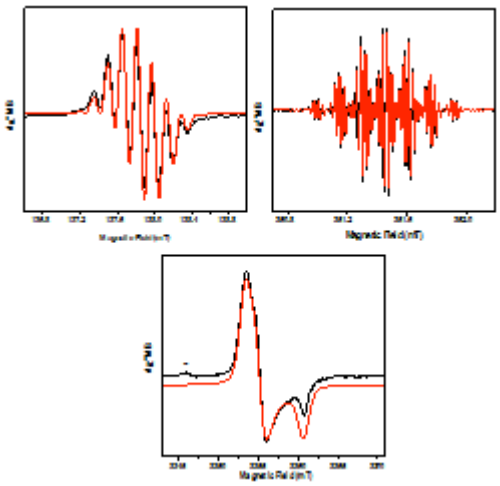

Fig. 1: RT MF-EPR spectra of acetosyringone (black line) formed with enzymatic oxidation, paired with its best simulation (red line) at: A: S-band (3.8GHz); B: X-band (9.8GHz); C: W-band (94GHz).

In this study, a Multifrequency (MF) EPR study on Coriolopsis gallica laccase using S-(3.8GHz), X-(9.4GHz) and W-band (94.8GHz) aided by simulations has been carried out, in order to obtain a complete and clear assignment of the g and A tensors. Since now, the only structural characterization of mediator radicals was performed on ABTS and VIOL and on a precursor radical such as 4-methyamino benzoic acid. More recently, 3,5-dimethoxy-4-hydroxyacetophenone

(acetosyringone), a lignin derived phenol, was extensively characterized by MF-EPR spectroscopy showing high stability and supporting the o-dimethoxyphenols as potential laccase mediators. A correlation between the substituents on the aromatic ring and the signal intensity of the radical generated was observed, pointing out the key factors of radical stability that are essential to improve the mediator efficiency. The great radical stability of such phenoxy radicals makes them particularly interesting for biotechnological applications and represent a good example for the design of new stable laccase mediators. It is well known that sterically hindered phenols by bulky alkyl substituents in the ortho position relative to the hydroxyl group of the phenol, change some typical properties of phenols, such as water and alkalis solubility and also reactivity. These bulky ortho-substituents prevent the reaction of the hydrogen of the OH group with other molecules, influencing also the ability to form an intramolecular hydrogen bond and preventing the association with other molecules. In addition, the radicals that do not contain α-hydrogen atoms in the ortho-substituents have an extremely high stability. The ether oxygen could participate in the overall conjugation and this stabilizes the radical to a sufficient extent. In this way, following a previous studies onto acetosyringone, the reaction of C. gallica laccase and four selected 2,6-dimethoxyphenol substrates were studied by EPR spectroscopy. All of them are laccase substrates and they are enzymatically transformed. Syringaldazine showed to be the faster substrate due to its high catalytic affinity to the enzyme. Syringaldehyde showed good values in both, catalytic rate and catalytic efficiency. A different situation was encountered working with 2,6-DMP, where the absence of substituent in para position, capable to delocalize the unpaired electron, does not stabilize the radical intermediate and no EPR signal was recorded after enzymatic oxidation.

In collaboration with Prof. Rafael Vazquez-Duhalt and Prof. M. Ayala Aceves, the research will be extended to the analysis and characterization of radical intermediates formed during the synthesis of polymers and their degradation with enzymes and the study of free radical intermediate formed on nanoparticles surface where enzymes have been immobilised.

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2C – Catalytic mechanism and structural determinants of oxidases for biotechnological processes

R. Pogni, M.C. Baratto, A. Sinicropi, C. Bernini, M.L. Parisi, A.T. Martinez, R. Basosi

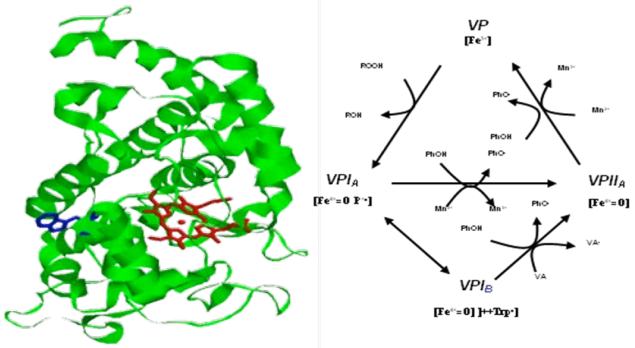
Extended catalytic cycle of VP

Aims

The aim of this project concerns the characterization through EPR techniques, combined to computational analysis, of native and mutated enzymes (oxidoreductases such as peroxidases and laccases) in order to get a better insight into the catalytic mechanism.

