Consorzio Interuniversitario
per lo Sviluppo dei Sistemi
a Grande Interfase

Report 2017

Last update December 2016
Editing by Filippo Baldereschi
Printed in July 2017

Summary

CSGI Research Activity *1*
Structure and Organization of CSGI *3*
Academic Units and Associated Centers *4*
CSGI Patents *7*
CSGI Registered Trade Marks *9*
Prospective CSGI Activity in 2017-2018 ..... *10*
List of Publications 2014-2016 ..... *11*
Conferences 2014-2016 ..... *58*
Theses (undergraduate, master and phd) *75*

1A: Hard Matter (Nanomaterials and Solid Interfaces)

Spontaneous aggregation of soil organic matter and its interaction with iron oxide particles *87*
Adhesion promoters for bitumen *89*
Design, synthesis and applications of new organic sensitizers for non-conventional photovoltaic cells *91*
Production and characterization of photoactive materials *93*
Ordered mesoporous silica in nanomedicine: effect of functionalization and interactions with proteins *95*
Carbon based nanostructures for innovative hydrogen storage systems *97*
Reversible hydrogen sorption for borohydrides infiltrated in silica matrices *99*
Nanostructured scaffolds for tissue engineering *101*
Nanohybrids P3HT-based systems *103*
Calcium phosphate-based nanostructures: synthesis in composite materials, stabilization and interaction with biologically relevant soft matter *105*
Advanced nanostructured materials for eco-sustainable cements: investigation of the structural properties and innovative strategies for their improvement *107*
A green integrated microwave-assisted synthesis of hexagonally ordered silica sieves using a geothermal waste as silicon source *109*
Microwave assisted synthesis of hexagonally ordered mesoporous silica modified by isomorphic incorporation of yttrium *111*
Tuning the pore size, surface area and hydrophobicity of template-based mesoporous silica sba-15 ..... *113*
Nanostrategies for early diagnosis and treatment of FKBP12-related neurodegenerative amyloidosis *115*
Surface engineering of nanostructured oxide systems for solar energy conversion . *117*
Electrical investigation of molecular wires *119*

1B: Soft Matter (Nanomaterials and Liquid Interfaces)

Rheology and rheo-nmr-imaging of lecithin-based viscoelastic solutions. *121*
Phyto-liposomes as biocompatible carriers for natural drugs *123*
Formulation of liposomes functionalized with specific protein and effective in targeting highly proliferative cells *125*
Effect of resveratrol on platelet aggregation by fibrinogen protection: NMR, IR and SEM experiments *127*

Effect of quercetin-loaded liposomes on induced oxidative stress in human spermatozoa 129
In vitro assays for the "ORAC" classification 131
Interaction of antimicrobial peptides with lipid membranes 133
EPR investigations of enzyme-ligand complex in copper containing proteins 135
Loading, protection and release of hydrophylic molecules entrapped in liposome based multishell nanocapsules 136
Coumarin derivative for sensing application: nucleotides identification using a micellar system 138
Cubosomes and hexosomes in theranostic nanomedicine 140
Poly(vinyl alcohol)-based microgels prepared through salting out: rationalising the aggregation process 142
Neuroprotective effect of poly-unsaturated fatty acids: structure, dynamics and interaction with amyloid peptides of omega-3 containing lipid bilayers 144
Characterization of protein-NPs interaction and development of aptamer functionalized NPs 146
Effect of cardiolipin on lipid bilayers 147
Bioinspired eumelanin-based nanomaterials for antimicrobial applications 148
Protein trapping within nanostructured surface 150
Role of polymer molecular weight on the removal process using amphiphilic formulations 152
Structure-property relation in oil soluble dispersants for lubricant media 154
Relation between structural and diffusional properties in classical and semi-IPN hydrogels 156
Biomimetic membranes and interaction with nanosystems 158
Lipid-spions mixed assemblies as smart drug delivery systems 160
Poly(ethylene glycol)-graft-poly(vinyl acetate) single-chain nanoparticles for the encapsulation of small molecules 161
Delivery of nucleic acid-based therapeutics for the treatment of antibiotic-resistant pathogens 163
Complexation of short ds RNA/DNA oligonucleotides with gemini micelles: a time resolved saxs and computational study 165
Nitric oxide assisted c60-SIMS for molecular depth profiling of polyelectrolyte multilayers 167

1C: Theory and Modelling

Active sites of copper-trafficking proteins: density functional structural and spectroscopy studies on copper(i) models 169
Biopolymers and biomacromolecules solvent 171
In silico design of dyes for DSSC 173
Computational spectroscopy of protein radicals 175
A complex system's view of the rebound effect in energy efficiency 177
Leather production ultrasound-assisted as best available technology to reduce damages to workers health 179
Specific ion effects in protein systems 180
Simulation of sims depth profiles of organic solids by transport diffusion model 182
Automated data mining of secondary ion mass spectra 184

2A: Art Restoration, Environmental Remediation and Textile Chemistry

Environmental assessment of total reinjection system for deep high temperature/high pressure geothermal resources 186
Biomass adsorbent for removal of toxic metal 188
Synergies in chemical, optical and biological conditions causing the formation of black water blooms 190
Micro and macroscale drivers of nutrient pollution in freshwater environments in north and south america 191
LCA of integrated agro-industrial chains for energy and biochemicals production from micro-algae and terrestrial oilseed crops 192
Energy efficiencies and LCA studies on technologically advanced energy devices and grid system 194
Nanomaterials for enzymes immobilization 196
Visible light activated carbon doped titanium dioxide for cleaning of olive mill wastewaters 198
Physico-chemical analysis and characterization of ancient mortars and other archaeological materials 200
Organogels for the cleaning of artifacts 202
Chemical hydrogels for the cleaning of artifacts 204
Film forming pva-based cleaning systems for the removal of corrosion products from historical bronzes 206
Calcium and barium hydroxide nanoparticles for the consolidation of wall paintings 208
Nanomaterials for the cleaning and ph adjustment of leather 210
Nanocomposite materials for the consolidation and strengthening of cellulose-based artifacts 212
Nanotechnology for the deacidification of cellulose-based works of art 214
A stabilizer-free nonpolar dispersion for the deacidification of contemporary art on paper 216
Amphiphile-based nanofluids for the removal of organic coatings from works of art 218
Nanostructured fluids for the conservation of cultural heritage: understanding the mechanism of organic coatings removal 220
Nanofluids and chemical hydrogels for the selective removal of overpaintings and undesired graffiti from street art 222

2B: Metals and Ceramics

Effect of mechanical energy on solid state synthesis of ternary oxides 224
New cathode materials for technological applications 225
Synthesis and characterization of nano-biomaterials 227

2C: Biotechnology

Chemical characterization and antioxidant properties of olive pomaces and olive leaves 229
Chemical characterization of peaches and nectarines 231
A multidisciplinary project for the study of historical landscapes: new archaeological and physicochemical data from the "colline metallifere" district 233

Identification of catalytic protein radicals in LRET mechanism of peroxidases and variants *235*
Biotechnological applications of oxidases *237*
A comparative study of chromatographic matrices for affinity chromatography of CRM197 ..... *239*
Enzyme-containing paints inhibit the growth of marine microorganisms *241*
The multifaceted benefits of protein co-expression in escherichia coli *243*
Oleuropein degradation by olive leaf protein extract *245*
Thermodynamics properties and photodegradation kinetics of indocyanine green in aqueous solution *247*
In vivo near-infrared fluorescence imaging of aqueous humor outflow structures *249*
Physico-chemical properties of pharmaceutical systems *251*
Phospholamban (PLN) regulation of sarco/endoplasmic reticulum Ca-ATPase (SERCA) *253*
Interaction of antitumor drugs with P-type ATPases *255*
Glutathione, glutathione disulfide and s-glutathionylated proteins in cell cultures *257*
Graphene/nanoparticles hybrid system for the controlled immobilization of biomarkers for early diagnosis of neurodegenerative diseases *259*

Author index *261*

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. It is also 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 (such as Nanorestart, Dna-Trap, Issflow, ShaleXEnvironment, Bioclean, Icarus), 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, L'Oreal, Solay, Eni SpA, bioMérieux Italia SpA, Lamberti SpA, Giuliani SpA, CTG Italcementi, King Saud University, Martelli Srl, Rifinizione S. Stefano, AMSA, Pierre Fabre, Farmabios, Fater SpA, University of Florida, È Così, Lachesis, MBN SpA, Novartis, W.A.D.A., Morphotec, Perkin Elmer, Grünenthal Gmbh, Comune di Firenze, Teletron Euroricerche, VTT, etc… The main results of these collaborations have 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 many applications of Nanotechnology, in the conservation of cultural heritage, and in the making of nanophasic powders (with MBN) to produce 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 promoted by the Mexican Federal Government for the conservation of monuments (Puebla Cathedral, Maya and Aztec heritage, the archaeological site of Calakmul, Campeche), have been conducted in association with Mexican museums and conservation institutions.

CSGI is also very active 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 and symposia. During the years 2014-2016, CSGI has issued 14 PhD scholarships, 39 fellowships, and 62 post-doc grants, and is actively participating in one European Master Program: 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 to produce: nanophasic systems (i) innovative textiles, (ii) nanophasic alloys, (iii) ceramics and nanophasic or nanostructured composites (with low temperature and low energy costs);

- setup of new additives for cement products and cement formulations. These projects are mainly carried out in collaboration with CTG-Italcementi and MIT, and are aimed at investigating and optimizing (i) the cement hydration process and the production of new additives, (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 recovery 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 (2011-2014): CSGI ranking

CSGI was one of the 9 Consortia that voluntary submitted their candidature, for the second time in a raw, 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 2011-2014. 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. VQR 2006-2010 and 2011-2014 resulted in the largest-scale evaluations of research in Italy's history.
The VQR examined research outcomes in 14 disciplinary areas of study published between 2011 and 2014 by 96 universities, 18 research centers and 19 other institutions to identify the significance of the Italian research output and how it compares globally. By reviewing a significant number of Italian research outcomes,

ANVUR could gain a greater understanding of Italian research strengths, impact and neglected fields of study.
CSGI ranked in the first position among the other Italian Consortia for Chemical Sciences (Area 03) for the period 2011-2014.
In the disciplines related to Chemical Sciences (the core of the CSGI research), CSGI resulted as excellent (about 85% of the submitted products were judged as excellent and the remaining products were classified 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.

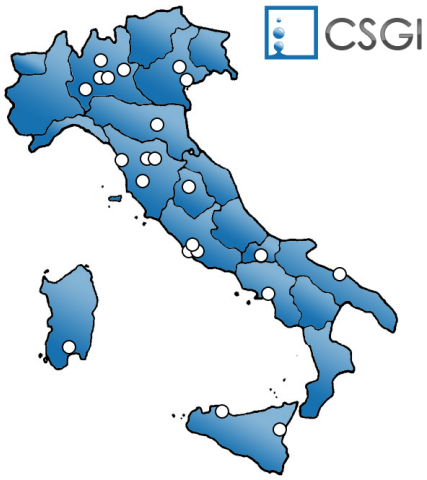
Website
http://www.csgi.unifi.it/

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 "Aldo Moro"
- 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
  - Opificio delle Pietre Dure
  - Polytechnic Institute of Milan
  - University of Bologna
  - University of Brescia
  - University of Milan, Bicocca
  - University of Palermo
  - University of Perugia
  - University of Rome, La Sapienza
  - University of Rome, Tor Vergata
  - University of Rome - TRE
  - 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 4 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 various European projects.
CSGI owns two research Laboratories, located in Vascon di Carbonera (Nanophases Laboratory).

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
Tufts University
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 Valladolid
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 SpA
bioMérieux Italia SpA
Bioscreen Technology srl
Bitossi
BTG-Holland
Chemia
Chiesi Farmaceutici SpA
Chimet S.p.A.
Comune di Firenze
Consorzio delle Buone Idee
Cover
D'Appolonia
Dynamotive
Elf-Atochem
ENEA (Energy Department – Casaccia)
Eniricerche
Eni SpA
Enitecnologie
EUBIA (Bruxelles)
Fater SpA
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 SpA
Italfarmaco
JRC (Joint Research Centre of the European Commission)
Kucept Ltd (UK)
Lamberti SpA
Ely-Lilly
Lima
Lombardia
Mapei
Mariplast
Martelli Srl
MBN Nanomaterialia
Merk
Microtec (Germany)
Nanovector Srl
Nicox
Novuspharma Omrod Diesel (UK)
Orion Pharma
Pharmacia-Upjon (USA and Sweden)
Pharmaness
Philips
Procarta Biosystems Ltd
Procter & Gamble
Rifiniture BP
S.I.F.I.
Sem
Siemens AG
Sigma-tau
Sintech
SIR Industriale
Sirio Panel
Solvay
Soprintendenze ai Beni Artistici e Storici di: FI-PO-PT, SI-GR, PI-LU-MS
Tecnotessile SpA
Tecrea Ltd (UK)
TIL (Tooling International Ltd UK)
TNO (Netherlands)
Transfergomma (Padova)
VTT (Finland).
WIP (Germany)

CSGI Patents

1) Baglioni Piero, Dei Luigi, Ferroni Enzo, Giorgi Rodorico – "Sospensioni stabili di idrossido di calcio". Italian Patent FI/96/A000255, deposit date 31/10/1996.

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, Italian Patent N. 0001328470, 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, Italian Patent N. 0001368154/2009, 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) Ranieri Rossi, Daniela Giustarini – "Metodo per la misura del glutatione su sangue prelevato tramite digitopuntura" Italian Patent N. 0001420029 deposit date 18/06/2013.

30) 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.

31) Bettini Ruggero, Hochkoeppler Alejandro, Melegari Cecilia, Primiceri Giuseppe, Stefan Alessandra – "Composizioni farmaceutiche con ridotto impatto ambientale." Italian patent IT 0001415653, deposit date 12/05/2015.

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

3) Nanorestore Gel® International Class 01, 03, 37 Registration n. 12696308 del 12/08/2014 RIF. 30346

4) Nanorestore Cleaning® International Class 01, 03, 37 Registration n. 013603006 del 07/05/2015 RIF. 30836

5) Nanorestore Plus® International Class 01, 37, 40 Registration n. 014414262 del 30/11/2015 RIF. 30836

Prospective CSGI Activity in 2017-2018

CSGI is involved in several European projects (FP7 and H2020), in several international and national projects, and in collaborations with industries and SME (small and medium enterprises).
CSGI is developing its own research activity to optimize the application of research projects inspired by the urging demands of small and medium size companies.
CSGI is actively working to offer a valid support to the Italian industrial system to set and develop of projects and pre-industrial processes.

List of Publications 2014-2016

1. 1,2-Benzisothiazole Derivatives Bearing 4-, 5-, or 6-Alkyl/arylcarboxamide Moieties Inhibit Carbonic Anhydrase Isoform IX (CAIX) and Cell Proliferation under Hypoxic Conditions. Coviello, V; Marchi, B; Sartini, S; Quattrini, L; Marini, AM; Simorini, F; Taliani, S; Salerno, S; Orlandi, P; Fioravanti, A; Di Desidero, T; Vullo, D; Da Settimo, F; Supuran, CT; Bocci, G; La Motta, C. *Journal Of Medicinal Chemistry* 59, 6547-6552 (2016).
2. 2LiBH(4)-MgH2 nanoconfined into carbon aerogel scaffold impregnated with $ZrCl_4$ for reversible hydrogen storage. Utke, R; Thiangviriya, S; Javadian, P; Jensen, TR; Milanese, C; Klassen, T; Dornheim, M. *Materials Chemistry And Physics* 169, 136-141 (2016).
3. 4-Arylbenzenesulfonamides as Human Carbonic Anhydrase Inhibitors (hCAIs): Synthesis by Pd Nanocatalyst-Mediated Suzuki-Miyaura Reaction, Enzyme Inhibition, and X-ray Crystallographic Studies. Cornelio, B; Laronze-Cochard, M; Ceruso, M; Ferraroni, M; Rance, GA; Carta, F; Khlobystov, AN; Fontana, A; Supuran, CT; Sapi, J. *Journal Of Medicinal Chemistry* 59, 721-732 (2016).
4. 5,6-Dihydroxyindole-2-carboxylic-Acid-TiO2 Charge Transfer Complexes in the Radical Polymerization of Melanogenic Precursor(s). Vitiello, G; Pezzella, A; Calcagno, V; Silvestri, B; Raiola, L; D'Errico, G; Costantini, A; Branda, F; Luciani, G. *Journal Of Physical Chemistry C* 120, 6262-6268 (2016).
5. 7-Aryl-triazolyl-substituted sulfocoumarins are potent, selective inhibitors of the tumor-associated carbonic anhydrase IX and XII. Nocentini, A; Ceruso, M; Carta, F; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1226-1233 (2016).
6. 9,10-Dibromo-N-aryl-9,10-dihydro-9,10-[3,4]epipyrroloanthracene-12,14-diones: Synthesis and Investigation of Their Effects on Carbonic Anhydrase Isozymes I, II, IX, and XII. Goksu, H; Topal, M; Keskin, A; Gultekin, MS; Celik, M; Gulcin, I; Tanc, M; Supuran, CT. *Archiv Der Pharmazie* 349, 466-474 (2016).
7. A Combined Crystallographic and Theoretical Study Explains the Capability of Carboxylic Acids to Adopt Multiple Binding Modes in the Active Site of Carbonic Anhydrases. Langella, E; D'Ambrosio, K; D'Ascenzio, M; Carradori, S; Monti, SM; Supuran, CT; De Simone, G. *Chemistry-A European Journal* 22, 97-100 (2016).
8. A continuous spectrophotometric enzyme-coupled assay for deoxynucleoside triphosphate triphosphohydrolases. Singh, D; Schaaper, RM; Hochkoeppler, A. *Analytical Biochemistry* 496, 43-49 (2016).
9. A Divalent PAMAM-Based Matrix Metalloproteinase/Carbonic Anhydrase Inhibitor for the Treatment of Dry Eye Syndrome. Richichi, B; Baldoneschi, V; Burgalassi, S; Fragai, M; Vullo, D; Akdemir, A; Dragoni, E; Louka, A; Mamusa, M; Monti, D; Berti, D; Novellino, E; De Rosa, G; Supuran, CT; Nativi, C. *Chemistry-A European Journal* 22, 1714-1721 (2016).
10. A generation-attraction model for renewable energy flows in Italy: A complex network approach. Valori, L; Giannuzzi, GL; Facchini, A; Squartini, T; Garlaschelli, D; Basosi, R. *European Physical Journal-Special Topics* 225, 1913-1927 (2016).
11. A magnificent enzyme superfamily: carbonic anhydrases, their purification and characterization. Guler, OO; Capasso, C; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 689-694 (2016).
12. A new insight into black blooms: Synergies between optical and chemical factors. Duan, HT; Loiselle, SA; Li, ZC; Shen, QS; Du, YX; Ma, RH. *Estuarine Coastal And Shelf Science* 175, 118-125 (2016).
13. A new potassium-based intermediate and its role in the desorption properties of the K-Mg-N-H system. Santoru, A; Garroni, S; Pistidda, C; Milanese, C; Girella, A; Marini, A; Masolo, E; Valentoni, A; Bergemann, N; Le, TT; Cao, H; Haase, D; Balmes, O; Taube, K; Mulas, G; Enzo, S; Klassen, T; Dornheim, M. *Physical Chemistry Chemical Physics* 18, 3910-3920 (2016).
14. A new procedure for the cloning, expression and purification of the beta-carbonic anhydrase from the pathogenic yeast Malassezia globosa, an anti-dandruff drug target. Del Prete, S; De Luca, V; Vullo, D; Osman, SM; AlOthman, Z; Carginale, V; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1156-1161 (2016).
15. A novel library of saccharin and acesulfame derivatives as potent and selective inhibitors of carbonic anhydrase IX and XII isoforms. Carradori, S; Secci, D; De Monte, C; Mollica, A; Ceruso, M; Akdemir, A; Sobolev, AP; Codispoti, R; De Cosmi, F; Guglielmi, P; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 1095-1105 (2016).
16. A novel MODIS algorithm to estimate chlorophyll a concentration in eutrophic turbid lakes. Zhang, YC; Ma, RH; Duan, HT; Loiselle, S; Zhang, MW; Xu, JD. *Ecological Indicators* 69, 138-151 (2016).
17. A step-by-step protocol for assaying protein carbonylation in biological samples. Colombo, G; Clerici, M; Garavaglia, ME; Giustarini, D; Rossi, R; Milzani, A; Dalle-Donne, I. *Journal Of*

Chromatography B-Analytical Technologies In The Biomedical And Life Sciences 1019, 178-190 (2016).