Results

Lignin-degrading peroxidases, a group of biotechnologically interesting enzymes, oxidize high redox potential aromatics via an exposed protein radical. Direct detection of a protein radical (Trp radical) in a ligninolytic peroxidase as a catalytic site, was obtained, for the first time by our group, in *Pleurotos eryngii* and *Bjerkandera adusta* Versatile peroxidases (VP) by low temperature EPR. On this basis an extension of the basic catalytic cycle of peroxidases was proposed.



The resting state and peroxide-activated forms of the native enzymes and different variants obtained by Trp164 site directed mutagenesis of *P. eryngii* VP were analyzed by multifrequency EPR to address the their role in the catalytic cycle.

A new type of Lignin Peroxidase (LiP), recently found in the white-rot basidiomycete *Trametopsis cervina*, has been characterized. Its first molecular characterization showed that T. cervina lacks the conserved catalytic tryptophan and contains one tyrosine residue (Tyr181) at a position where tyrosine residues were never found in other LiP and VP sequences. Low temperature EPR of the peroxide-activated T. cervina LiP successfully detected a protein radical at Tyr-181. These results provide the first structure-function information on the only ligninolytic peroxidase described to date that has a catalytic tyrosine.

More recently, Pristine LiP showed a lag period in VA (veratryl alcohol) oxidation. However, VA-LiP (LiP after turnover with H_2O_2/VA) lacked this lag, and H_2O_2-LiP (H_2O_2-pre-treated LiP) was inactive. MS analyses revealed that VA-LiP includes one VA molecule covalently bound to the side chain of Tyr181, whereas H_2O_2-LiP contains hydroxylated Tyr181. No adduct is formed in the Y171N variant. EPR spectroscopy after peroxide activation of the pre-treated LiPs showed protein radicals

other than the tyrosine radical found in pristine LiP, which were assigned to a tyrosine–VA adduct radical in VA-LiP and a dihydroxyphenyalanine radical in H_2O_2-LiP. Both radicals are able to oxidize large low-redox-potential substrates, but H_2O_2-LiP is unable to oxidize high-redox-potential substrates. Transient state kinetics showed that the tyrosine–VA adduct strongly promotes (>100-fold) substrate oxidation by compound II, the rate-limiting step in catalysis. The novel activation mechanism is involved in ligninolysis, as demonstrated using lignin model substrates. This is the first report on autocatalytic modification, resulting in functional alteration, among class II peroxidases.
Due to steric hinderance factors and redox potential between 0.5 and 0.8 V, laccase can oxidises only low redox potential compounds. To overcome this problem, small molecule, called mediators, act as electron shuttle between the enzyme and the substrate, extending the range of substrates susceptible to the enzymatic action. Using predictive methods, some mediator molecules have been selected as good candidates for the catalytic mechanism of the laccase from trametes versicolor and coriolopsis gallica. Some dimethoxyphenol mediators have been analysed by EPR spectroscopy thanks to their stable radical intermediates formation and their well-structured and intensive EPR signals. The study allowed obtaining a relationship between molecular structure and radical formation that elucidate the oxidation reaction process mediated by laccase.

This project has been partially funded by Project PRIN 2009 prot. 2009STNWX3_001.

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2C – PON Project 02_00355_2964193 "Development of innovative Micro and Nano-Technologies and Advanced Systems for Healthcare (HIPPOCRATES)"

Distretto Tecnologico Sicilia Micro e Nano Sistemi
Partners: CNR – Consiglio Nazionale delle Ricerche (CNR IBB; CNR IBIM; CNR ICB; CNR IMM; CNR IPCF; CNR ISN; CNR IBF; CNR ISMN); Consorzio Interuniversitario Nazionale delle Biostrutture e Biosistemi (INBB); Parco Scientifico e Tecnologico della Sicilia scpa (PST Sicilia); Università degli Studi di Catania (UNICT); Università degli Studi di Messina (UNIME); Università degli Studi di Palermo (UNIPA); STMicroelectronics S.r.l. (ST); S.I.F.I. – Società Industria Farmaceutica Italiana S.p.A. (SIFI); Engineering – Ingegneria Informatica S.p.A. (Engineering); Istituto Mediterraneo per i Trapianti e Terapie ad Alta Specializzazione S.r.l. (ISMETT); Infracom IT S.p.A. (Infracom); Consorzio Catania Ricerche (CCR); Italtel S.p.A. (Italtel); Etna Hitech S.c.p.A. (EHT)
1) PON Hippocrates –Biosensor for Early diagnosis of sepsis
Operating Unit: M&Nbit Laboratory, Dpt. of Biological and Environmental Sciences, University of Messina. Resp. Prof. S. Guglielmino

Aims

The Project Hippocrates aims to develop, test and validate, technologically innovative systems based on micro-and nano-technologies, with the final goal of an early detection, prevention and effective treatment of diseases.
Besides, the project aims to launch, through integrated ICT, the construction of a software infrastructure consistent with the adoption of a patient centric model.
In particular, the project aims to address the following research lines:
1. Development of advanced technological solutions for in vitro diagnosis using miniaturized and high performance (sensitivity, 'specificity', etc) biosensors for nucleic acids and proteins that can also be used by unskilled personnel at competitive costs;
2. Development of "smart" molecular systems for targeted and personalized pharmacological therapy, through drug delivery systems able to improve both bioavailability and the therapeutical index of the active administered obtaining a controlled and targeted release;
3. Development of an information infrastructure for the direct transmission of clinical data of biosensors and drug delivery systems to electronic health record, which represents a high level of integration of clinical information of individual patients

contributing, therefore, the full adoption centric model of a patient who, for health systems, is a desirable at both national and European level.

Results

PON Hippocrates - Early diagnosis of sepsis

The Operating Unit of Messina is involved in early diagnosis of sepsis, with the aim to identify molecular probes to be used for binding and concentration of blood markers.

In detail, for sepsis diagnosis, molecular probes, based on genetically-modified bacteriophages able to recognize and bind the surface of sepsis ethiological agents (*Escherichia coli*, *Listeria monocytogenes*, *Staphylococcus aureus* and *Staphylococcus epidermidis*) were selected.

Moreover, three prototypes of biosensor have been designed. In two prototypes, the bond between probes and pathogens is revealed by CMOS technology and RAMAN spectroscopy, respectively; the third prototype is a PCR-base Lab-on-Chip (LoC), which is actually under study.

2C – Project IM-MILK

Operating Unit: M&Nbit Laboratory, Dpt. of Biological and Environmental Sciences, University of Messina. Resp. Prof. S. Guglielmino

Aims

The aim is the construction of a microsensor for detecting *Escherichia coli* in raw milk to be used by farmers for self-certification of quality control.
In food analysis, the low concentration of bacterial pathogens is critical for their detection. Among the techniques of cell separation, immunomagnetic separation is a cell-separation technique where magnetisable micro- or nano-beads are first coated with antibody, then selectively bond to the target cell. Yet, antibodies suffer a few drawbacks as explained below. Antibodies are often used as biosensing selective element Polyclonal antibodies obtained from immunised animals are often cross-reactive, whereas monoclonal antibodies are selective, but costly. Generally, antibodies are susceptible to environment conditions and often of low availability. An effective alternative to antibodies are random phage peptides, displayed on the surface of filamentous bacteriophages. They are foreign peptides whose coding has been introduced in the genome through recombinant modification. Phage-displayed peptides can act as antibody alternative. Phage peptides are durable, of standardised forms and low-cost. In addition, they are prone to simple immobilisation through physical adsorption and to reproducible orientation onto surfaces. Phage-display has become routinely used for the isolation of peptide ligands to a wide variety of targets, including bacteria cells.

Results

The Operating Unit of Messina is involved in production of molecular probes and their immobilization on several types of beads, by which capture and concentrate *E. coli* in raw milk.
Actually, the best solution is represented by T4 phage-coated tosyl-activated Dynabeads, where the phage was consistently bound to Dynabeads, showing no variations in lytic activity.
Other technical solutions are currently under study.