18. A Superior All-Natural Antioxidant Biomaterial from Spent Coffee Grounds for Polymer Stabilization, Cell Protection, and Food Lipid Preservation. Panzella, L; Cerruti, P; Ambrogi, V; Agustin-Salazar, S; D'Errico, G; Carfagna, C; Goya, L; Ramos, S; Martin, MA; Napolitano, A; d'Ischia, M. *Acs Sustainable Chemistry & Engineering* 4, 1169-1179 (2016).
19. Acetylcholinesterase and carbonic anhydrase inhibitory properties of novel urea and sulfamide derivatives incorporating dopaminergic 2-aminotetralin scaffolds. Oumlzgeris, B; Goksu, S; Kose, LP; Gulcin, I; Salmas, RE; Durdagi, S; Tumer, F; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 2318-2329 (2016).
20. Acetylcholinesterase and carbonic anhydrase isoenzymes I and II inhibition profiles of taxifolin. Gocer, H; Topal, F; Topal, M; Kucuk, M; Teke, D; Gulcin, I; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 441-447 (2016).
21. Active Components of Essential Oils as Anti-Obesity Potential Drugs Investigated by in Silico Techniques. Supuran, CT; Alcaro, S. *Journal Of Agricultural And Food Chemistry* 64, 5295-5300 (2016).
22. Alkaline nanoparticles for the deacidification and pH control of books and manuscripts. Giorgi, R; Chelazzi, D; Xing, H; Poggi, G; Baglioni, P. *Nanoscience and Cultural Heritage, eds. Philippe Dillmann, Ludovic Bellot-Gurlet, Irène Nenner, Atlantis Press-Springer*, 253-281 (2016).
23. Amido/ureidosubstituted benzenesulfonamides-isatin conjugates as low nanomolar/subnanomolar inhibitors of the tumor-associated carbonic anhydrase isoform XII. Eldehna, WM; Fares, M; Ceruso, M; Ghabbour, HA; Abou-Seri, SM; Abdel-Aziz, HA; Abou El Ella, DA; Supuran, CT. *European Journal Of Medicinal Chemistry* 110, 259-266 (2016).
24. A new RNA Aptamer against CA125 tumor marker: kinetic characterization by Surface Plasmon Resonance. Lamberti, I; Scarano, S; Esposito, CL; Antoccia, A; Antonini, G; Tanzarella, C; De Franciscis, V; Minunni M. *issue on Nucleic Acid Aptamers, Methods* 97, 58-68 (2016).
25. An improved neutron autoradiography set-up for 10B concentration measurements in biological samples. Postuma, I; Bortolussi, S; Protti, N; Ballarini, F; Altieri, S; Bruschi, P; Ciani, L; Ristori, S; Panza, L; Ferrari, C. Rep. Pract. Onc. Radiother. 21, 123-8 (2016).
26. An Overview of the Carbonic Anhydrases from Two Pathogens of the Oral Cavity: Streptococcus mutans and Porphyromonas gingivalis. Capasso, C; Supuran, CT. *Current Topics In Medicinal Chemistry* 16, 2359-2368 (2016).
27. An Unusual Natural Product Primary Sulfonamide: Synthesis, Carbonic Anhydrase Inhibition, and Protein X-ray Structures of Psammaplin C. Mujumdar, P; Teruya, K; Tonissen, KF; Vullo, D; Supuran, CT; Peat, TS; Poulsen, SA. *Journal Of Medicinal Chemistry* 59, 5462-5470 (2016).
28. An Update on Natural Products with Carbonic Anhydrase Inhibitory Activity. Karioti, A; Carta, F; Supuran, CT. *Current Pharmaceutical Design* 22, 1570-1591 (2016).
29. Anion inhibition profiles of alpha-, beta- and gamma-carbonic anhydrases from the pathogenic bacterium Vibrio cholerae. Del Prete, S; Vullo, D; De Luca, V; Carginale, V; di Fonzo, P; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry* 24, 3413-3417 (2016).
30. Anion inhibition profiles of the complete domain of the eta-carbonic anhydrase from Plasmodium falciparum. Del Prete, S; Vullo, D; De Luca, V; Carginale, V; di Fonzo, P; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry* 24, 4410-4414 (2016).
31. Anion inhibition studies of the beta-carbonic anhydrase from the pathogenic bacterium Vibrio cholerae. Vullo, D; Del Prete, S; De Luca, V; Carginale, V; Ferraroni, M; Dedeoglu, N; Osman, SM; AlOthman, Z; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 26, 1406-1410 (2016).
32. Anions as Triggers in Controlled Release Protocols from Mesoporous Silica Nanoparticles Functionalized with Macrocyclic Copper(II) Complexes. El Sayed, S; Milani, M; Milanese, C; Licchelli, M; Martinez-Manez, R; Sancenon, F. *Chemistry-A European Journal* 22, 13935-13945 (2016).
33. Antimony-phosphomolybdate ATPase assay. Bartolommei, G; Tadini-Buoninsegni, F. *Methods in Molecular Biology* 1377, 111-120 (2016).
34. A physico-chemical timer: autonomous time-delayed microfluidic valves for environmental applications. Tuccitto, N. *Microfluidics and Nanofluidics* 20, 129 (2016).
35. Are specific buffer effects the new frontier of Hofmeister phenomena? Insights from lysozyme adsorption on ordered mesoporous silica. Cugia, F; Sedda, S; Pitzalis, F; Parsons, DF; Monduzzi, M; Salis, A. *Rsc Advances* 6, 94617-94621 (2016).
36. Arteriolar Diameters in Glaucomatous Eyes with Single-Hemifield Damage. Russo, A; Costagliola, C; Rizzoni, D; Ghilardi, N; Turano, R; Semeraro, F. *Optometry And Vision Science* 93, 504-509 (2016).

37. A transport and reaction model for simulating cluster secondary ion mass spectrometry depth profiles of organic solids. Tuccitto, N; Zappalà, G; Vitale, S; Torrisi, V; Licciardello, A. *Journal of Physical Chemistry C* 120, 9263-9269 (2016).
38. A wavelet-PCA method saves high mass resolution information in data treatment of SIMS molecular depth profiles. Tuccitto, N; Zappalà , G; Vitale, S; Torrisi, V; Licciardello, A. *Surface and Interface Analysis* 48, 317-327 (2016).
39. Benzoxaborole as a new chemotype for carbonic anhydrase inhibition. Alterio, V; Cadoni, R; Esposito, D; Vullo, D; Di Fiore, A; Monti, SM; Caporale, A; Ruvo, M; Sechi, M; Dumy, P; Supuran, CT; De Simone, G; Winum, JY. *Chemical Communications* 52, 11983-11986 (2016).
40. Bioanalytical approaches in early diagnosis of Alzheimer's disease: from novel immunochemical to bio-mimetic emerging receptors. Scarano, S; Lisi, S; Ravelet, C; Peyrin, E; Minunni M. *Analytica Chimica Acta* (2016).
41. Biomass - an Overview. Bonechi, C; Donati, A; Leone, G; Magnani, A; Tamasi, G; Rossi, C. *Chapter in Bioenergy – A technology prospect forward the future, edited by F. Dalena, A. Basile, C. Rossi, Elsevier* (2016).
42. Biomimetic Metal Phenolates. Tamasi, G; Cini, R. *Chapter in Patai's Chemistry of Functional Groups, The Chemistry of Metal Phenolates Volume 2, edited by I. Marek (Guest editor J. Zabicky), John Wiley & Sons, Ltd. Chichester, UK* , - (2016).
43. Bortezomib inhibits bacterial and fungal beta-carbonic anhydrases. Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 4406-4409 (2016).
44. $Ca(BH_4)_2$-Mg_2NiH_4: on the pathway to a $Ca(BH_4)_2$ system with a reversible hydrogen cycle. Bergemann, N; Pistidda, C; Milanese, C; Emmler, T; Karimi, F; Chaudhary, AL; Chierotti, MR; Klassen, T; Dornheim, M. *Chemical Communications* 52, 4836-4839 (2016).
45. Calcium hydroxide nanoparticles from solvothermal reaction for the deacidification of degraded waterlogged wood. Poggi, G; Toccafondi, N; Chelazzi, D; Canton, P; Giorgi, R; Baglioni, P. *Journal Of Colloid And Interface Science* 473, 1-8 (2016).
46. Calcium hydroxide nanoparticles in hydroalcoholic gelatin solutions (GeolNan) for the deacidification and strengthening of papers containing iron gall ink. Poggi, G; Sistach, MC; Marin, E; Garcia, JF; Giorgi, R; Baglioni, P. *Journal Of Cultural Heritage* 18, 250-257 (2016).
47. Caratterizzazione chimica, varietale e geografica di pesche e nettarine mediante metodologie di analisi chimica e trattamento statistico dei dati. Tamasi, G; Bonechi, C; Magnani, A; Leone, G; Lamponi, S; Gallucci, G; Rossi, C. *Capitolo in Direct Food: Applicazioni avanzate per la valorizzazione dei prodotti agroalimentari della filiera corta* (2016).
48. Carbonic anhydrase activators: Activation of the beta-carbonic anhydrase from Malassezia globosa with amines and amino acids. Vullo, D; Del Prete, S; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 26, 1381-1385 (2016).
49. Carbonic anhydrase inhibition and cytotoxicity studies of Mannich base derivatives of thymol. Gul, HI; Yamali, C; Yasa, AT; Unluer, E; Sakagami, H; Tanc, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1375-1380 (2016).
50. Carbonic anhydrase inhibition and the management of neuropathic pain. Supuran, CT. *Expert Review Of Neurotherapeutics* 16, 961-968 (2016).
51. Carbonic anhydrase inhibition for the management of cerebral ischemia: in vivo evaluation of sulfonamide and coumarin inhibitors. Mannelli, LD; Micheli, L; Carta, F; Cozzi, A; Ghelardini, C; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 894-899 (2016).
52. Carbonic anhydrase IX correlates with survival and is a potential therapeutic target for neuroblastoma. Ameis, HM; Drenckhan, A; Freytag, M; Izbicki, JR; Supuran, CT; Reinshagen, K; Holland-Cunz, S; Gros, SJ. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 404-409 (2016).
53. Carbonic anhydrases are producers of S-nitrosothiols from inorganic nitrite and modulators of soluble guanylyl cyclase in human platelets. Hanff, E; Bohmer, A; Zinke, M; Gambaryan, S; Schwarz, A; Supuran, CT; Tsikas, D. *Amino Acids* 48, 1695-1706 (2016).
54. Carboxymethylinulin-Chitosan Nanoparticles for the Delivery of Antineoplastic Mitoxantrone. Merli, D; Pivi, F; Profumo, A; Quadrelli, P; Milanese, C; Risi, G; Visai, L. *Chemmedchem* 11, 2436-2444 (2016).
55. Challenging Organic Syntheses and Pharmacological Applications of Natural Products and their Derivatives - Part II. Mori, M; Supuran, CT. *Current Pharmaceutical Design* 22, 1559-1560 (2016).
56. Characterisation and Antioxidant Activity of Crude Extract and Polyphenolic Rich Fractions from C. incanus Leaves. Gori, A; Ferrini, F; Marzano, MC; Tattini, M; Centritto, M; Baratto, MC; Pogni, R; Brunetti, C. *International Journal Of Molecular Sciences* 17 (2016).
57. Cisplatin-protein interactions: unexpected drug binding to N-terminal amine and lysine side chains. Russo Krauss, I; Ferraro, G; Merlino, A. *Inorganic Chemistry* 55, 7814-7816 (2016).

58. Class I Hydrophobin Vmh2 Adopts Atypical Mechanisms to Self-Assemble into Functional Amyloid Fibrils. Gravagnuolo, AM; Longobardi, S; Luchini, A; Appavou, MS; De Stefano, L; Notomista, E; Paduano, L; Giardina, P. *Biomacromolecules* 17, 954-964 (2016).
59. Cloning, characterization and anion inhibition studies of a gamma-carbonic anhydrase from the Antarctic bacterium Colwellia psychrerythraea. De Luca, V; Vullo, D; Del Prete, S; Carginale, V; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry* 24, 835-840 (2016).
60. Cloning, expression and biochemical characterization of a beta-carbonic anhydrase from the soil bacterium Enterobacter sp B13. Eminoglu, A; Vullo, D; Asik, A; Colak, DN; Supuran, CT; Canakci, S; Belduz, AO. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1111-1118 (2016).
61. Cloning, expression, purification and sulfonamide inhibition profile of the complete domain of the eta-carbonic anhydrase from Plasmodium falciparum. Del Prete, S; Vullo, D; De Luca, V; Carginale, V; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry Letters* 26, 4184-4190 (2016).
62. Comparative Life Cycle Assessment study on environmental impact of oil production from microalgae and terrestrial oilseed crops. Spinelli, D; Jez, S; Busi, E; Fierro, A; Basosi, R. *J Energy Conversion and Management* under revision (2016).
63. Comparison of Smartphone Ophthalmoscopy With Slit-Lamp Biomicroscopy for Grading Vertical Cup-to-Disc Ratio. Russo, A; Mapham, W; Turano, R; Costagliola, C; Morescalchi, F; Scaroni, N; Semeraro, F. *Journal Of Glaucoma* 25, E777-E781 (2016).
64. Comparison of the sulfonamide inhibition profiles of the alpha-, beta- and gamma-carbonic anhydrases from the pathogenic bacterium Vibrio cholerae. Del Prete, S; Vullo, D; De Luca, V; Carginale, V; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry Letters* 26, 1941-1946 (2016).
65. Confined aqueous media for the cleaning of cultural heritage: innovative gels and amphiphile-based nanofluids. Bonelli, N; Chelazzi, D; Baglioni, M; Giorgi, R; Baglioni, P. *Nanoscience and Cultural Heritage, eds. Philippe Dillmann, Ludovic Bellot-Gurlet, Irène Nenner, Atlantis Press-Springer*, 283-311 (2016).
66. Controlled graphene oxide assembly on silver nanocubes monolayers for SERS detection: dependence on nanocubes packing procedure. Banchelli, M; Tiribilli, B ; Pini, R; Dei, L; Matteini P; Caminati G. *Beilstein J. Nanotechnol.* 7, 9-21 (2016).
67. Controlled Veiling of Silver Nanocubes with Graphene Oxide for Improved Surface-Enhanced Raman Scattering Detection. Banchelli, M; Tiribilli, B; de Angelis, M; Pini, R; Caminati G; Matteini, P. *ACS Appl. Mater. Interfaces* 8, 2628-2634 (2016).
68. Coral Carbonic Anhydrases: Regulation by Ocean Acidification. Zoccola, D; Innocenti, A; Bertucci, A; Tambutte, E; Supuran, CT; Tambutte, S. *Marine Drugs* 14 (2016).
69. Coupling non invasive and fast sampling of proteins from work of art surfaces to surface plasmon resonance biosensing: Differential and simultaneous detection of egg components for cultural heritage diagnosis and conservation. Scarano, S; Carretti, E; Dei, L; Baglioni, P; Minunni, M. *Biosensors & Bioelectronics* 85, 83-89 (2016).
70. Data in support of Gallium (Ga(3+)) antibacterial activities to counteract E. coli and S. epidermidis biofilm formation onto pro-osteointegrative titanium surfaces. Cochis, A; Azzimonti, B; Sorrentino, R; Della Valle, C; De Giglio, E; Bloise, N; Visai, L; Bruni, G; Cometa, S; Pezzoli, D; Candiani, G; Rimondini, L; Chiesa, R. *Data Brief* 6, 758-762 (2016).
71. Decoration of silicon nanowires with silver nanoparticles for ultrasensitive surface enhanced Raman scattering. D'Andrea, C; Lo Faro, MJ; Bertino, G; Ossi, PM; Neri, F; Trusso, S; Musumeci, P; Galli, M; Cioffi, N; Irrera, A; Priolo, F; Fazio, B. *Nanotechnology* 27 (2016).
72. Deposition of morphology-tailored PbS thin films by surfactant-enhanced aerosol assisted chemical vapor deposition. Khan, MD; Hameed, S; Haider, N; Afzal, A; Sportelli, MC; Cioffi, N; Malik, MA; Akhtar, J. *Materials Science In Semiconductor Processing* 46, 39-45 (2016).
73. Design of Decorated Self-Assembling Peptide Hydrogels as Architecture for Mesenchymal Stem Cells. Zamuner, A; Cavo, M; Scaglione, S; Messina, GML; Russo, T; Gloria, A; Marletta, G; Dettin, M. *Materials* 9, 727-745 (2016).
74. Design of lipidic platforms anchored within nanometric cavities by peptide hooks. Messina, GML; De Zotti, M; Lettieri, R; Gatto, E; Venanzi, M; Formaggio, F; Toniolo, C; Marletta, G. *RSC Adv.* 6, 46984-46993 (2016).
75. Design of smart GE11-PLGA/PEG-PLGA blend nanoparticulate platforms for parenteral administration of hydrophilic macromolecular drugs: synthesis, preparation and in vitro/ex vivo characterization. Colzani, B; Speranza G; Dorati, R; Conti, B; Modena T; Bruni, G; Zagato E; Vermeulen L; Dakwar Genta GR; Braeckmans K; Genta I. *International Journal of Pharmaceutics* 511, 1112-1123 (2016).
76. Development of 3-(4-aminosulphonyl)-phenyl-2-mercapto-3-H-quinazolin-4-ones as inhibitors of carbonic anhydrase isoforms involved in tumorigenesis and glaucoma. Alafeefy, AM; Carta, F;

Ceruso, M; Al-Tamimi, AMS; Al-Kahtani, AA; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 1402-1407 (2016).