2C – P-type ATPases as pharmacological targets

F. Tadini-Buoninsegni, G. Bartolommei, M.R. Moncelli
(University of Florence, Department of Chemistry)

Aims

Study of the effects of molecules with pharmacological interests on P-type ATPases. Determination of the drug affinity for the protein. Investigation of the mechanism of action. Role of ATPases in anticancer treatment.

Results

P-type ATPases are membrane proteins that translocate ions across cell membranes. Ion transport is directly coupled to ATP hydrolysis and a phosphorylated intermediate is formed during the enzymatic cycle. Considering the physiological importance of P-type ATPases, it is clear that defects in their mechanism of action may cause severe diseases. Moreover, these transporters represent potential pharmacological targets and play a key role in pharmacokinetics by increasing or rather interfering with the effectiveness of certain drugs.

We are currently investigating the transport mechanism of several P-type ATPases, as well as the effects of various molecules that can modulate (by inhibition or activation) the activity of these transporters.

Recently, in collaboration with colleagues of the Prassis-Sigma Tau Research Institute in Milan we have carried out a study on SERCA2a, a calcium ATPase isoform found in the heart sarcolemma [1]. We demonstrated that the new drug Istaroxime enhances SERCA2a activity, Ca^{2+} uptake and the Ca^{2+}-dependent charge movements into dog healthy and failing cardiac SR vesicles (Fig. 1).

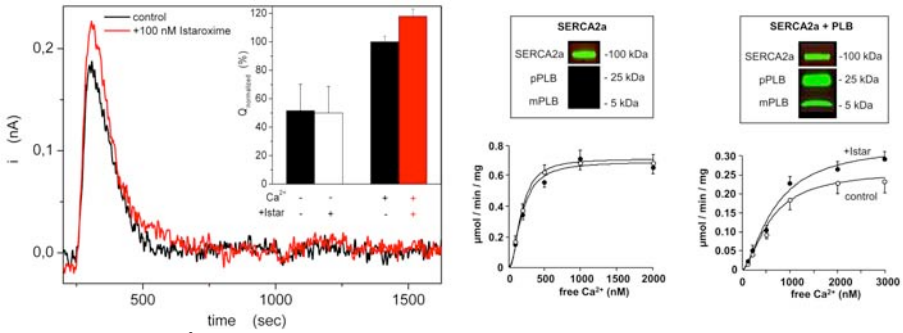

Fig. 1: Increase of Ca^{2+}-dependent charge movements in SERCA2 by Istaroxime (right). Drug-dependent enhancement of calcium transport seems related to the presence of a small (52 aa) regulatory membrane protein called phospholamban, PLB (left). PLB can exist in monomeric (mPLB) as well as pentameric (pPLB) forms.

To our knowledge, this is the first example of a SERCA activator that may be used to restore impaired ATPase activity. This research has received very positive editorial attention as highlighted by the commentary that will appear in the same journal issue [2].

Another interesting research topic is the human copper ATPase and its role in mediating resistance of cancer cells to anti-tumor drugs. This protein catalyzes the ATP-dependent copper transport across cellular membranes and exists in two main isoforms, ATP7A and ATP7B. Inactivation of either ATP7A or ATP7B is associated with severe metabolic disorders, known as Menkes (ATP7A) and Wilson (ATP7B) diseases.
Our research aims at investigating the mechanism of interaction of platinum-based drugs (e.g. cisplatin and oxaliplatin) with recombinant human ATP7A and ATP7B, obtained by heterologous expression in COS-1 cells. We measured ATP-dependent charge movements on COS-1 microsomes containing ATP7A or ATP7B adsorbed on a solid supported membrane (Fig. 2).

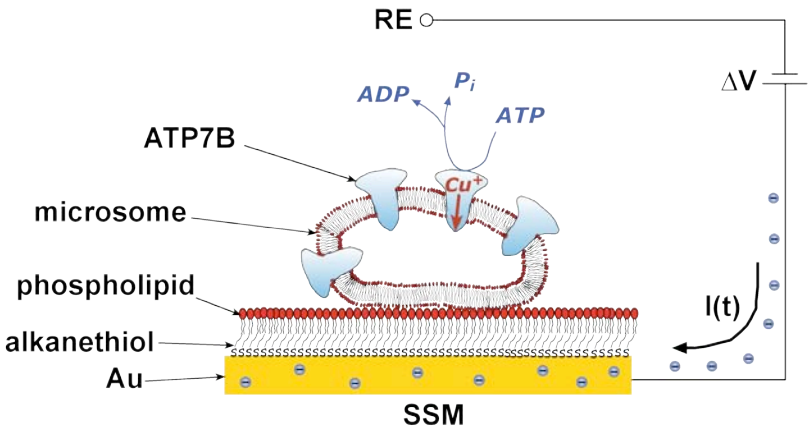

Fig. 2: Schematic representation of a microsome containing ATP7B adsorbed on a solid supported membrane, SSM (not drawn to scale).

Our results show that a charged platinum species undergoes vectorial displacement within the enzyme upon ATP utilization (formation of the phosphoenzyme intermediate required), analogous to the copper transport cycle. We also found that copper interferes with platinum transport and viceversa. We propose a mechanism for the electrogenic platinum transport by ATP7A/B [3].

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2C – Biomolecules Integration in Electronic Devices for Ultrasensitive Biosensors Development

M. Magliulo, A. Mallardi, K. Manoli, G. Palazzo, L. Torsi

Aims

Bio-systems interfaced to an electronic device is presently one of the most challenging research activity that has relevance not only for fundamental studies but also for the development of highly performing bio-sensors. Particularly, the development of new strategies ensuring a stable and well-oriented integration of biomolecules in electronic devices is a major challenge for the development of ultrasensitive biosensors. Innovative methods to integrate biorecognition elements in organic field effect transistor (OFET) devices are explored. Two completely novel approaches comprising a Functional Biological Interlayer (FBI-OFET) or Electrolyte gated-OFET (EGOFET) integrating bio-recognition elements were recently proposed by the Torsi's group.

Results

Functional Biological Interlayer (FBI)-OFET (Fig. 1) comprises a biological layer, acting as biosensor recognition element, which is fully integrated into the device structure, residing underneath the organic semiconductor film, right at the interface were the OFET two-dimensional transport occurs. A streptavidin embedding FBI-OFET capable to perform label-free selective detection of biotin at 3 ppt was proposed. The response is logarithmic spanning over five orders of magnitude of analyte concentration. The FBI-OFETs can operate also with an antibody interlayer as well as with an *ad hoc* designed micro-fluidic system. These occurrences, along with the proven extremely high sensitivity and selectivity, open to FBI-OFETs consideration as disposable electronic strip-tests for assays in biological fluids requiring very low detection limits.

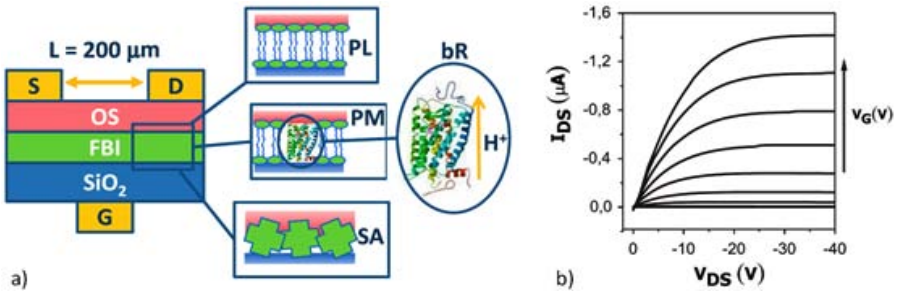

Fig. 1: FBI-OFET embedding different biorecognition layer, namely phospholipids, bacteriorhodopsin and streptavidin (a) along with typical I-V characteristic curves obtained for a streptavidin FBI-OFET (b).

Another interesting general platform for biosensing is the bio-electrolyte gated OFET (BIOEGOFET). This device is fabricated by anchoring a capturing bio-layer capable to control ionic diffusion into the OSC (Fig. 2). The OSC surface modification is achieved by a plasma enhanced vapor chemical deposition (PE-CVD). These -COOH groups are eventually used to stably anchor phospholipid (PL) layer containing a fraction of PL bearing amino group or biotin (biotinylated PL) to the OSC surface. The non-polar nature of the deposited PL bilayer interior minimizes ionic diffusion

through the membrane, eventually limiting the OSC doping, while the biotinylated PLs conveniently furnish the binding sites for streptavidin or avidin capturing proteins that can be further used for biothynilated bio-receptors immobilization (antibodies or nucleic acids).