77. Development of certain new 2-substituted-quinazolin-4-yl-aminobenzenesulfonamide as potential antitumor agents. Alafeefy, AM; Ahmad, R; Abdulla, M; Eldehna, WM; Al-Tamimi, AMS; Abdel-Aziz, HA; Al-Obaid, O; Carta, F; Al-Kahtani, AA; Supuran, CT. *European Journal Of Medicinal Chemistry* 109, 247-253 (2016).
78. Development of novel cyclic peptides as pro-apoptotic agents. Brindisi, M; Maramai, S; Brogi, S; Fanigliulo, E; Butini, S; Guarino, E; Casagni, A; Lamponi, S; Bonechi, C; Nathwani, SM; Finetti, F; Ragonese, F; Arcidiacono, P; Campiglia, P; Valenti, S; Novellino, E; Spaccapelo, R; Morbidelli, L; Zisterer, DM; Williams, CD; Donati, A; Baldari, C; Campiani, G; Ulivieri, C; Gemma, S. *European Journal Of Medicinal Chemistry* 117, 301-320 (2016).
79. Different duplex/quadruplex junctions determine the properties of anti-thrombin aptamers with mixed fold. Russo Krauss, I; Spiridonova, V; Pica, A; Napolitano, V; Sica, F. *Nucleic Acid Research* 44, 983-991 (2016).
80. Discovery and microassay of a nitrite-dependent carbonic anhydrase activity by stable-isotope dilution gas chromatography-mass spectrometry. Zinke, M; Hanff, E; Bohmer, A; Supuran, CT; Tsikas, D. *Amino Acids* 48, 245-255 (2016).
81. Discovery of HIV Type1 Aspartic Protease Hit Compounds through Combined Computational Approaches. Xanthopoulos, D; Kritsi, E; Supuran, CT; Papadopoulos, MG; Leonis, G; Zoumpoulakis, P. *Chemmedchem* 11, 1646-1652 (2016).
82. Discovery of New Potential Anti-Infective Compounds Based on Carbonic Anhydrase Inhibitors by Rational Target-Focused Repurposing Approaches. Annunziato, G; Angeli, A; D'Alba, F; Bruno, A; Pieroni, M; Vullo, D; De Luca, V; Capasso, C; Supuran, CT; Costantino, G. *Chemmedchem* 11, 1904-1914 (2016).
83. Discovery of Strecker-type alpha-aminonitriles as a new class of human carbonic anhydrase inhibitors using differential scanning fluorimetry. Krasavin, M; Stavniichuk, R; Zozulya, S; Borysko, P; Vullo, D; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1707-1711 (2016).
84. Dithiocarbamates with potent inhibitory activity against the Saccharomyces cerevisiae beta-carbonic anhydrase. Bozdag, M; Carta, F; Vullo, D; Isik, S; AlOthman, Z; Osman, SM; Scozzafava, A; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 132-136 (2016).
85. Drug interaction considerations in the therapeutic use of carbonic anhydrase inhibitors. Supuran, CT. *Expert Opinion On Drug Metabolism & Toxicology* 12, 423-431 (2016).
86. Dynamic encapsulation and activation of carbonic anhydrase in multivalent dynameric host matrices. Zhang, Y; Legrand, YM; Petit, E; Supuran, CT; Barboiu, M. *Chemical Communications* 52, 4053-4055 (2016).
87. Dynamical behaviors of structural, constrained and free water in calcium- and magnesium-silicate-hydrate gels. Le, PS; Fratini, E; Ito, K; Wang, Z; Mamontov, E; Baglioni, P; Chen, SH. *Journal Of Colloid And Interface Science* 469, 157-163 (2016).
88. Editorial: Electrolytes and specific ion effects. New and old horizons. Lo Nostro, P; Ninham, BW. *Current Opinion In Colloid & Interface Science* 23, A1-A5 (2016).
89. Effect of electrolytes on proteins physisorption on ordered mesoporous silica materials. Salis, A; Medda, L; Cugia, F; Monduzzi, M. *Colloids And Surfaces B-Biointerfaces* 137, 77-90 (2016).
90. Effect of ionic strength on intra-protein electron transfer reactions: The case study of charge recombination within the bacterial reaction center. Giustini, M; Parente, M; Mallardi, A; Palazzo, G. *Biochimica Et Biophysica Acta-Bioenergetics* 1857, 1541-1549 (2016).
91. Effect of Quercetin-loaded liposomes on induced oxidative stress in human spermatozoa. Moretti, E; Mazzi, L; Bonechi, C; Salvatici, MC; Iacoponi, F; Rossi, C; Collodel, G. *Reproductive Toxicology* 60, 140-147 (2016).
92. Effect of Resveratrol on Platelet Aggregation by Fibrinogen Protection. Bonechi, C; Lamponi, S; Donati, A; Tamasi, G; Consumi, M; Leone, G; Rossi, C; Magnani, A. *Biophysical Chemistry* submitted (2016).
93. Effect of temperature on the interaction of cisplatin with the model protein hen egg white lysozyme. Ferraro, G; Pica, A; Russo Krauss, I; Amoresano, A; Merlino, A. *Journal of Biological Inorganic Chemistry* 21, 433-442 (2016).
94. Effect of the gate metal work function on water-gated ZnO thin-film transistor performance. Singh, M; Mulla, MY; Santacroce, MV; Magliulo, M; Di Franco, C; Manoli, K; Altamura, D; Giannini, C; Cioffi, N; Palazzo, G; Scamarcio, G; Torsi, L. *Journal Of Physics D-Applied Physics* 49 (2016).
95. Effects of adhesion promoters on the contact angle of bitumen-aggregate interface. Rossi, CO; Caputo, P; Baldino, N; Lupi, FR; Miriello, D; Angelico, R. *International Journal Of Adhesion And Adhesives* 70, 297-303 (2016).
96. Effects of dipotassium-trioxohydroxytetrafluorotriborate, K-2[B3O3F4OH], on cell viability and gene expression of common human cancer drug targets in a melanoma cell line. Pojskic, L; Haveric,

S; Lojo-Kadric, N; Hadzic, M; Haveric, A; Galic, Z; Galic, B; Vullo, D; Supuran, CT; Milos, M. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 999-1004 (2016).

97. Electrochemical study of Na2Fe1-xMnxP2O7 (x= 0, 0.25, 0.5, 0.75, 1) as cathode material for rechargeable Na-ion batteries. Tealdi, C; Ricci, M; Ferrara C; Bruni, G; Quartarone E; Mustarelli, P. *Batteries, Special Issue: Rechargeable Battery Technologies-From Materials to Applications* 2, 1 (2016).
98. Electrodeposition and characterization of p and n sulphide semiconductors. Innocenti, M; Picca, RA; Vizza, F; Lavacchi, A; Montegrossi, G; Foresti, M; Di Benedetto, F; Giaccherini, A; Cioffi, N; Caporali, S; Cinotti, S; Berretti, E. *Journal of the Electrochemical Society* 163, D3034-D3039 (2016).
99. Electrophoretic deposition of Au NPs on MWCNT-based gas sensor for tailored gas detection with enhanced sensing properties. Dilonardo, E; Penza, M; Alvisi, M; Di Franco, C; Rossi, R; Palmisano, F; Torsia, L; Cioffi, N. *Sensors And Actuators B-Chemical* 223, 417-428 (2016).
100. Electrophysiological measurements on solid supported membranes. Tadini-Buoninsegni, F; Bartolommei, G. *Methods in Molecular Biology* 1377, 293-303 (2016).
101. Electrospun fibers as potential carrier systems for enhanced drug release of perphenazine. Bruni, G; Maggi, L; Tammaro, L; Di Lorenzo, R; Friuli, V; D'Aniello, S; Maietta, M; Berbenni, V; Milanese, C; Girella, A; Marini, A. *International Journal Of Pharmaceutics* 511, 190-197 (2016).
102. Energy landscape in protein folding and unfolding. Mallamace, F; Corsaro, C; Mallamace, D; Vasi, S; Vasi, C; Baglioni, P; Buldyrev, SV; Chen, SH; Stanley, HE. *Proceedings Of The National Academy Of Sciences Of The United States Of America* 113, 3159-3163 (2016).
103. Environmental sustainability evaluation of innovative self-cleaning textiles. Busi, E; Maranghi, S; Corsi, L; Basosi, R. *Journal Of Cleaner Production* 133, 439-450 (2016).
104. Enzymatic reactions in confined environments. Kuchler, A; Yoshimoto, M; Luginbuhl, S; Mavelli, F; Walde, P. *Nature Nanotechnology* 11, 409-420 (2016).
105. Escherichia coli DnaE Polymerase Couples Pyrophosphatase Activity to DNA Replication. Lapenta, F; Silva, AM; Brandimarti, R; Lanzi, M; Gratani, FL; Gonzalez, PV; Perticarari, S; Hochkoeppler, A. *Plos One* 11 (2016).
106. Etica delle Sperimentazioni Scientifiche, I risultati del Workshop Nazionale a Pisa. Domenici, V; Minunni, M; Tine, MR. *La Chimica e l'Industria, attualità* (2016).
107. Evaluation of gas-sensing properties of ZnO nanostructures electrochemically doped with Au nanophases. Dilonardo, E; Penza, M; Alvisi, M; Di Franco, C; Palmisano, F; Torsi, L; Cioffi, N. *Beilstein Journal Of Nanotechnology* 7, 22-31 (2016).
108. Evidence for a plasma-accessible carbonic anhydrase in the lumen of salmon heart that may enhance oxygen delivery to the myocardium. Alderman, SL; Harter, TS; Wilson, JM; Supuran, CT; Farrell, AP; Brauner, CJ. *Journal Of Experimental Biology* 219, 719-724 (2016).
109. Expression and characterization of a recombinant psychrophilic gamma-carbonic anhydrase (NcoCA) identified in the genome of the Antarctic cyanobacteria belonging to the genus Nostoc. De Luca, V; Del Prete, S; Vullo, D; Carginale, V; Di Fonzo, P; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 810-817 (2016).
110. Fabricating energy devices with low environmental impacts. Innocenti, M; Di Benedetto, F; Lavacchi, A; Cioffi, N; Felici, R; Pardi, LA. *SPIE Newsroom-Nanotechnology* (2016).
111. Fast analysis of nine PAHs in beer by ultrasound-vortex-assisted dispersive liquid-liquid micro-extraction coupled with gas chromatography-ion trap mass spectrometry. Russo, MV; Avino, P; Perugini, L; Notardonato, I. *RSC Advances* 6, 13920-13927 (2016).
112. Fe_3O_4@SiO_2 core-shell nanoparticles for biomedical purposes: adverse effects on blood cells. Grandi, S; Achilli, C; Guidetti, GF; Ciana, A; Tomasi, C; Capsoni, D; Minetti, G. *Biomaterials Science* 4, 1417-1421 (2016).
113. Filling nanoporous polymer thin films: an easy route toward the full control of the 3D nanostructure. Li-Destri, G; Tummino, A; Malfatti Gasperini, AA; Parellada Monreal, L; Messina, GML; Spampinato, V; Ceccone, G; Konovalov, O. *RSC Adv*. 6, 9175-9179 (2016).
114. Flow-induced structures observed in a viscoelastic reverse wormlike micellar system by magnetic resonance imaging and NMR velocimetry. Angelico, R; Gentile, L; Ranieri, GA; Rossi, CO. *Rsc Advances* 6, 33339-33347 (2016).
115. Fluorescent lactose-derived catanionic aggregates: synthesis, characterisation and potential use as antibacterial agents. Bettoschi, A; Brisson, A; Caltagirone, C; Falchi, AM; Isaia, F; Lippolis, V; Loi, G; Loi, M; Murgia, S; Pilia, R; Serra, C; Tan, S. *Rsc Advances* 6, 23340-23344 (2016).
116. Fluorescent sulfonamide carbonic anhydrase inhibitors incorporating 1,2,3-triazole moieties: Kinetic and X-ray crystallographic studies. Carta, F; Ferraroni, M; Scozzafava, A; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 104-112 (2016).
117. Formulation of liposomes functionalized with the Lotus lectin and effective in targeting highly proliferative cells. Della Giovampaola, C; Capone, A; Ermini, L; Lupetti, P; Vannuccini, E; Finetti,

F; Donnini, S; Ziche, M; Magnani, A; Leone, G; Rossi, C; Rosati F; Bonechi, C. *BBA General Subjects* submitted (2016).

118. From the analysis of pharmacologic vitreolysis to the comprehension of ocriplasmin safety. Morescalchi, F; Gambicorti, E; Duse, S; Costagliola, C; Semeraro, F. *Expert Opinion On Drug Safety* 15, 1267-1278 (2016).
119. Functional calcium phosphate composites in nanomedicine. Ridi, F; Meazzini, I; Castroflorio, B; Bonini, M; Berti, D; Baglioni, P. *Advances in Colloid and Interface Science* submitted (2016).
120. Functionalization of silicon nanowire arrays by silver nanoparticles for the laser desorption ionization mass spectrometry analysis of vegetable oils. Picca, RA; Calvano, CD; Lo Faro, MJ; Fazio, B; Trusso, S; Ossi, PM; Neri, F; D'Andrea, C; Irrera, A; Cioffi, N. *Journal Of Mass Spectrometry* 51, 849-856 (2016).
121. Functionalized SPIONs: the surfactant nature modulates the self-assembly and cluster formation. Luchini, A; Heenan, RK; Paduano, L; Vitiello, G. *Physical Chemistry Chemical Physics* 18, 18441-18449 (2016).
122. Geometric structures, fractal self-similarity, squeezed coherent states and electrodynamics. Vitiello, G. *Xxiii International Conference On Integrable Systems And Quantum Symmetries (Isqs-23)* 670 (2016).
123. Giant Vesicles as Compartmentalized Bio-reactors: A 3D Modelling Approach. Mavelli, F; Altamura, E; Stano, P. *Advances In Artificial Life, Evolutionary Computation And Systems Chemistry* 587, 184-196 (2016).
124. Global Analysis of Type Three Secretion System and Quorum Sensing Inhibition of Pseudomonas savastanoi by Polyphenols Extracts from Vegetable Residues. Biancalani, C; Cerboneschi, M; Tadini-Buoninsegni, F; Campo, M; Scardigli, A; Romani, A; Tegli, S. *Plos One* 11 (2016).
125. Glucose-assisted synthesis and wet-chemistry preparation of pyrophosphate cathodes for rechargeable Na-ion batteries. Tealdi, C; Ricci, M; Ferrara C; Bruni, G; Berbenni V; Quartarone E; Mustarelli, P. *RSC Advances* 6, 99735-99742 (2016).
126. Glutathione loaded solid lipid nanoparticles: preparation and in vitro evaluation as delivery systems of the antioxidant peptide to immunocompetent fish cells. Trapani, A; Tripodo, G; Mandracchia, D; Cioffi, N; Ditaranto, N; Cerezuela, R; Esteban, MA. *Journal of Cellular Biotechnology* 2, 1-14 (2016).
127. Health-related quality of life in patients with primary open-angle glaucoma. An Italian multicentre observational study. Floriani, I; Quaranta, L; Rulli, E; Katsanos, A; Varano, L; Frezzotti, P; Rossi, GCM; Carmassi, L; Rolle, T; Ratiglia, R; Gandolfi, S; Fossarello, M; Uva, M; Hollander, L; Poli, D; Grignolo, F; Roberto, A; Clivio, L; Galli, F; Carlucci, L; Riva, I; Delcassi, L; Carchedi, T; Talarico, S; Motolese, I; Bagaglia, SA; Lanteri, S; Bossolesi, L; Piccini, R; Rossi, A; Tagliavini, V; Ungaro, N; Cuccu, A; Zucca, I; Bonacci, E; Cardarella, G; Tognetto, D; Vattovani, O; Vallon, P; Iannacone, F; Fontana, L; Marchi, S; Manni, GL; Jannetta, D; Roberti, G; Rossetti, L; Maggiolo, E; Oneta, O; Sborgia, C; Cantatore, F; Mastropasqua, L; Agnifili, L; Campos, E; Gizzi, C; Giannaccare, G; Pucci, V; Cassamali, M; Costagliola, C; Traverso, C; Scotto, R; Musolino, M; Landi, L; Bagnis, A. *Acta Ophthalmologica* 94, e278-e286 (2016).
128. High Quality Grappa from Chianti and Montepulciano Areas (Tuscany, Italy). Monitoring the Leaching of Copper from Distillation Columns. Tamasi, G; Bonechi, C; Donati, A; Magnani, A; Cini, R; Rossi, C. *Food Chemistry* in press (2016).
129. High-resolution high-speed nanoindentation mapping of cement pastes: Unravelling the effect of microstructure on the mechanical properties of hydrated phases. Sebastiani, M; Moscatelli, R; Ridi, F; Baglioni, P; Carassiti, F. *Materials & Design* 97, 372-380 (2016).
130. Hofmeister effects at low salt concentration due to surface charge transfer. Parsons, DF; Salis, A. *Current Opinion In Colloid & Interface Science* 23, 41-49 (2016).
131. How many carbonic anhydrase inhibition mechanisms exist?. Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 345-360 (2016).
132. Hyaluronan-coated polybenzofulvene brushes as biomimetic materials. Cappelli, A; Paolino, M; Grisci, G; Razzano, V; Giuliani, G; Donati, A; Bonechi, C; Mendichi, R; Battiato, S; Samperi, F; Scialabba, C; Giammona, G; Makovec, F; Licciardi, M. *Polymer Chemistry* 7, 6529-6544 (2016).
133. Hyaluronan-Coated Polymer Brushes as Biomimetic Drug Delivery Systems. Cappelli, A; Paolino, M; Grisci, G; Razzano, V; Giuliani, G; Donati, A; Bonechi, C; Mendichi, R; Battiato, S; Samperi, F; Scialabba, C; Giammona, G; Makovec, F; Licciardi, M. *Polymer Chemistry* in press (2016).
134. Hydroxamic acid derivatives: a promising scaffold for rational compound optimization in Chagas disease. de Menezes, DD; Calvet, CM; Rodrigues, GC; Pereira, MCD; Almeida, IR; de Aguiar, AP; Supuran, CT; Vermelho, AB. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 964-973 (2016).
135. Immediate stabilization of human blood for delayed quantification of endogenous thiols and disulfides. Giustarini, D; Galvagni, F; Orlandini, M; Fanti, P; Rossi, R. *Journal Of Chromatography B-Analytical Technologies In The Biomedical And Life Sciences* 1019, 51-58 (2016).

136. Improving impedimetric nucleic acid detection by using enzyme-decorated liposomes and nanostructured screen-printed electrodes. Voccia, D; Bettazzi, F; Fratini, E; Berti, D; Palchetti, I. *Analytical And Bioanalytical Chemistry* 408, 7271-7281 (2016).
137. Improving the performances of NafionTM-based membranes for microbial fuel cells with silica-based, organically-functionalized mesostructured fillers. Angioni, S; Millia, L; Bruni, G; Tealdi, C; Mustarelli, P; Quartarone E. *Journal of Power Sources* 334, 120-127 (2016).
138. In silico modeling of beta-carbonic anhydrase inhibitors from the fungus Malassezia globosa as antidandruff agents. Singh, S; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 417-424 (2016).
139. In situ photodeposited nanoCu on TiO2 as a catalyst for hydrogen production under UV/visible radiation. Clarizia, L; Vitiello, G; Luciani, G; Di Somma, I; Andreozzi, R; Marotta, R. *Applied Catalysis A-General* 518, 142-149 (2016).
140. In vitro imaging of beta-cells using fluorescent cubic bicontinuous liquid crystalline nanoparticles. Miceli, V; Meli, V; Blanchard-Desce, M; Bsaibess, T; Pampalone, M; Conaldi, PG; Caltagirone, C; Obiols-Rabasa, M; Schmidt, J; Talmon, Y; Casu, A; Murgia, S. *Rsc Advances* 6, 62119-62127 (2016).
141. In Vivo Near-Infrared Fluorescence Imaging of Aqueous Humor Outflow Structures. Zeppa, L; Ambrosone, L; Guerra, G; Fortunato, M; Costagliola, C. *Journal Of Ophthalmology* (2016).
142. Indazole, Pyrazole, and Oxazole Derivatives Targeting Nitric Oxide Synthases and Carbonic Anhydrases. Maccallini, C; Di Matteo, M; Vullo, D; Ammazzalorso, A; Carradori, S; De Filippis, B; Fantacuzzi, M; Giampietro, L; Pandolfi, A; Supuran, CT; Amoroso, R. *Chemmedchem* 11, 1695-1699 (2016).
143. Influence of free fatty acid content on the oxidative stability of red palm oil. De Leonardis, A; Cuomo, F; Macciola, V; Lopez, F. *Rsc Advances* 6, 101098-101104 (2016).
144. Influence of hypoxia-dependent factors on the progression of neuroblastoma. Ameis, HM; Drenckhan, A; Freytag, M; Izbicki, JR; Supuran, CT; Reinshagen, K; Holland-Cunz, S; Gros, SJ. *Pediatric Surgery International* 32, 187-192 (2016).
145. Inhibition of carbonic anhydrase from Trypanosoma cruzi for the management of Chagas disease: an underexplored therapeutic opportunity. Supuran, CT. *Future Medicinal Chemistry* 8, 311-324 (2016).
146. Inhibition of carbonic anhydrase isoforms I, II, IV, VII and XII with carboxylates and sulfonamides incorporating phthalimide/phthalic anhydride scaffolds. El-Azab, AS; Abdel-Aziz, AAM; Ayyad, RR; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 20-25 (2016).
147. Inhibition of carbonic anhydrase isoforms I, II, IX and XII with secondary sulfonamides incorporating benzothiazole scaffolds. Petrou, A; Geronikaki, A; Terzi, E; Guler, OO; Tuccinardi, T; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1306-1311 (2016).
148. Inhibitory effects of benzimidazole containing new phenolic Mannich bases on human carbonic anhydrase isoforms hCA I and II. Gul, HI; Yazici, Z; Tanc, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1540-1544 (2016).
149. Inhibitory effects of isatin Mannich bases on carbonic anhydrases, acetylcholinesterase, and butyrylcholinesterase. Ozgun, DO; Yamali, C; Gul, HI; Taslimi, P; Gulcin, I; Yanik, T; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1498-1501 (2016).
150. Injectable composites via functionalization of 1D nanoclays and biodegradable coupling with a polysaccharide hydrogel. Del Buffa, S; Rinaldi, E; Carretti, E; Ridi, F; Bonini, M; Baglioni, P. *Colloids And Surfaces B-Biointerfaces* 145, 562-566 (2016).
151. Interaction between a cationic bolaamphiphile and DNA: The route towards nanovectors for oligonucleotide antimicrobials. Mamusa, M; Resta, C; Barbero, F; Carta, D; Codoni, D; Hatzixanthis, K; McArthur, M; Berti, D. *Colloids And Surfaces B-Biointerfaces* 143, 139-147 (2016).
152. Interaction of anions with a newly characterized alpha carbonic anhydrase from Halomonas sp. Orhan, F; Senturk, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1119-1123 (2016).
153. Investigation of Industrial Polyurethane Foams Modified with Antimicrobial Copper Nanoparticles. Sportelli, MC; Picca, RA; Ronco, R; Bonerba, E; Tantillo, G; Pollini, M; Sannino, A; Valentini, A; Cataldi, TRI; Cioffi, N. *Materials* 9 (2016).
154. Investigation of Li and H dynamics in Li_6C_{60} and $Li_6C_{60}Hy$. Maidich, L; Pontiroli, D; Gaboardi, M; Lenti, S; Magnani, G; Riva, G; Carretta, P; Milanese, C; Marini, A; Ricco, M; Sanna, S. *Carbon* 96, 276-284 (2016).
155. InVivo Evaluation of Selective Carbonic Anhydrase Inhibitors as Potential Anticonvulsant Agents. Bruno, E; Buemi, MR; De Luca, L; Ferro, S; Monforte, AM; Supuran, CT; Vullo, D; De Sarro, G; Russo, E; Gitto, R. *Chemmedchem* 11, 1812-1818 (2016).
156. Isatin analogs as novel inhibitors of Candida spp. beta-carbonic anhydrase enzymes. Akdemir, A; Guzel-Akdemir, O; Karali, N; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 1648-1652 (2016).

157. Kinetic and docking studies of cytosolic/tumor-associated carbonic anhydrase isozymes I, II and IX with some hydroxylic compounds. Durdagi, S; Korkmaz, N; Isik, S; Vullo, D; Astley, D; Ekinci, D; Salmas, RE; Senturk, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1214-1220 (2016).
158. Kinetic and X-ray crystallographic investigations of substituted 2-thio-6-oxo-1,6-dihydropyrimidine-benzenesulfonamides acting as carbonic anhydrase inhibitors. Vullo, D; Supuran, CT; Scozzafava, A; De Simone, G; Monti, SM; Alterio, V; Carta, F. *Bioorganic & Medicinal Chemistry* 24, 3643-3648 (2016).
159. Kinetic and X-ray crystallographic investigations on carbonic anhydrase isoforms I, II, IX and XII of a thioureido analog of SLC-0111. Lomelino, CL; Mahon, BP; McKenna, R; Carta, F; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 976-981 (2016).
160. Label free Affinity sensing: application to food analysis. Scarano, S; Mariani, S; Minunni, M. *special issue of ACTA IMEKO on International Conference 1st IMEKOFOODS Metrology Promoting Objective and Measurable Food Quality and Safety in Rome ACTA IMEKO* 5, 36-44 (2016).
161. Label-free C-reactive protein electronic detection with an electrolyte-gated organic field-effect transistor-based immunosensor. Magliulo, M; De Tullio, D; Vikholm-Lundin, I; Albers, WM; Munter, T; Manoli, K; Palazzo, G; Torsi, L. *Analytical And Bioanalytical Chemistry* 408, 3943-3952 (2016).
162. Laser Ablation Synthesis of Hybrid Cu/Ag Nanoparticles for prospective application as nanoantimicrobial agents for food packaging. Picca, RA; Di Maria, A; Riháková, L; Volpe, A; Sportelli, MC; Lugarà, PM; Ancona, A; Cioffi, N. *MRS Advances* (2016).
163. LCA di sistemi solari innovativi: DSSC. Basosi, R; Maranghi, S; Parisi, ML. *Life Cycle Assessment applicata al sistema edificio-impianto, AICARR* in press (2016).
164. LCA of 1,4-Butanediol Produced via Direct Fermentation of Sugars from Wheat Straw Feedstock within a Territorial Biorefinery. Forte, A; Zucaro, A; Basosi, R; Fierro, A. *Materials* 9 (2016).
165. Legionella pneumophila Carbonic Anhydrases: Underexplored Antibacterial Drug Targets. Supuran, CT. *Pathogens* 5 (2016).
166. Life Cycle Assessment of second generation bioethanol produced from low-input dedicated crops of Arundo donax L. Zucaro, A; Forte, A; Basosi, R; Fagnano, M; Fierro, A. *Bioresource Technology* 219, 589-599 (2016).
167. Lipoplexes from Non-Viral Cationic Vectors: DOTAP-DOPE Liposomes and Gemini Micelles in Non-Viral Gene Delivery Vectors: Methods and Protocols. Falsini, S; Ristori, S; ("Methods in Molecular Biology" Series), G. Candiani Ed., ISSN: 1064-3745, Springer NY, 1445, 33-43 (2016).
168. Magnetic field responsive drug release from magnetoliposomes in biological fluids. Nappini, S; Fogli, S; Castroflorio, B; Bonini, M; Bombelli, FB; Baglioni, P. *Journal Of Materials Chemistry B* 4, 716-725 (2016).
169. MALDI-TOF mass spectrometry analysis of proteins and lipids in Escherichia coli exposed to copper ions and nanoparticles. Calvano, CD; Picca, RA; Bonerba, E; Tantillo, G; Cioffi, N; Palmisano, F. *Journal Of Mass Spectrometry* 51, 828-840 (2016).
170. Mesoporous Silica Nanoparticles Functionalized with Hyaluronic Acid and Chitosan Biopolymers. Effect of Functionalization on Cell Internalization. Salis, A; Fanti, M; Medda, L; Nairi, V; Cugia, F; Piludu, M; Sogos, V; Monduzzi, M. *Acs Biomaterials Science & Engineering* 2, 741-751 (2016).
171. Metabolism and microenvironment in cancer plasticity. Baldini, N; Sonveaux, P; De Milito, A; Supuran, CT; Otto, AM; Stock, CM; Pedersen, SF; Favicchio, R; Avnet, S. *Cancer & Metabolism* 4 (2016).
172. Metal-decorated silicon nanowires as novel platform for laser-desorption-ionization mass spectrometry. Picca, RA; Lo Faro, MJ; Calvano, CD; Fazio, B; Sportelli, MC; Trusso, S; Ossi, PM; Neri, F; D'Andrea, C; Irrera, A; Cioffi, N. *SPIE Newsroom-Nanotechnology* (2016).
173. Methane Adsorption in Model Mesoporous Material, SBA-15, Studied by Small-Angle Neutron Scattering. Chiang, WS; Fratini, E; Baglioni, P; Georgi, D; Chen, JH; Liu, Y. *Journal Of Physical Chemistry C* 120, 4354-4363 (2016).
174. Method for Determining the Activation Energy Distribution Function of Complex Reactions by Sieving and Thermogravimetric Measurements. Bufalo, G; Ambrosone, L. *Journal Of Physical Chemistry B* 120, 244-249 (2016).
175. MgO/SiO2 and Portland cement formulations: mutual effects on hydration processes and products. Martini, F; Tonelli, M; Calucci, L; Geppi, M; Ridi, F; Borsacchi, M. *Cement & Concrete Composites* submitted (2016).
176. Microcapsules for Confining Fluids: Prediction of Shell Stability from Advanced SAXS Investigations. Ambrosi, M; Fratini, E; Baglioni, P; Vannucci, C; Bartolini, A; Pintens, A; Smets, J. *Journal Of Physical Chemistry C* 120, 13514-13522 (2016).
177. Microwave assisted synthesis of novel acridine-acetazolamide conjugates and investigation of their inhibition effects on human carbonic anhydrase isoforms hCA I, II, IV and VII. Ulus, R; Aday, B; Tanc, M; Supuran, CT; Kaya, M. *Bioorganic & Medicinal Chemistry* 24, 3548-3555 (2016).

178. Molecular Surface Analysis and Depth-Profiling of Polyethylene Modified by an Atmospheric Ar-D2O Post-Discharge. Cristaudo, V; Collette, S; Tuccitto, N; Poleunis, C; Melchiorre, LC; Licciardello, A; Reniers, F; Delcorte, A. *Plasma Processes and Polymers* 13, 1104-1117 (2016).
179. Monothiocarbamates Strongly Inhibit Carbonic Anhydrases in Vitro and Possess Intraocular Pressure Lowering Activity in an Animal Model of Glaucoma. Vullo, D; Durante, M; Di Leva, FS; Cosconati, S; Masini, E; Scozzafava, A; Novellino, E; Supuran, CT; Carta, F. *Journal Of Medicinal Chemistry* 59, 5857-5867 (2016).
180. Morpho-Chemical Characterization and Surface Properties of Carcinogenic Zeolite Fibers. Mattioli,M; Giordani, M; Dogan, M; Cangiotti, M; Avella, G; Giorgi, R; Umran Dogan, A; Ottaviani, MF. *Journal of Hazardous Materials* 306, 140-148 (2016).
181. Multifunctional Magnetoliposomes for Sequential Controlled Release. Salvatore, A; Montis, C; Berti, D; Baglioni, P. *Acs Nano* 10, 7749-7760 (2016).
182. Multimeric xanthates as carbonic anhydrase inhibitors. Abellan-Flos, M; Tanc, M; Supuran, CT; Vincent, SP. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 946-952 (2016).
183. Multiscale Characterization of Some Commercial Carbon Blacks and Diesel Engine Soot. Ferraro, G; Fratini, E; Rausa, R; Fiaschi, P; Baglioni, P. *Energy & Fuels* 30, 9859-9866 (2016).
184. Mycobacterial carbonic anhydrase inhibition with phenolic acids and esters: kinetic and computational investigations. Cau, Y; Mori, M; Supuran, CT; Botta, M. *Organic & Biomolecular Chemistry* 14, 8322-8330 (2016).
185. N-Nitrosulfonamides: A new chemotype for carbonic anhydrase inhibition. Nocentini, A; Vullo, D; Bartolucci, G; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 3612-3617 (2016).
186. Nanomaterials for the cleaning and pH adjustment of vegetable-tanned leather. Baglioni, M; Bartoletti, A; Bozec, L; Chelazzi, D; Giorgi, R; Odlyha, M; Pianorsi, D; Poggi, G; Baglioni, P. *Applied Physics A-Materials Science & Processing* 122 (2016).
187. Nanostructured TiO2 surfaces promote human bone marrow mesenchymal stem cells differentiation to osteoblasts. Vercellino, M; Ceccarelli, G; Cristofaro, F; Balli, M; Bertoglio, F; Bruni, G; Benedetti, L; Avanzini, MA; Imbriani, M; Visai L. *Nanomaterials* 6, 124 (2016).
188. Nanotechnologies for the restoration of alum-treated archaeological wood. Andriulo, F; Braovac, S; Kutzke, H; Giorgi, R; Baglioni, P. *Applied Physics A-Materials Science & Processing* 122 (2016).
189. Needle-free jet injection of intact phospholipid vesicles across the skin: a feasibility study. Schlich, M; Lai, F; Murgia, S; Valenti, D; Fadda, AM; Sinico, C. *Biomedical Microdevices* 18 (2016).
190. New formulations to enhance lovastatin release from Red Yeast Rice (RYR). Leone, G; Bonechi, C; Consumi, M; Lamponi, S; Pepi, S; Rossi, C; Magnani, A; Tamasi, G; Donati, A. *Journal of Drug Delivery Science and Technology* in press (2016).
191. New light on bacterial carbonic anhydrases phylogeny based on the analysis of signal peptide sequences. Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1254-1260 (2016).
192. New materials for Li-ion batteries: synthesis and spectroscopic characterization of $Li_2(FeMnCo)SiO_4$ cathode materials. Ferrari, S; Mozzati, MC; Lantieri, M; Spina, G; Capsoni, D; Bini, M. *Scientific Reports* 6, 1-12 (2016).
193. Non-Classical Inhibition of Carbonic Anhydrase. Lomelino, CL; Supuran, CT; McKenna, R. *International Journal Of Molecular Sciences* 17 (2016).
194. Not only pH. Specific buffer effects in biological systems. Salis, A; Monduzzi, M. *Current Opinion In Colloid & Interface Science* 23, 1-9 (2016).
195. Novel sulfonamide bearing coumarin scaffolds as selective inhibitors of tumor associated carbonic anhydrase isoforms IX and XII. Chandak, N; Ceruso, M; Supuran, CT; Sharma, PK. *Bioorganic & Medicinal Chemistry* 24, 2882-2886 (2016).
196. Nucleolipid bilayers: A quartz crystal microbalance and neutron reflectometry study. Montis, C; Gerelli, Y; Fragneto, G; Nylander, T; Baglioni, P; Berti, D. *Colloids And Surfaces B-Biointerfaces* 137, 203-213 (2016).
197. Olive Mill Wastewater (OMW) Phenol Compounds Degradation by Means of a Visible Light Activated Titanium Dioxide-Based Photocatalyst. Cuomo, F; Venditti, F; Cinelli, G; Ceglie, A; Lopez, F. *Zeitschrift Fur Physikalische Chemie-International Journal Of Research In Physical Chemistry & Chemical Physics* 230, 1269-1280 (2016).
198. On the microscopic and mesoscopic perturbations of lipid bilayers upon interaction with the MPER domain of the HIV glycoprotein gp41. Oliva, R; Emendato, A; Vitiello, G; De Santis, A; Grimaldi, M; D'Ursi, AM; Busi, E; Del Vecchio, P; Petraccone, L; D'Errico, G. *Biochimica Et Biophysica Acta-Biomembranes* 1858, 1904-1913 (2016).
199. On the role of a coumarin derivative for sensing applications: Nucleotide identification using a micellar system. Bettoschi, A; Ceglie, A; Lopez, F; Meli, V; Murgia, S; Tamburro, M; Caltagirone, C; Cuomo, F. *Journal Of Colloid And Interface Science* 477, 8-15 (2016).