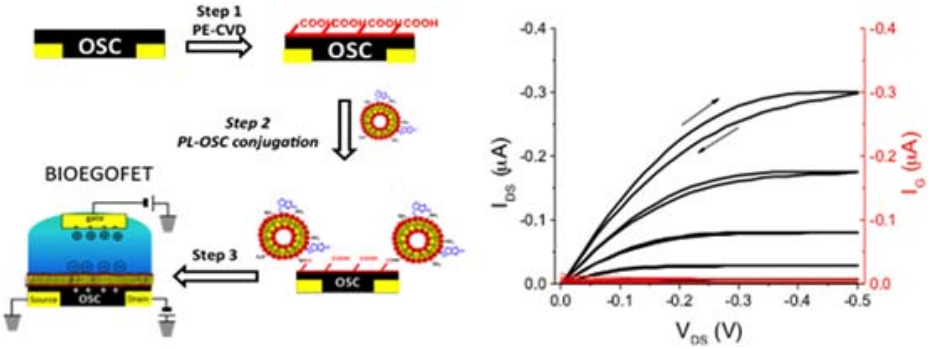

Fig. 2: Scheme of phospholipid BIOEGOFET fabrication along with typical source-drain current-voltage characteristics (black curves) and gate currents (red curves) in presence of PBS.

Such BIOEGOFET retains good field-effect performances (Fig. 2) and can lead to stable and reliable label-free electronic sensing in electrolyte solution with physiologically relevant ionic strength.

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2C – Optical biososensors and bioassays based on immobilized proteins

G. Palazzo, M. Giustini, A. Mallardi (CNR-IPCF)

Aims

Chemical compounds determination in medical, food and environmental samples often requires sophisticated analytical methods, expensive equipments and/or polluting solvent employment. Optical sensors based on biomolecules have been proven to be promising tools for this purpose, because of their advantages such as selectivity, low cost, fast and cheap screening of samples.

Results

Proteins can be immobilized in ordered films on a transparent solid support by means of an alternate deposition with charged polymers: this leads to the formation of the so-called polyelectrolyte multilayers. Such films are readily prepared by "layer-by-layer" (LbL) assembly, a simple process based on the sequential adsorption, driven by electrostatic interactions or by chemical affinity, on a support. The obtained surfaces are still transparent in UV and visible regions and they can be used in optical detection methods. The effect of herbicides on the optical response of photosynthetic proteins to illumination is exploited to develop herbicide biosensor. Other studies are oriented to develop low cost, portable and disposable paper-based bioassays. A first assay for phenolic compounds is based on an enzymatic assay. The tyrosinase enzyme has been immobilized on a filter paper by simple over-spotting with 3-methyl-2-benzothiazolinone hydrazone (MBTH), that allows the detection of phenols by forming stable colored adducts with their enzymatic oxidation products. Analyte detection can be achieved by eye and quantification can be simply obtained by using a camera phone and an image analysis software.

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2C – Direct binding of Resveratrol to SIRT1 studied by Small Angle Neutron Scattering and Nuclear Magnetic Resonance

C. Bonechi, S. Martini, A. Donati, C. Rossi, S. Ristori

Aims

To probe the ability of trans-resveratrol (trans-3,5,4'-trihydroxystilbene, Resv) to interact directly with the human sirtuin SIRT1 and to assess if this interaction can occur at the SIRT1 active site

Results

Polyphenols potent antioxidants and, in particular, those derived from plant sources are used in medicine for their well known beneficial effects on human health. Resveratrol (Resv) is a phenolic compound found in grapes, mulberries and cocoa, which is able to exert cardiovascular protection as well as anti-proliferative and anti-inflammatory action. However, the most intriguing property of which Resv has been credited is life span extension in lower organisms. This, in turn, is connected with the activity of sirtuins, a class of histone deacetylase proteins involved in the mimicking of calory restriction.

Seven sirtuins have been identified in mammals and, among these, SIRT1 is regulates important processes, such as glucose and insulin production. Previous screening over 20,000 molecules led to recognize resveratrol as one of the strongest enhancer of SIRT1 activity in vitro.