200. On the use of uniaxial tests on the sclera to understand the difference between emmetropic and highly myopic eyes. Romano, MR; Romano, V; Pandolfi, A; Costagliola, C; Angelillo, M. *Meccanica*, 1-10 (2016).
201. Organic bioelectronics probing conformational changes in surface confined proteins. Macchia, E; Alberga, D; Manoli, K; Mangiatordi, GF; Magliulo, M; Palazzo, G; Giordano, F; Lattanzi, G; Torsi, L. *Scientific Reports* 6 (2016).
202. PEGylated Bis-Sulfonamide Carbonic Anhydrase Inhibitors Can Efficiently Control the Growth of Several Carbonic Anhydrase IX-Expressing Carcinomas. Akocak, S; Alam, MR; Shabana, AM; Sanku, RKK; Vullo, D; Thompson, H; Swenson, ER; Supuran, CT; Hies, MA. *Journal Of Medicinal Chemistry* 59, 5077-5088 (2016).
203. PET Imaging of Carbonic Anhydrase IX Expression of HT-29 Tumor Xenograft Mice with Ga-68-Labeled Benzenesulfonamides. Lau, J; Zhang, ZX; Jenni, S; Kuo, HT; Liu, ZB; Vullo, D; Supuran, CT; Lin, KS; Benard, F. *Molecular Pharmaceutics* 13, 1137-1146 (2016).
204. Pharmacological targeting of glucose-6-phosphate dehydrogenase in human erythrocytes by Bay 11-7082, parthenolide and dimethyl fumarate. Ghashghaeinia, M; Giustarini, D; Koralkova, P; Koberle, M; Alzoubi, K; Bissinger, R; Hosseinzadeh, Z; Dreischer, P; Bernhardt, I; Lang, F; Toulany, M; Wieder, T; Mojzikova, R; Rossi, R; Mrowietz, U. *Scientific Reports* 6 (2016).
205. Phase transitions in hydrophobe/phospholipid mixtures: hints at connections between pheromones and anaesthetic activity. Borsacchi, S; Geppi, M; Macchi, S; Ninham, BW; Fratini, E; Ambrosi, M; Baglioni, P; Lo Nostro, P. *Physical Chemistry Chemical Physics* 18, 15375-15383 (2016).
206. Phosphocholine-decorated superparamagnetic iron oxide nanoparticles: defining the structure and probing in vivo applications. Luchini, A; Irace, C; Santamaria, R; Montesarchio, D; Heenan, RK; Szekely, N; Flori, A; Menichetti, L; Paduano, L. *Nanoscale* 8, 10078-10086 (2016).
207. Phospholamban Interaction with SR Ca-ATPase Investigated by Pre-Steady State Charge Measurements. Smeazzetto, S; Young, HS; Trieber, CA; Moncelli, MR; Tadini-Buoninsegni, F. *Biophysical Journal* 110, 541A-541A (2016).
208. Phospholamban spontaneously reconstitutes into giant unilamellar vesicles where it generates a cation selective channel. Smeazzetto, S; Tadini-Buoninsegni, F; Thiel, G; Berti, D; Montis, C. *Physical Chemistry Chemical Physics* 18, 1629-1636 (2016).
209. Phytoliposome-Based Silibinin Delivery System as a Promising Strategy to Prevent Hepatitis C Virus Infection. Ripoli, M; Angelico, R; Sacco, P; Ceglie, A; Mangia, A. *Journal Of Biomedical Nanotechnology* 12, 770-780 (2016).
210. Pitfalls in the analysis of the physiological antioxidant glutathione (GSH) and its disulfide (GSSG) in biological samples: An elephant in the room. Giustarini, D; Tsikas, D; Colombo, G; Milzani, A; Dalle-Donne, I; Fanti, P; Rossi, R. *Journal Of Chromatography B-Analytical Technologies In The Biomedical And Life Sciences* 1019, 21-28 (2016).
211. Plait point in ternary system with a miscibility gap: Analysis of the procedures involved in its determination and development of novel procedures. Mangiapia, G; Sartorio, R; Lungu, RP. *Fluid Phase Equilibria* 409, 49-58 (2016).
212. Potentialities of LCA for urban systems sustainability assessment. Maranghi, S; Parisi, ML; Basosi, R . *In Atti del X Convegno della Rete Italiana LCA - Life Cycle Thinking, sostenibilità ed economia circolare*, 54-62 (2016).
213. Prediction of mutual diffusion coefficients in binary liquid systems with one self-associating component from viscosity data and intra-diffusion coefficients at infinite dilution. Zhu, Q; D'Agostino, C; Ainte, M; Mantle, MD; Gladden, LF; Ortona, O; Paduano, L; Ciccarelli, D; Moggridge, GD. *Chemical Engineering Science* 147, 118-127 (2016).
214. Preferential interaction of the Alzheimer peptide A beta-(1-42) with Omega-3-containing lipid bilayers: structure and interaction studies. Emendato, A; Spadaccini, R; De Santis, A; Guerrini, R; D'Errico, G; Picone, D. *Febs Letters* 590, 582-591 (2016).
215. Preparation and enhanced conducting properties of open networks of poly(3-hexylthiophene)/carbon nanotube hybrids. Sfuncia, G; Tuccitto, N; Marletta, G. *RSC Advances* 6, 51485-51492 (2016).
216. Properties of Glauconite/Polyaniline Composite Prepared in Aqueous Solution of Citric Acid. Yatsyshyn, M; Saldan, I; Milanese, C; Makogon, V; Zeffiro, A; Bellani, V; Di Lorenzo, R; Cofrancesco, P; Girella, A; Dondi, D; Reshetnyak, O; Korniy, S. *Journal Of Polymers And The Environment* 24, 196-205 (2016).
217. Purification, Conformational Analysis, and Properties of a Family of Tigerinin Peptides from Skin Secretions of the Crowned Bullfrog Hoplobatrachus occipitalis. McLaughlin, CM; Lampis, S; Mechkarska, M; Coquet, L; Jouenne, T; King, JD; Mangoni, ML; Lukic, ML; Scorciapino, MA; Conlon, JM. *Journal Of Natural Products* 79, 2350-2356 (2016).
218. Pyrazolylbenzo[d]imidazoles as new potent and selective inhibitors of carbonic anhydrase isoforms hCA IX and XII. Kumar, S; Ceruso, M; Tuccinardi, T; Supuran, CT; Sharma, PK. *Bioorganic & Medicinal Chemistry* 24, 2907-2913 (2016).

219. Pyridazinone substituted benzenesulfonamides as potent carbonic anhydrase inhibitors. Yaseen, R; Ekinci, D; Senturk, M; Hameed, AD; Ovais, S; Rathore, P; Samim, M; Javed, K; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 26, 1337-1341 (2016).
220. Rapid and Reliable Method for Analyzing Acaricides in Honey-Based Products. Notardonato, I; Avino, P; Cinelli, G; Russo, MV. *Food Analytical Methods* 9, 1675-1685 (2016).
221. Rational design of functionalized polyacrylate-based high internal phase emulsions for analytical and biomedical uses. Brusotti, G; Calleri, E; Milanese, C; Catenacci, L; Marrubini, G; Sorrenti, M; Girella, A; Massolini, G; Tripodo, G. *Polymer Chemistry* 7, 7436-7445 (2016).
222. Recent advances in the synthesis and characterization of nano-antimicrobials. Sportelli MC; Picca RA; Cioffi N. *Trends in Analytical Chemistry* 84, 131-138 (2016).
223. Recombinant thermoactive phosphoenolpyruvate carboxylase (PEPC) from Thermosynechococcus elongatus and its coupling with mesophilic/thermophilic bacterial carbonic anhydrases (CAs) for the conversion of CO2 to oxaloacetate. Del Prete, S; De Luca, V; Capasso, C; Supuran, CT; Carginale, V. *Bioorganic & Medicinal Chemistry* 24, 220-225 (2016).
224. Reduction of vitreous prostaglandin e-2 levels after topical administration of indomethacin 0.5%, bromfenac 0.09%, and nepafenac 0.1%. Russo, A; Morescalchi, F; Vezzoli, S; Bernini, M; Turano, R; Costagliola, C; De Ferrari, F; Semeraro, F. *Retina-The Journal Of Retinal And Vitreous Diseases* 36, 1227-1231 (2016).
225. Regulation of HIF1 alpha under Hypoxia by APE1/Ref-1 Impacts CA9 Expression: Dual Targeting in Patient-Derived 3D Pancreatic Cancer Models. Logsdon, DP; Grimard, M; Luo, MH; Shahda, S; Jiang, YL; Tong, Y; Yu, ZS; Zyromski, N; Schipani, E; Carta, F; Supuran, CT; Korc, M; Ivan, M; Kelley, MR; Fishel, ML. *Molecular Cancer Therapeutics* 15, 2722-2732 (2016).
226. Resolvins and aliamides: lipid autacoids in ophthalmology - what promise do they hold?. Hesselink, JMKl; Chiosi, F; Costagliola, C. *Drug Design Development And Therapy* 10, 3133-3141 (2016).
227. Reverse Wormlike Micelles. In Wormlike Micelles: New Systems, Advances in Characterisation and Applications, (Royal Society of Chemistry. Angelico, R; Murgia, S; Palazzo, G. *RSC Soft Matter Series, Ed. C. A. Dreiss, Y. Feng* ISSN: 2048-7681, ISBN: 9781782625162 (2016).
228. Reversible hydrogen sorption in the composite made of magnesium borohydride and silica aerogel. Rueda, M; Sanz-Moral, LM; Girella, A; Cofrancesco, P; Milanese, C; Martin, A. *International Journal Of Hydrogen Energy* 41, 15245-15253 (2016).
229. Review of magnesium hydride-based materials: development and optimisation. Crivello, JC; Dam, B; Denys, RV; Dornheim, M; Grant, DM; Huot, J; Jensen, TR; de Jongh, P; Latroche, M; Milanese, C; Milcius, D; Walker, GS; Webb, CJ; Zlotea, C; Yartys, VA. *Applied Physics A-Materials Science & Processing* 122, (2016).
230. Rosmarinic acid inhibits some metabolic enzymes including glutathione S-transferase, lactoperoxidase, acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase isoenzymes. Gulcin, I; Scozzafava, A; Supuran, CT; Koksal, Z; Turkan, F; Cetinkaya, S; Bingol, Z; Huyut, Z; Alwasel, SH. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1698-1702 (2016).
231. Salts of 5-amino-2-sulfonamide-1,3,4-thiadiazole, a structural and analog of acetazolamide, show interesting carbonic anhydrase inhibitory properties, diuretic, and anticonvulsant action. Diaz, JRA; Cami, GE; Liu-Gonzalez, M; Vega, DR; Vullo, D; Juarez, A; Pedregosa, JC; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1102-1110 (2016).
232. Satellite analysis to identify changes and drivers of CyanoHABs dynamics in Lake Taihu. Zhang, YC; Ma, RH; Duan, HT; Loiselle, S; Xu, JD. *Water Science And Technology-Water Supply* 16, 1451-1466 (2016).
233. SBA-15 mesoporous silica highly functionalized with propylsulfonic pendants: A thorough physico-chemical characterization. Cattaneo, AS; Ferrara, C; Villa, DC; Angioni, S; Milanese, C; Capsoni, D; Grandi, S; Mustarelli, P; Allodi, V; Mariotto, G; Brutti, S; Quartarone, E. *Microporous And Mesoporous Materials* 219, 219-229 (2016).
234. Selective protein trapping within hybrid nanowells. Messina, GML; Passiu, C; Rossi, A; Marletta, G. *Nanoscale* 8, 16511-16519 (2016).
235. Shallow Anterior Chamber After Trabeculectomy: Risk Reduction by Use of Removable Compression Sutures. Savastano, MC; Savastano, A; Sbordone, S; Forte, R; Piccirillo, V; Costagliola, C; Savastano, S. *Journal Of Glaucoma* 25, 223-227 (2016).
236. Shellac/nanoparticles dispersions as protective materials for wood. Weththimuni, ML; Capsoni, D; Malagodi, M; Milanese, C; Licchelli, M. *Applied Physics A* 122, 1-12 (2016).
237. SIMS characterization of surface-modified nanostructured titania electrodes for solar energy conversion devices. Vitale, S; Zappalà, G; Tuccitto, N; Torrisi, A; Napolitani, E; Licciardello, A. *Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics* 34, 0001 (2016).
238. Simulating the active sites of copper-trafficking proteins. Density functional structural and spectroscopy studies on copper(I) complexes with thiols, carboxylato, amide and phenol ligands.

Tamasi, G; Bonechi, C; Rossi, C; Cini, R; Magnani, A. *Journal Of Coordination Chemistry* 69, 404-424 (2016).

239. Small Angle X-ray and Neutron Scattering: Powerful Tools for Studying the Structure of Drug-Loaded Liposome. Di Cola, E; Grillo, I; Ristori S. *Pharmaceutics* 8, 10-26 (2016).
240. Specific Anion Effects on the Kinetics of Iodination of Acetone. Lo Nostro, P; Mazzini, V; Ninham, BW; Ambrosi, M; Dei, LG; Baglioni, P. *Chemphyschem* 17, 2567-2571 (2016).
241. Spirobisnaphthalenes effectively inhibit carbonic anhydrase. Gocer, H; Aslan, A; Gulcin, I; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 503-507 (2016).
242. State of Water in Hydrating Tricalcium Silicate Pastes: The Effect of a Cellulose Ether. Del Buffa, S; Fratini, E; Ridi, F; Faraone, A; Baglioni, P. *Journal Of Physical Chemistry C* 120, 7612-7620 (2016).
243. Structural characterization of magnesium silicate hydrate: towards the design of eco-sustainable cements. Tonelli, M; Martini, F; Calucci, L; Fratini, E; Geppi, M; Ridi, F; Borsacchi, S; Baglioni, P. *Dalton Transactions* 45, 3294-3304 (2016).
244. Structural Insights into the Quadruplex-Duplex 3' Interface formed from a Telomeric Repeat: A Potential Molecular Target. Russo Krauss, I; Ramaswamy, S; Neidle, S; Haider, S; Parkinson, GN. *Journal of the American Chemical Society* 138, 1226-1233 (2016).
245. Structure and rheology of gel nanostructures from a vitamin C-based surfactant. Carretti, E; Mazzini, V; Fratini, E; Ambrosi, M; Dei, LG; Baglioni, P; Lo Nostro, P. *Physical Chemistry Chemical Physics* 18, 8865-8873 (2016).
246. Sulfamide derivatives with selective carbonic anhydrase VII inhibitory action. Villalba, ML; Palestro, P; Ceruso, M; Funes, JLG; Talevi, A; Blanch, LB; Supuran, CT; Gavernet, L. *Bioorganic & Medicinal Chemistry* 24, 894-901 (2016).
247. Sulfonamide inhibition studies of the alpha-carbonic anhydrase from the gammaproteobacterium Thiomicrospira crunogena XCL-2, TcruCA. Vullo, D; Bhatt, A; Mahon, BP; McKenna, R; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 26, 401-405 (2016).
248. Sulfonamide inhibition studies of the beta-carbonic anhydrase from the newly discovered bacterium Enterobacter sp B13. Eminoglu, A; Vullo, D; Asik, A; Colak, DN; Canakci, S; Belduz, AO; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 26, 1821-1826 (2016).
249. Sulfonamide inhibition studies of the beta-carbonic anhydrase from the pathogenic bacterium Vibrio cholerae. Del Prete, S; Vullo, D; De Luca, V; Carginale, V; Ferraroni, M; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry* 24, 1115-1120 (2016).
250. Sulfonamide inhibition studies of the gamma-carbonic anhydrase from the Antarctic bacterium Colwellia psychrerythraea. Vullo, D; De Luca, V; Del Prete, S; Carginale, V; Scozzafava, A; Osman, SM; AlOthman, Z; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 26, 1253-1259 (2016).
251. Sulfonamides incorporating heteropolycyclic scaffolds show potent inhibitory action against carbonic anhydrase isoforms I, II, IX and XII. Barresi, E; Salerno, S; Marini, AM; Taliani, S; La Motta, C; Simorini, F; Da Settimo, F; Vullo, D; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 921-927 (2016).
252. Supramolecular Polymer Networks Based on Calix[5]arene Chained Poly(p-phenyleneethynylene) and C60 Fulleropyrrolidine. Fraix, A; Torrisi, V; Marletta, G; Sortino, S; Mineo, PG; Tomaselli, GA; Ballistreri, FP; Trusso Sfrazzetto, G; Pappalardo, A. *Supramol. Chem.* 28, 485-492 (2016).
253. Surface characterization of textiles modified by copper and zinc oxide nano-antimicrobials. Ditaranto, N; Picca, RA; Sportelli, MC; Sabbatini, L; Cioffi, N. *Surface And Interface Analysis* 48, 505-508 (2016).
254. Surface Modification of MWCNT and their Reaction with Aniline by Oxidative Condensation. Kovalyshyn, Y; Konovska, M; Krupak, A; Milanese, C; Saldan, I;. Reshetnyak, O. *Research & Reviews: Journal of Chemistry* 5, 75-83 (2016).
255. Surface-Functionalization of Nanostructured Cellulose Aerogels by Solid State Eumelanin Coating. Panzella, L; Melone, L; Pezzella, A; Rossi, B; Pastori, N; Perfetti, M; D'Errico, G; Punta, C; d'Ischia, M. *Biomacromolecules* 17, 564-571 (2016).
256. Surface patterning: self-organization at the molecular level. Zhavnerko, G; Marletta, G. *Encyclopedia of Surface and Colloid Science (3rd Edition), Publisher: CRC Press, Boca Raton, USA; ISBN: 978-1-4665-9045-8* 10, 7087-7100 (2016).
257. Sustainability evaluation of innovative self-cleaning textiles. Busi, E; Maranghi, S; Corsi, L; Basosi, R. *Journal of Cleaner Production* 133, 439-450 (2016).
258. Synthesis 4-[2-(2-mercapto-4-oxo-4H-quinazolin-3-yl)-ethyl]-benzenesulfonamides with subnanomolar carbonic anhydrase II and XII inhibitory properties. Bozdag, M; Alafeefy, AM; Carta, F; Ceruso, M; Al-Tamimi, AMS; Al-Kahtani, AA; Alasmary, FAS; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 4100-4107 (2016).
259. Synthesis and bioactivity studies on new 4-(3-(4-Substitutedphenyl)-3a,4-dihydro-3H-indeno[1,2-c]pyrazol-2-yl) benzenesulfonamides. Gul, HI; Tugrak, M; Sakagami, H; Taslimi, P; Gulcin, I; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1619-1624 (2016).

260. Synthesis and carbonic anhydrase I, II, IV and XII inhibitory properties of N-protected amino acid - sulfonamide conjugates. Kucukbay, FZ; Kucukbay, H; Tanc, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1476-1483 (2016).
261. Synthesis and carbonic anhydrase inhibitory effects of new N-glycosylsulfonamides incorporating the phenol moiety. Riafrecha, LE; Bua, S; Supuran, CT; Colinas, PA. *Bioorganic & Medicinal Chemistry Letters* 26, 3892-3895 (2016).
262. Synthesis and carbonic anhydrase inhibitory properties of amino acid - coumarin/quinolinone conjugates incorporating glycine, alanine and phenylalanine moieties. Kucukbay, FZ; Kucukbay, H; Tanc, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1198-1202 (2016).
263. Synthesis and in Vivo Biological Evaluation of Ga-68-Labeled Carbonic Anhydrase IX Targeting Small Molecules for Positron Emission Tomography. Sneddon, D; Niemans, R; Bauwens, M; Yaromina, A; van Kuijk, SJA; Lieuwes, NG; Biemans, R; Pooters, I; Pellegrini, PA; Lengkeek, NA; Greguric, I; Tonissen, KF; Supuran, CT; Lambin, P; Dubois, L; Poulsen, SA. *Journal Of Medicinal Chemistry* 59, 6431-6443 (2016).
264. Synthesis and inhibition potency of novel ureido benzenesulfonamides incorporating GABA as tumor-associated carbonic anhydrase IX and XII inhibitors. Ceruso, M; Antel, S; Scozzafava, A; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 205-211 (2016).
265. Synthesis and inhibitory properties of some carbamates on carbonic anhydrase and acetylcholine esterase. Yilmaz, S; Akbaba, Y; Ozgeris, B; Kose, LP; Goksu, S; Gulcin, I; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1484-1491 (2016).
266. Synthesis of 4-(2-substituted hydrazinyl)benzenesulfonamides and their carbonic anhydrase inhibitory effects. Gul, HI; Kucukoglu, K; Yamali, C; Bilginer, S; Yuca, H; Ozturk, I; Taslimi, P; Gulcin, I; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 568-573 (2016).
267. Synthesis of 4-(thiazol-2-ylamino)-benzenesulfonamides with carbonic anhydrase I, II and IX inhibitory activity and cytotoxic effects against breast cancer cell lines. Gawad, NMA; Amin, NH; Elsaadi, MT; Mohamed, FMM; Angeli, A; De Luca, V; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 3043-3051 (2016).
268. Synthesis of 4-[2-(3,4-dimethoxybenzyl)cyclopentyl]-1,2-dimethoxybenzene Derivatives and Evaluations of Their Carbonic Anhydrase Isoenzymes Inhibitory Effects. Artunc, T; Cetinkaya, Y; Gocer, H; Gulcin, I; Menzek, A; Sahin, E; Supuran, CT. *Chemical Biology & Drug Design* 87, 594-607 (2016).
269. Synthesis of 4-sulfamoylphenyl-benzylamine derivatives with inhibitory activity against human carbonic anhydrase isoforms I, II, IX and XII. Durgun, M; Turkmen, H; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry* 24, 982-988 (2016).
270. Synthesis of $Bi_4Ti_3O_{12}$ by high energy milling of Bi_2O_3-TiO_2 (anatase) mixtures. Berbenni, V; Milanese, C; Bruni, G; Girella, A; Marini, A. *Journal Of Thermal Analysis And Calorimetry* 126, 1507-1511 (2016).
271. Synthesis of N-alkyl (aril)-tetra pyrimidine thiones and investigation of their human carbonic anhydrase I and II inhibitory effects. Sujayev, A; Kose, LP; Garibov, E; Gulcin, I; Farzaliev, V; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1192-1197 (2016).
272. Synthesis of some tetrahydropyrimidine-5-carboxylates, determination of their metal chelating effects and inhibition profiles against acetylcholinesterase, butyrylcholinesterase and carbonic anhydrase. Sujayev, A; Garibov, E; Taslimi, P; Gulcin, I; Gojayeva, S; Farzaliyev, V; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1531-1539 (2016).
273. Synthesis, characterization and carbonic anhydrase inhibitory activity of novel benzothiazole derivatives. Kucukbay, FZ; Bugday, N; Kucukbay, H; Tanc, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1221-1225 (2016).
274. Synthesis, structural and optical characterization of $APbX_3$ (A=methylammonium, dimethylammonium, trimethylammonium; X=I, Br, Cl) hybrid organic-inorganic materials. Mancini, A; Quadrelli, P; Amoroso, G; Milanese, C; Boiocchi, M; Sironi, A; Patrini, M; Guizzetti, G; Malavasi, L. *Journal Of Solid State Chemistry* 240, 55-60 (2016).
275. Tailoring ionic-electronic transport in PEO-Li_4C_{60}: Towards a new class of all solid-state mixed conductors. Cattaneo, AS; Dall'Asta, V; Pontiroli, D; Ricco, M; Magnani, G; Milanese, C; Tealdi, C; Quartarone, E; Mustarelli, P. *Carbon* 100, 196-200 (2016).
276. Targeting the pH regulatory mechanisms of breast cancer cells. Meehan, J; Ward, C; Jarman, E; Xintaropoulou, C; Martinez-Perez, C; Turnbull, A; Supuran, C; Dixon, M; Kunkler, I; Langdon, SP. *Cancer Research* 76 (2016).
277. Technological Potential of Lactobacillus Strains Isolated from Fermented Green Olives: In Vitro Studies with Emphasis on Oleuropein-Degrading Capability. Iorizzo, M; Lombardi, SJ; Macciola, V; Testa, B; Lustrato, G; Lopez, F; De Leonardis, A. *Thescientificworldjournal* 2016, 1917592-1917592 (2016).

278. The anticonvulsant sulfamide JNJ-26990990 and its S,S-dioxide analog strongly inhibit carbonic anhydrases: solution and X-ray crystallographic studies. Di Fiore, A; De Simone, G; Alterio, V; Riccio, V; Winum, JY; Carta, F; Supuran, CT. *Organic & Biomolecular Chemistry* 14, 4853-4858 (2016).
279. The degradation of wall paintings and stone: Specific ion effects. Baglioni, P; Giorgi, R; Chelazzi, D. *Current Opinion In Colloid & Interface Science* 23, 66-71 (2016).
280. The DnaE Polymerase from Deinococcus radiodurans features RecA-dependent DNA Polymerase activity. Randi, L; Perrone, A; Maturi, M; Dal Piaz, F; Camerani, M; Hochkoeppler, A. *Bioscience Reports* (2016).
281. The effect of caffeic acid phenethyl ester (CAPE) on metabolic enzymes including acetylcholinesterase, butyrylcholinesterase, glutathione S-transferase, lactoperoxidase, and carbonic anhydrase isoenzymes I, II, IX, and XII. Gulcin, I; Scozzafava, A; Supuran, CT; Akincioglu, H; Koksal, Z; Turkan, F; Alwasel, S. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1095-1101 (2016).
282. The effects of some avermectins on bovine carbonic anhydrase enzyme. Kose, LP; Gulcin, I; Ozdemir, H; Atasever, A; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 773-778 (2016).
283. The effects of some bromophenols on human carbonic anhydrase isoenzymes. Taslimi, P; Gulcin, I; Oztaskin, N; Cetinkaya, Y; Goksu, S; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 603-607 (2016).
284. The expression of the Cuphea palustris thioesterase CpFatB2 in Yarrowia lipolytica triggers oleic acid accumulation. Stefan, A; Hochkoeppler, A; Ugolini, L; Lazzeri, L; Conte, E. *Biotechnology Progress* 32, 26-35 (2016).
285. The history and rationale of using carbonic anhydrase inhibitors in the treatment of peptic ulcers. In memoriam Ioan Puscas (1932-2015). Buzas, GM; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 527-533 (2016).
286. The human carbonic anhydrase isoenzymes I and II (hCA I and II) inhibition effects of trimethoxyindane derivatives. Taslimi, P; Gulcin, I; Ozgeris, B; Goksu, S; Tumer, F; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 152-157 (2016).
287. The human carbonic anhydrase isoenzymes I and II inhibitory effects of some hydroperoxides, alcohols, and acetates. Kose, LP; Gulcin, I; Yildirim, A; Atmaca, U; Celik, M; Alwasel, SH; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1248-1253 (2016).
288. The impact of alkanes on the structure of Triton X100 micelles. Giorgio, G; Colafemmina, G; Mavelli, F; Murgia, S; Palazzo, G. *Rsc Advances* 6, 825-836 (2016).
289. The impact of interfaces in laminated packaging on transport of carboxylic acids. Gardebjer, S; Geback, T; Andersson, T; Fratini, E; Baglioni, P; Bordes, R; Viriden, A; Nicholas, M; Loren, N; Larsson, A. *Journal Of Membrane Science* 518, 305-312 (2016).
290. The inhibitory effects of phenolic Mannich bases on carbonic anhydrase I and II isoenzymes. Yamali, C; Tugrak, M; Gul, HI; Tanc, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 1678-1681 (2016).
291. The memory-driven order-disorder transition of a 3D-supramolecular architecture based on calix[5]arene and porphyrin derivatives. Tuccitto, N; Sfrazzetto, GT; Gangemi, CMA; Ballistreri, FP; Toscano, RM; Tomaselli, GA; Pappalardo, A; Marletta, G. *Chemical Communications* 52, 11681-11684 (2016).
292. The novel cannabinoid antagonist SM-11 reduces hedonic aspect of food intake through a dopamine-dependent mechanism. Fois, GR; Fattore, L; Murineddu, G; Salis, A; Pintore, G; Asproni, B; Pinna, G A; Diana, M. *Pharmacological Research* 113, 108-115 (2016).
293. The role of non-covalent sulfur-oxygen interactions in phenoxyl radicals stabilization: Synthesis of super tocopherol-like antioxidants. Menichetti, S; Amorati, R; Meoni, V; Tofani, L; Caminati, G; Viglianisi, C. *Organic Letters*, in press (2016).
294. The synthesis of (Z)-4-oxo-4-(arylamino)but-2-enoic acids derivatives and determination of their inhibition properties against human carbonic anhydrase I and II isoenzymes. Oktay, K; Kose, LP; Sendil, K; Gultekin, MS; Gulcin, I; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 31, 939-945 (2016).
295. Thermodynamic Analysis of Ethanol Reforming for Hydrogen Production. Tamasi, G; Bonechi, C; Magnani, A; Leone, G; Donati, A; Pepi, S; Rossi, C. *Chapter in Bioenergy – A technology prospect forward the future, edited by F. Dalena, A. Basile, C. Rossi, Elsevier* (2016).
296. Thermodynamic properties and photodegradation kinetics of indocyanine green in aqueous solution. Di Nezza, F.; Guerra, G.; Costagliola, C.; Zeppa, L.; Ambrosone, L. *Dyes And Pigments* 134, 342-347 (2016).
297. Thioxocoumarins Show an Alternative Carbonic Anhydrase Inhibition Mechanism Compared to Coumarins. Ferraroni, M; Carta, F; Scozzafava, A; Supuran, CT. *Journal Of Medicinal Chemistry* 59, 462-473 (2016).

298. Through-bond effects in the ternary complexes of thrombin sandwiched by two DNA aptamers. Pica, A; Russo Krauss, I; Parente, V; Tateishi-Karimata, H; Nagatoishi, S; Tsumoto, K; Sugimoto, N; Sica, F. *Nucleic Acids Research* doi: 10.1093/nar/gkw1113 (2016).
299. To the Memory of Marco Mascini: His Contribution to Biosensors Technology. Marrazza G; Minunni, M; Palchetti, I. *TrAC Trends in Analytical Chemistry* 79, 2-8 (2016).
300. Toward sensitive immuno-based detection of Tau protein by surface plasmon resonance coupled to carbon nanostructures as signal amplifiers. Lisi, S; Scarano, S; Fedeli, S; Cicchi, S; Pascale, E; Ravelet, C; Peyrin, E; Minunni, M. *Biosens. Bioelectron.* (2016).
301. Traditional Portland cement and innovative MgO-based cement: a promising combination?. Tonelli, M; Martini, F; Calucci, L; Fratini, E; Geppi, M; Ridi, F; Borsacchi, S; Baglioni, P. *Physics and Chemistry of the Earth* under review (2016).
302. Tryptophan-surface modification of versatile peroxidase from Bjerkandera adusta enhances its catalytic performance. Sanchez-Alejandro, F; Juarez-Moreno, K; Baratto, MC; Basosi, R; Vazquez-Duhalt, R. *Journal Of Molecular Catalysis B-Enzymatic* 124, 45-51 (2016).
303. Tuning the Composition of Alloy Nanoparticles Through Laser Mixing: The Role of Surface Plasmon Resonance. Messina, G; Sinatra, M; Bonanni, V; Brescia, R; Alabastri, A; Pineider, F; Campo, G; Sangregorio, C; Li Destri, G; Sfuncia, G; Marletta, G; Condorelli, M; Proietti Zaccaria, R; De Angelis, F; Compagnini, G. *J. Phys. Chem. C* 120, 12810-12818; (2016).
304. Wool fibril sponges with perspective biomedical applications. Patrucco, A; Cristofaro, F; Simionati, M; Zoccola, M; Bruni, G; Fassina, L; Visai, L; Magenes, G; Mossotti, R; Montarsolo, A; Tonin, C. *Materials Science and Engineering C* 61, 42-50 (2016).
305. [F-18]VM4-037 MicroPET Imaging and Biodistribution of Two In Vivo CAIX-Expressing Tumor Models. Peeters, SGJA; Dubois, L; Lieuwes, NG; Laan, D; Mooijer, M; Schuit, RC; Vullo, D; Supuran, CT; Eriksson, J; Windhorst, AD; Lambin, P. *Molecular Imaging And Biology* 17, 615-619 (2015).
306. 5-Aryl-1H-pyrazole-3-carboxylic acids as selective inhibitors of human carbonic anhydrases IX and XII. Cvijetic, IN; Tanc, M; Juranic, IO; Verbic, TZ; Supuran, CT; Drakulic, BJ. *Bioorganic & Medicinal Chemistry* 23, 4649-4659 (2015).
307. 6-Substituted 1,2-benzoxathiine-2,2-dioxides are isoform-selective inhibitors of human carbonic anhydrases IX, XII and VA. Tanc, M; Carta, F; Scozzafava, A; Supuran, CT. *Organic & Biomolecular Chemistry* 13, 77-80 (2015).
308. 6-Substituted Sulfocoumarins Are Selective Carbonic Anhdydrase IX and XII Inhibitors with Significant Cytotoxicity against Colorectal Cancer Cells. Grandane, A; Tanc, M; Mannelli, LD; Carta, F; Ghelardini, C; Zalubovskis, R; Supuran, CT. *Journal Of Medicinal Chemistry* 58, 3975-3983 (2015).
309. 7-Amino-3,4-dihydro-1H-quinolin-2-one, a compound similar to the substituted coumarins, inhibits alpha-carbonic anhydrases without hydrolysis of the lactam ring. Vullo, D; Isik, S; Bozdag, M; Carta, F; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 773-777 (2015).
310. A central role for intermolecular dityrosine cross-linking of fibrinogen in high molecular weight advanced oxidation protein product (AOPP) formation. Colombo, G; Clerici, M; Giustarini, D; Portinaro, N; Badalamenti, S; Rossi, R; Milzani, A; Dalle-Donne, I. *Biochimica Et Biophysica Acta-General Subjects* 1850, 1-12 (2015).
311. A class of sulfonamide carbonic anhydrase inhibitors with neuropathic pain modulating effects. Carta, F; Mannelli, LD; Pinard, M; Ghelardini, C; Scozzafava, A; McKenna, R; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 1828-1840 (2015).
312. A coarse grain model for alfa-synuclein aggregation. Procacci, P; Caminati, G., *Ed. Italian National Agency for New Technologies, Energy and Sustainable Economic Development*, 98-107 (2015).
313. A failed tentative to design a super carbonic anhydrase having the biochemical properties of the most thermostable CA (SspCA) and the fastest (SazCA) enzymes. De Luca, V; Del Prete, S; Carginale, V; Vullo, D; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 989-994 (2015).
314. A hydrogel capsule as gate dielectric in flexible organic field-effect transistors. Dumitru, LM; Manoli, K; Magliulo, M; Ligonzo, T; Palazzo, G; Torsi, L. *Apl Materials* 3 (2015).
315. A Key Opinion Leader interview: insight into the research and career of Prof. Claudiu T Supuran. Palmer, C; Supuran, CT. *Expert Opinion On Therapeutic Patents* 25, 501-505 (2015).
316. A new affinity gel for the purification of alpha-carbonic anhdrases. Sahin, A; Isik, S; Arslan, O; Supuran, CT; Guler, OO. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 224-228 (2015).
317. A new class of quinazoline-sulfonamides acting as efficient inhibitors against the alpha-carbonic anhydrase from Trypanosoma cruzi. Alafeefy, AM; Ceruso, M; Al-Jaber, NA; Parkkila, S; Vermelho, AB; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 581-585 (2015).