Here we showed for the first time the direct interaction of Resv with SIRT1 in D_2O solution and, more specifically, with a 27 aminoacid peptide (pSIRT1) having the same sequence of the SIRT1 active site:

Gly-Ile-Pro-Asp-Phe-Arg-Ser-Arg-Asp-Gly-Ile-Tyr-Ala-Arg-Leu-Ala-Arg-Asp-Phe-Pro-Asp-Leu-Pro-Asp-Pro-Gln-Ala

pSIRT1 was synthetized for the purpose of mimicking the interaction of Resv with this relevant protein subunit.

In the SANS diagrams the low-q intensity increased for Resv:SIRT1 molar ratio in the range 25-100 (figure 1a), while at higher ratios precipitation occurred. The extra intensity, being related to size increase of scattering objects, suggested that Resv is able to act as a bridging unit among sirtuin molecules in solution.

A similar effect was observed when Resv was added to pSIRT1 solution in D_2O (figure 1b). In this case the growing of aggregates was visible at lower molar ratios and precipitation occurred at Resv:pSIRT1 ≥ 5.

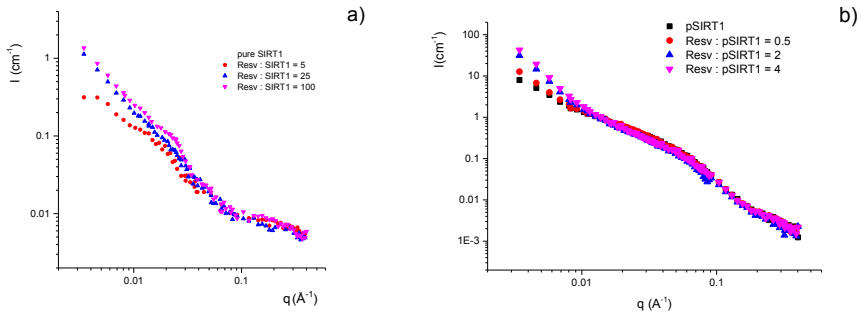

Fig. 1

These preliminary data indicated that association between Resv and the active site of SIRT1 actually occurs. Therefore we decided to investigate further the modality of this interaction by high resolution NMR.
The ^{1}H spectrum of Resv:pSIRT1=4:1 in D_2O is reported in Figure 2.

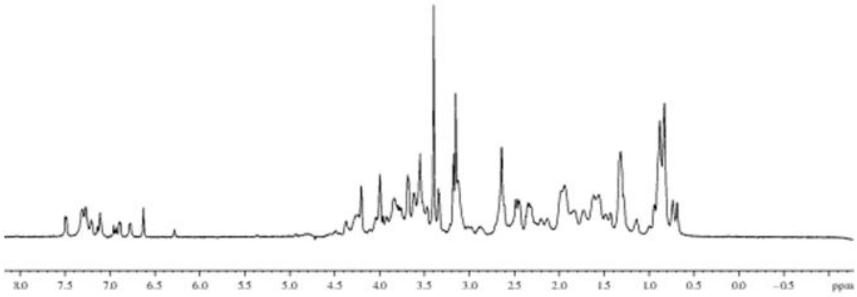

Fig. 2: Proton NMR spectrum of RSV: pSIRT1 = 4:1 in D2O recorded at 600 MHz and 298 K.

The Resv protons resonate at low field (7.48, 6.96, 6.93, 6.88, 6.61, 6.27 ppm). Other peaks in this region were attributed to the signals from aromatic protons in the Tyr and Phe aminoacids.
The interaction between Resv and pSIRT1 was also investigated by recording NOESY spectra at varying Resv:pSIRT1 ratios, with the aim of emphasizing the dipolar interactions occurring in aqueous solution. In the NOESY spectrum of the Resv:pSIRT1=4:1 sample the H_4 (6.27 ppm) of Resv clearly showed a cross-peak with the methyl group of isoleucine 11, resonating at 0.85 ppm. Moreover Resv signals at 7.48 and 6.88 ppm ($H_{2',6'}$ and $H_{3',5'}$ respectively) showed dipolar coupling with the peptide proton signals at 1.30, 1.59, 1.93 ppm. These data gave information on the interaction site between SIRT1 and Resv in solution. Distance bounds, calculated from the nuclear Overhauser effect (NOE) crosspeak intensities, were also used to restrain the structure of the two structures during simulations of molecular dynamics.

References

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