318. A new lead compound for the development of Carbonic Anhydrase inhibitors. Di Fiore, A; De Simone, G; Vergara, A; Caterino, M; Alterio, V; Monti, SM; Ombouma, J; Dumy, P; Supuran, CT; Winum, JY. *Protein Science* 24, 50-50 (2015).
319. A Novel Device to Exploit the Smartphone Camera for Fundus Photography. Russo, A; Morescalchi, F; Costagliola, C; Delcassi, L; Semeraro, F. *Journal Of Ophthalmology* (2015).
320. A Remote Sensing Approach to Estimate Vertical Profile Classes of Phytoplankton in a Eutrophic Lake. Xue, K; Zhang, YC; Duan, HT; Ma, RH; Loiselle, S; Zhang, MW. *Remote Sensing* 7, 14403-14427 (2015).
321. A Simple Protein Synthesis Model for the PURE System Operation. Mavelli, F; Marangoni, R; Stano, P. *Bulletin Of Mathematical Biology* 77, 1185-1212 (2015).
322. A Spectroscopic Study of the Aggregation State of the Human Antimicrobial Peptide LL-37 in Bacterial versus Host Cell Model Membranes. Bonucci, A; Caldaroni, E; Balducci, E; Pogni, R. *Biochemistry* 54, 6760-6768 (2015).
323. A sulfur-based transport pathway in Cu+-ATPases. Mattle, D; Zhang, LM; Sitsel, O; Pedersen, LT; Moncelli, MR; Tadini-Buoninsegni, F; Gourdon, P; Rees, DC; Nissen, P; Meloni, G. *Embo Reports* 16, 728-740 (2015).
324. A thermodynamic signature of lipid segregation in biomembranes induced by a short peptide derived from glycoprotein gp36 of feline immunodeficiency virus. Oliva, R; Del Vecchio, P; Stellato, MI; D'Ursi, AM; D'Errico, G; Paduano, L; Petraccone, L. *Biochimica Et Biophysica Acta-Biomembranes* 1848, 510-517 (2015).
325. Acetazolamide for the treatment of idiopathic intracranial hypertension. Supuran, CT. *Expert Review Of Neurotherapeutics* 15, 851-856 (2015).
326. Acetazolamide protects steatotic liver against cold ischemia reperfusion injury. Bejaoui, M; Pantazi, E; De Luca, V; Panisello, A; Folch-Puy, E; Capasso, C; Supuran, C; Rosello-Catafau, J. *Transplant International* 28, 260-260 (2015).
327. Acetazolamide Protects Steatotic Liver Grafts against Cold Ischemia Reperfusion Injury. Bejaoui, M; Pantazi, E; De Luca, V; Panisello, A; Folch-Puy, E; Serafin, A; Capasso, C; Supuran, CT; Rossello-Catafau, J. *Journal Of Pharmacology And Experimental Therapeutics* 355, 191-198 (2015).
328. Activatory coupling among oscillating droplets produced in microfluidic based device. Tomasi, R ; Noël, JM; Zenati, A; Rossi, F; Cabuil, V; Ristori, S; Kanoufi, F; Abou-Hassan, A. *Int. J. Unconv. Computing* 11, 21-34 (2015).
329. Adsorbent properties of olive mill wastes for chromate removal. Mosca, M; Cuomo, F; Lopez, F; Palumbo, G; Bufalo, G; Ambrosone, L. *Desalination And Water Treatment* 54, 275-283 (2015).
330. alpha-Carbonic Anhydrases Possess Thioesterase Activity. Tanc, M; Carta, F; Scozzafava, A; Supuran, CT. *Acs Medicinal Chemistry Letters* 6, 292-295 (2015).
331. Ammonia-storage in lithium intercalated fullerides. Pontiroli, D; D'Alessio, D; Gaboardi, M; Magnani, G; Milanese, C; Duyker, SG; Peterson, VK; Sharma, N; Ricco, M. *Journal Of Materials Chemistry A* 3, 21099-21105 (2015).
332. Amphiphile-based nanofludis for the removal of styrene/acrylate coatings: cleaning of stucco decoration in the Uaxactun archeological site (Guatemala). Baglioni, M; Jáidar Benavides, Y; Desprat-Drapela, A; Giorgi, R. *Journal of Cultural Heritage* 16, 861-868 (2015).
333. An amine-oxide surfactant-based microemulsion for the cleaning of works of art. Baglioni, M; Benavides, YJ; Berti, D; Giorgi, R; Keiderling, U; Baglioni, P. *Journal Of Colloid And Interface Science* 440, 204-210 (2015).
334. An analytical model for bio-electronic organic field-effect transistor sensors (vol 103, 103301, 2013). Macchia, E; Giordano, F; Magliulo, M; Palazzo, G; Torsi, L. *Applied Physics Letters* 106 (2015).
335. An overview of the alpha-, beta- and gamma-carbonic anhydrases from Bacteria: can bacterial carbonic anhydrases shed new light on evolution of bacteria?. Capasso, C; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 325-332 (2015).
336. An Overview of the Selectivity and Efficiency of the Bacterial Carbonic Anhydrase Inhibitors. Capasso, C; Supuran, CT. *Current Medicinal Chemistry* 22, 2130-2139 (2015).
337. Anion and sulfonamide inhibition studies of an alpha-carbonic anhydrase from the Antarctic hemoglobinless fish Chionodraco hamatus. Cincinelli, A; Martellini, T; Vullo, D; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 5485-5489 (2015).
338. Anion inhibition studies of the dandruff-producing fungus Malassezia globosa beta-carbonic anhydrase MgCA. Del Prete, S; Vullo, D; Osman, SM; AlOthman, Z; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 5194-5198 (2015).
339. Antibiotic delivery by liposomes from prokaryotic microorganisms: Similia cum similis works better. Colzi, I; Gonnelli, C; Troyan, AT; Perito, B; Casalone, E; Romoli, R; Pieraccini, G; Škalko-Basnet, N; Adessi, A; Rossi, F; Ristori, S. *Eur. J. Pharm. Biopharm.* 94, 411-18 (2015).
340. A regenerable optical biosensor for the ultrasensitive and selective detection of unamplified human genomic DNA with gold nanostars. Mariani, S; Scarano, S; Spadavecchia, J; Minunni, M. *Biosensor and Bioelectronics* 74, 981-988 (2015).

341. Ascaris lumbricoides beta carbonic anhydrase: a potential target enzyme for treatment of ascariasis. Emameh, RZ; Kuuslahti, M; Vullo, D; Barker, HR; Supuran, CT; Parkkila, S. *Parasites & Vectors* 8 (2015).
342. Au/In2O3 and Au/ZrO2 composite nanoparticles via in situ sacrificial gold electrolysis. Afzal, A; Di Franco, C; Mesto, E; Ditaranto, N; Cioffi, N; Scordari, F; Scamarcio, G; Torsi, L. *Materials Express* 5, 171-179 (2015).
343. Bacterial, fungal and protozoan carbonic anhydrases as drug targets. Capasso, C; Supuran, CT. *Expert Opinion On Therapeutic Targets* 19, 1689-1704 (2015).
344. Basidiomycete DyPs: Genomic diversity, structural-functional aspects, reaction mechanism and environmental significance. Linde, D; Ruiz-Duenas, FJ; Fernandez-Fueyo, E; Guallar, V; Hammel, KE; Pogni, R; Martinez, AT. *Archives Of Biochemistry And Biophysics* 574, 66-74 (2015).
345. Benzenesulfonamides incorporating bulky aromatic/heterocyclic tails with potent carbonic anhydrase inhibitory activity. Bozdag, M; Alafeefy, AM; Vullo, D; Carta, F; Dedeoglu, N; Al-Tamimi, AMS; Al-Jaber, NA; Scozzafava, A; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 7751-7764 (2015).
346. Bio-functionalization of ZnO water gated thin-film transistors. Singh, M; Mulla, MY; Manoli, K; Magliulo, M; Ditaranto, N; Cioffi, N; Palazzo, G; Torsi, L; Santacroce, MV; Di Franco, C; Scamarcio, G. *2015 6Th Ieee International Workshop On Advances In Sensors And Interfaces (Iwasi)*, 261-265 (2015).
347. Biochemical characterization of recombinant beta-carbonic anhydrase (PgiCAb) identified in the genome of the oral pathogenic bacterium Porphyromonas gingivalis. Del Prete, S; Vullo, D; De Luca, V; AlOthman, Z; Osman, SM; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 366-370 (2015).
348. C-glycosides incorporating the 6-methoxy-2-naphthyl moiety are selective inhibitors of fungal and bacterial carbonic anhydrases. Riafrecha, LE; Vullo, D; Supuran, CT; Colinas, PA. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 857-861 (2015).
349. Capacitance-modulated transistor detects odorant binding protein chiral interactions. Mulla, MY; Tuccori, E; Magliulo, M; Lattanzi, G; Palazzo, G; Persaud, K; Torsi, L. *Nature Communications* 6 (2015).
350. Carbamoylphosphonates inhibit autotaxin and metastasis formation in vivo. Reich, R; Hoffman, A; Suresh, RR; Shai, O; Frant, J; Maresca, A; Supuran, CT; Breuer, E. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 767-772 (2015).
351. Carbonic anhydrase and acetylcholinesterase inhibitory effects of carbamates and sulfamoylcarbamates. Gocer, H; Akincioglu, A; Goksu, S; Gulcin, I; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 316-320 (2015).
352. Carbonic Anhydrase Glycoinhibitors belonging to the Aminoxysulfonamide Series. Ombouma, J; Vullo, D; Dumy, P; Supuran, CT; Winum, JY. *Acs Medicinal Chemistry Letters* 6, 819-821 (2015).
353. Carbonic Anhydrase Inhibitors with Dual-Tail Moieties To Match the Hydrophobic and Hydrophilic Halves of the Carbonic Anhydrase Active Site. Tanpure, RP; Ren, B; Peat, TS; Bornaghi, LF; Vullo, D; Supuran, CT; Poulsen, SA. *Journal Of Medicinal Chemistry* 58, 1494-1501 (2015).
354. Carbonic anhydrase inhibitors: Design, synthesis and structural characterization of new heteroaryl-N-carbonylbenzenesulfonamides targeting druggable human carbonic anhydrase isoforms. Buemi, MR; De Luca, L; Ferro, S; Bruno, E; Ceruso, M; Supuran, CT; Pospisilova, K; Brynda, J; Rezacova, P; Gitto, R. *European Journal Of Medicinal Chemistry* 102, 223-232 (2015).
355. Carbonic anhydrase inhibitors: Design, synthesis, kinetic, docking and molecular dynamics analysis of novel glycine and phenylalanine sulfonamide derivatives. Fidan, I; Salmas, RE; Arslan, M; Senturk, M; Durdagi, S; Ekinci, D; Senturk, E; Cosgun, S; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 7353-7358 (2015).
356. Carbonic anhydrase inhibitors: guaiacol and catechol derivatives effectively inhibit certain human carbonic anhydrase isoenzymes (hCA I, II, IX and XII). Scozzafava, A; Passaponti, M; Supuran, CT; Gulcin, I. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 586-591 (2015).
357. Carbonic anhydrase IX inhibition is an effective strategy for osteosarcoma treatment. Perut, F; Carta, F; Bonuccelli, G; Grisendi, G; Di Pompo, G; Avnet, S; Sbrana, FV; Hosogi, S; Dominici, M; Kusuzaki, K; Supuran, CT; Baldini, N. *Expert Opinion On Therapeutic Targets* 19, 1593-1605 (2015).
358. Carbonic anhydrase IX inhibitors in cancer therapy: an update. Supuran, CT; Winum, JY. *Future Medicinal Chemistry* 7, 1407-1414 (2015).
359. Carbonic Anhydrase Protects Fatty Liver Grafts against Ischemic Reperfusion Damage. Bejaoui, M; Pantazi, E; De Luca, V; Panisello, A; Folch-Puy, E; Hotter, G; Capasso, C; Supuran, CT; Rossello-Catafau, J. *Plos One* 10 (2015).
360. Carbonic anhydrases and their functional differences in human and mouse sperm physiology. Jose, O; Torres-Rodriguez, P; Forero-Quintero, LS; Chavez, JC; De la Vega-Beltran, JL; Carta, F;

Supuran, CT; Deitmer, JW; Trevino, CL. *Biochemical And Biophysical Research Communications* 468, 713-718 (2015).

361. Carboxylic Acids: a versatile classe of carbonic anhydrase inhibitors. De Simone, G; Carradori, S; Langella, E; Monti, SM; Supuran, CT; D'Ambrosio, K. *Protein Science* 24, 49-49 (2015).
362. Catalytic surface radical in dye-decolorizing peroxidase: a computational, spectroscopic and site-directed mutagenesis study. Linde, D; Pogni, R; Canellas, M; Lucas, F; Guallar, V; Baratto, MC; Sinicropi, A; Saez-Jimenez, V; Coscolin, C; Romero, A; Medrano, FJ; Ruiz-Duenas, FJ; Martinez, AT. *Biochemical Journal* 466, 253-262 (2015).
363. Cationic liposomes as efficient nanocarriers for the drug delivery of an anticancer cholesterol-based ruthenium complex. Vitiello, G; Luchini, A; D'Errico, G; Santamaria, R; Capuozzo, A; Irace, C; Montesarchio, D; Paduano, L. *Journal Of Materials Chemistry B* 3, 3011-3023 (2015).
364. $CH_3NH_3SnxPb_1$-xBr_3 Hybrid Perovskite Solid Solution: Synthesis, Structure, and Optical Properties. Mancini, A; Quadrelli, P; Milanese, C; Patrini, M; Guizzetti, G; Malavasi, L. *Inorganic Chemistry* 54, 8893-8895 (2015).
365. Challenging Organic Syntheses and Pharmacological Applications of Natural Products and their Derivatives. Mori, M; Supuran, CT. *Current Pharmaceutical Design* 21, 5451-5452 (2015).
366. Characterization of Wet Powder-Sprayed Zirconia/Calcium Phosphate Coating for Dental Implants. Pardun, K; Treccani, L; Volkmann, E; Li Destri, G; Marletta, G; Streckbein, P; Heiss, C; Rezwan, K. *Clin. Impl. Dent. Relat. Res.* 17, 186-198 (2015).
367. Chelating Surfaces for Native State Proteins Patterning: The Human Serum Albumin Case. Giamblanco, N; Tuccitto, N; Zappalà, G; Sfuncia, G; Licciardello, A; Marletta, G. *ACS Applied Materials and Interfaces* 7, 23353-23363 (2015).
368. Chemistry of Lipid A: At the Heart of Innate Immunity. Molinaro, A; Holst, O; Di Lorenzo, F; Callaghan, M; Nurisso, A; D'Errico, G; Zamyatina, A; Peri, F; Berisio, R; Jerala, R; Jimenez-Barbero, J; Silipo, A; Martin-Santamaria, S. *Chemistry-A European Journal* 21, 500-519 (2015).
369. Chromophore-Protein Coupling beyond Nonpolarizable Models: Understanding Absorption in Green Fluorescent Protein. Daday, C; Curutchet, C; Sinicropi, A; Mennucci, B; Filippi, C. *Journal Of Chemical Theory And Computation* 11, 4825-4839 (2015).
370. Cleaning of olive mill wastewaters by visible light activated carbon doped titanium dioxide. Cuomo, F; Venditti, F; Ceglie, A; De Leonardis, A; Macciola, V; Lopez, F. *Rsc Advances* 5, 85586-85591 (2015).
371. Click-tailed coumarins with potent and selective inhibitory action against the tumor-associated carbonic anhydrases IX and XII. Nocentini, A; Carta, F; Ceruso, M; Bartolucci, G; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 6955-6966 (2015).
372. Cloning, characterization and anion inhibition studies of a gamma-carbonic anhydrase from the Antarctic cyanobacterium Nostoc commune. De Luca, V; Del Prete, S; Carginale, V; Vullo, D; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry Letters* 25, 4970-4975 (2015).
373. Cloning, characterization and anion inhibition studies of a new gamma-carbonic anhydrase from the Antarctic bacterium Pseudoalteromonas haloplanktis. De Luca, V; Vullo, D; Del Prete, S; Carginale, V; Scozzafava, A; Osman, SM; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry* 23, 4405-4409 (2015).
374. Cloning, characterization and anion inhibition study of a beta-class carbonic anhydrase from the caries producing pathogen Streptococcus mutans. Dedeoglu, N; De Luca, V; Isik, S; Yildirim, H; Kockar, F; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 2995-3001 (2015).
375. Colorimetric Nanoplasmonic Assay To Determine Purity and Titrate Extracellular Vesicles. Maiolo, D; Paolini, L; Di Noto, G; Zendrini, A; Berti, D; Bergese, P; Ricotta, D. *Analytical Chemistry* 87, 4168-4176 (2015).
376. Comparative Attributional Life Cycle Assessment of Annual and Perennial Lignocellulosic Feedstocks Production Under Mediterranean Climate for Biorefinery Framework. Zucaro, A; Forte, A; Fagnano, M; Bastianoni, S; Basosi, R; Fierro, A. *Integrated Environmental Assessment And Management* 11, 397-403 (2015).
377. Comparison of Smartphone Ophthalmoscopy With Slit-Lamp Biomicroscopy for Grading Diabetic Retinopathy. Russo, A; Morescalchi, F; Costagliola, C; Delcassi, L; Semeraro, F. *American Journal Of Ophthalmology* 159, 360-364 (2015).
378. Comparison of Smartphone Ophthalmoscopy with Slit-lamp Biomicroscopy for Undilated Glaucoma Screening. Russo, A; Morescalchi, F; Delcassi, L; Costagliola, C; Semeraro, F. *Investigative Ophthalmology & Visual Science* 56 (2015).
379. Comparison of the thermochemical and mechanochemical transformations in the $2NaNH_2$-MgH_2 system. Pireddu, G; Valentoni, A; Minella, CB; Pistidda, C; Milanese, C; Enzo, S; Mulas, G; Garroni, S. *International Journal Of Hydrogen Energy* 40, 1829-1835 (2015).
380. Computational investigation of the selectivity of salen and tetrahydrosalen compounds towards the tumor-associated hCA XII isozyme. Akdemir, A; De Monte, C; Carradori, S; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 114-118 (2015).

381. Controlled Microwave Assisted Hydrothermal Synthesis of Magnetite Nanoparticles as Easily Transportable Magnetic Support for Catalysts. Rizzuti, A; Dassisti, M; Mastrorilli, P; Sportelli, MC; Cioffi, N; Picca, RA; Agostinelli, E; Varvaro, G; Caliandro, R. *Journal of Nanoparticle Research* 17, 408 (2015).
382. Copper(II)-catalysed oxidative carbonylation of aminols and amines in water: A direct access to oxazolidinones, ureas and carbamates. Casiello, M; Iannone, F; Cotugno, P; Monopoli, A; Cioffi, N; Ciminale, F; Trzeciak, AM; Nacci, A. *Journal Of Molecular Catalysis A-Chemical* 407, 8-14 (2015).
383. Covering silver nanocube monolayers with graphene oxide sheets: Towards an efficient SERS platform. Banchelli, M; Caminati, G; Tiribilli, B; Pini, R; Matteini, P. *Fotonica*, 1-4 (2015).
384. Crystal structure and kinetic studies of a tetrameric type II beta-carbonic anhydrase from the pathogenic bacterium Vibrio cholerae. Ferraroni, M; Del Prete, S; Vullo, D; Capasso, C; Supuran, CT. *Acta Crystallographica Section D-Biological Crystallography* 71, 2449-2456 (2015).
385. Crystal structure of the most catalytically effective carbonic anhydrase enzyme known, SazCA from the thermophilic bacterium Sulfurihydrogenibium azorense. De Simone, G; Monti, SM; Alterio, V; Buonanno, M; De Luca, V; Rossi, M; Carginale, V; Supuran, CT; Capasso, C; Di Fiore, A. *Bioorganic & Medicinal Chemistry Letters* 25, 2002-2006 (2015).
386. Cubosome formulations stabilized by a dansyl-conjugated block copolymer for possible nanomedicine applications. Murgia, S; Falchi, AM; Meli, V; Schillen, K; Lippolis, V; Monduzzi, M; Rosa, A; Schmidt, J; Talmon, Y; Bizzarri, R; Caltagirone, C. *Colloids And Surfaces B-Biointerfaces* 129, 87-94 (2015).
387. Cucurbita pepo L. extracts as a versatile hydrotropic source for the synthesis of gold nanoparticles with different shapes. Gonnelli, C; Cacioppo, F; Giordano, C; Capozzoli, L; Salvatici, MC; Colzi, I; Del Bubba, M; Ancillotti, C; Ristori, S. *Green Chem. Rev. & Lett.* 8, 39-47 (2015).
388. Current Trends about Inner Limiting Membrane Peeling in Surgery for Epiretinal Membranes. Semeraro, F; Morescalchi, F; Duse, S; Gambicorti, E; Russo, A; Costagliola, C. *Journal Of Ophthalmology* (2015).
389. Cyclodextrin complexation highly enhances efficacy of arylsulfonylureido benzenesulfonamide carbonic anhydrase inhibitors as a topical antiglaucoma agents. Bragagni, M; Bozdag, M; Carta, F; Scozzafava, A; Lanzi, C; Masini, E; Mura, P; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 6223-6227 (2015).
390. Demonstration of Lignin-to-Peroxidase Direct Electron Transfer: a transient-state kinetics, directed mutagenesis, epr, and nmr study. Saez-Jimenez, V; Baratto, MC; Pogni, R; Rencoret, J; Gutierrez, A; Santos, JI; Martinez, AT; Ruiz-Duenas, FJ. *Journal Of Biological Chemistry* 290, 23201-23213 (2015).
391. Dendrimers incorporating benzenesulfonamide moieties strongly inhibit carbonic anhydrase isoforms I-XIV. Carta, F; Osman, SM; Vullo, D; AlOthman, Z; Supuran, CT. *Organic & Biomolecular Chemistry* 13, 6453-6457 (2015).
392. Design and characterization of a composite material based on Sr(II)-loaded clay nanotubes included within a biopolymer matrix. Del Buffa, S; Bonini, M; Ridi, F; Severi, M; Losi, P; Volpi, S; Al Kayal, T; Soldani, G; Baglioni, P. *Journal Of Colloid And Interface Science* 448, 501-507 (2015).
393. Design and synthesis of benzothiazole-6-sulfonamides acting as highly potent inhibitors of carbonic anhydrase isoforms I, II, IX and XII. Ibrahim, DA; Lasheen, DS; Zaky, MY; Ibrahim, AW; Vullo, D; Ceruso, M; Supuran, CT; Abou El Ella, DA. *Bioorganic & Medicinal Chemistry* 23, 4989-4999 (2015).
394. Design and Validation of FRESH, a Drug Discovery Paradigm Resting on Robust Chemical Synthesis. Shi, Q; Kaiser, TM; Dentmon, ZW; Ceruso, M; Vullo, D; Supuran, CT; Snyder, JP. *Acs Medicinal Chemistry Letters* 6, 518-522 (2015).
395. Designing carbonic anhydrase inhibitors for the treatment of breast cancer. Supuran, CT; Winum, JY. *Expert Opinion On Drug Discovery* 10, 591-597 (2015).
396. Design of a dual aptamer-based recognition strategy for human matrix metalloproteinase 9 protein by piezoelectric biosensors. Scarano, S; Dausse, E; Crispo, F; Toulmé, JJ; Minunni M. *Analytica Chimica Acta* 897, 1-9 (2015).
397. Detection Beyond Debye's Length with an Electrolyte-Gated Organic Field-Effect Transistor. Palazzo, G; De Tullio, D; Magliulo, M; Mallardi, A; Intranuovo, F; Mulla, MY; Favia, P; Vikholm-Lundin, I; Torsi, L. *Advanced Materials* 27, 911-916 (2015).
398. Developing functionalized Fe3O4-Au nanoparticles: a physico-chemical insight. Luchini, A; Vitiello, G; Rossi, F; De Ballesteros, OR; Radulescu, A; D'Errico, G; Montesarchio, D; Fernandez, CD; Paduano, L. *Physical Chemistry Chemical Physics* 17, 6087-6097 (2015).
399. Development of ocular hypertension secondary to tamponade with light versus heavy silicone oil: A systematic review. Romano, V; Cruciani, M; Semeraro, F; Costagliola, C; Romano, MR. *Indian Journal Of Ophthalmology* 63, 227-232 (2015).
400. Diabetic Retinopathy: Vascular and Inflammatory Disease. Semeraro, F.; Cancarini, A.; dell'Omo, R.; Rezzola, S.; Romano, M. R.; Costagliola, C. *Journal Of Diabetes Research* (2015).

401. Dietary Intake of Proteins and Calories Is Inversely Associated With The Oxidation State of Plasma Thiols in End-Stage Renal Disease Patients. Fanti, P; Giustarini, D; Rossi, R; Cunningham, SED; Folli, F; Khazim, K; Cornell, J; Matteucci, E; Bansal, S. *Journal Of Renal Nutrition* 25, 494-503 (2015).
402. Dipotassium-trioxohydroxytetrafluorotriborate, K-2[B3O3F4OH], is a potent inhibitor of human carbonic anhydrases. Vullo, D; Milos, M; Galic, B; Scozzafava, A; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 341-344 (2015).
403. Direct genotyping of C3435T single nucleotide polymorphism in unamplified human MDR1 gene using a surface plasmon resonance imaging DNA sensor. Mariani, S; Scarano, S; Carrai, M; Barale, R; Minunni, M. *Analytical, Bioanalytical Chemistry* 407, 4023-4028 (2015).
404. Discovery of 1,1 '-Biphenyl-4-sulfonamides as a New Class of Potent and Selective Carbonic Anhydrase XIV Inhibitors. La Regina, G; Coluccia, A; Famiglini, V; Pelliccia, S; Monti, L; Vullo, D; Nuto, E; Aterio, V; De Simone, G; Monti, SM; Pan, PW; Parkkila, S; Supuran, CT; Rossello, A; Silvestri, R. *Journal Of Medicinal Chemistry* 58, 8564-8572 (2015).
405. Discovery of novel isatin-based sulfonamides with potent and selective inhibition of the tumor-associated carbonic anhydrase isoforms IX and XII. Guzel-Akdemir, O; Akdemir, A; Karali, N; Supuran, CT. *Organic & Biomolecular Chemistry* 13, 6493-6499 (2015).
406. Discovery of potent carbonic anhydrase and acetylcholine esterase inhibitors: Novel sulfamoylcarbamates and sulfamides derived from acetophenones. Akincioglu, A; Akincioglu, H; Gulcin, I; Durdagi, S; Supuran, CT; Goksu, S. *Bioorganic & Medicinal Chemistry* 23, 3592-3602 (2015).
407. Discrimination of human semen specimens by NMR data, sperm parameters, and statistical analysis. Bonechi, C; Collodel, G; Donati, A; Martini, S; Moretti, E; Rossi, C. *Systems Biology In Reproductive Medicine* 61, 353-359 (2015).
408. Disentangling mass and angle dependence in neutrino mixing. Blasone, M; Gargiulo, MV; Vitiello, G. *7Th International Workshop Dice2014 Spacetime - Matter - Quantum Mechanics* 626 (2015).
409. Distribution and incidence of algal blooms in Lake Taihu. Duan, HT; Loiselle, SA; Zhu, L; Feng, L; Zhang, YC; Ma, RH. *Aquatic Sciences* 77, 9-16 (2015).
410. Docetaxel-Loaded Fluorescent Liquid-Crystalline Nanoparticles for Cancer Theranostics. Meli, V; Caltagirone, C; Falchi, AM; Hyde, ST; Lippolis, V; Monduzzi, M; Obiols-Rabasa, M; Rosa, A; Schmidt, J; Talmon, Y; Murgia, S. *Langmuir* 31, 9566-9575 (2015).
411. Drosophila melanogaster: a model organism for controlling Dipteran vectors and pests. Emameh, RZ; Syrjanen, L; Barker, H; Supuran, CT; Parkkila, S. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 505-513 (2015).
412. Dual Cyclooxygenase and Carbonic Anhydrase Inhibition by Nonsteroidal Anti-Inflammatory Drugs for the Treatment of Cancer. De Monte, C; Carradori, S; Gentili, A; Mollica, A; Trisciuoglio, D; Supuran, CT. *Current Medicinal Chemistry* 22, 2812-2818 (2015).
413. Effect of Factor XIII-A G185T Polymorphism on Visual Prognosis after Photodynamic Therapy for Neovascular Macular Degeneration. Parmeggiani, F; Costagliola, C; Semeraro, F; Romano, MR; Rinaldi, M; Gallenga, CE; Serino, ML; Incorvaia, C; D'Angelo, S; De Nadai, K; Dell'Omo, R; Russo, A; Gemmati, D; Perri, P. *International Journal Of Molecular Sciences* 16, 19796-19811 (2015).
414. Effect of intravitreal ranibizumab injections on aqueous humour concentrations of vascular endothelial growth factor and pigment epithelium-derived factor in patients with myopic choroidal neovascularisation. Costagliola, C; Semeraro, F; dell'Omo, R; Romano, MR; Russo, A; Aceto, F; Mastropasqua, R; Porcellini, A. *British Journal Of Ophthalmology* 99, 1004-1008 (2015).
415. Effect of the plait point position on the shape of spinodal curve determined by wheeler-widom model. Lungu, RP; Sartorio, R; Mangiapia, G. *Romanian Journal Of Physics* 60, 1462-1473 (2015).
416. Effects of monoolein-based cubosome formulations on lipid droplets and mitochondria of HeLa cells. Falchi, AM; Rosa, A; Atzeri, A; Incani, A; Lampis, S; Meli, V; Caltagirone, C; Murgia, S. *Toxicology Research* 4, 1025-1036 (2015).
417. Efficacy and vitreous levels of topical NSAIDs. Semeraro, F; Russo, A; Gambicorti, E; Duse, S; Morescalchi, F; Vezzoli, S; Costagliola, C. *Expert Opinion On Drug Delivery* 12, 1767-1782 (2015).
418. Efficient Expression and Crystallization System of Cancer-Associated Carbonic Anhydrase Isoform IX. Leitans, J; Kazaks, A; Balode, A; Ivanova, J; Zalubovskis, R; Supuran, CT; Tars, K. *Journal Of Medicinal Chemistry* 58, 9004-9009 (2015).
419. Electrochemical deposition of gold on indium zirconate (InZrOx with In/Zr atomic ratio 1.0) for high temperature automobile exhaust gas sensors. Afzal, A; Andersson, M; Di Franco, C; Ditaranto, N; Cioffi, N; Scamarcio, G; Spetz, AL; Torsi, L. *Journal Of Solid State Electrochemistry* 19, 2859-2868 (2015).
420. Electrodeposited semiconductors at room temperature: an X-ray Absorption Spectroscopy study of Cu-, Zn-, S-bearing thin films. Di Benedetto, F; Cinotti, S; D'Acapito, F; Vizza, F; Foresti, ML; Guerri, A; Lavacchi, A; Montegrossi, G; Romanelli, M; Cioffi, N; Innocenti, M. *Electrochimica Acta* 179, 495-503 (2015).

421. Electrospun Scaffolds for Osteoblast Cells: Peptide-Induced Concentration Dependent Improvements of Polycaprolactone. Dettin, M; Zamuner, A; Roso, M; Gloria, A; Iucci, G; Messina, GML; D'Amora, U; Marletta, G; Modesti, M; Castagliuolo, I; Brun, P. *Plos one* 10(9):e0137505 (2015).
422. Electrosynthesis and characterization of ZnO nanoparticles as inorganic component in organic thin-film transistor active layers. Picca, RA; Sportelli, MC; Hotger, D; Manoli, K; Kranz, C; Mizaikoff, B; Torsi, L; Cioffi, N. *Electrochimica Acta* 178, 45-54 (2015).
423. Emerging interface dipole versus screening effect in copolymer/metal nano-layered systems. Torrisi, V; Ruffino, F; Liscio, A; Grimaldi, MG; Marletta, G. *Appl.Surf.Sci*. 359, 637-642 (2015).
424. Energy and water savings by exploiting nano-technological self cleaning textiles. Busi, E; Maranghi, S; Corsi, L: Basosi, R. *In proceedings of International conference on Life Cycle Assessment as reference methodology for assessing supply chains and supporting global sustainability challenges*, 6-8 (2015).
425. Environmental impact assessment of an eco-efficient production for coloured textiles. Parisi, ML; Fatarella, E; Spinelli, D; Pogni, R; Basosi, R. *Journal Of Cleaner Production* 108, 514-524 (2015).
426. Environmental life cycle analysis of non-conventional thin-film photovoltaics: the case of dye-sensitized solar devices. Parisi, ML; Basosi, R. *Energy Security and Development, Springer India*, 195-210 (2015).
427. Enzyme-assisted calcium phosphate biomineralisation on an inert alumina surface. Treccani, L; Aminian, A; Pardun, K; Volkmann, E; Li Destri, G; Marletta, G; Rezwan, K. *Acta Biomat*. 13, 335-343 (2015).
428. EPR and LC-MS studies on the mechanism of industrial dye decolorization by versatile peroxidase from Bjerkandera adusta. Baratto, MC; Juarez-Moreno, K; Pogni, R; Basosi, R; Vazquez-Duhalt, R. *Environmental Science And Pollution Research* 22, 8683-8692 (2015).
429. Eriocitrin and Apigenin as New Carbonic Anhydrase VA Inhibitors from a Virtual Screening of Calabrian Natural Products. Gidaro, MC; Alcaro, F; Carradori, S; Costa, G; Vullo, D; Supuran, CT; Alcaro, S. *Planta Medica* 81, 533-540 (2015).
430. Estimating Forest fAPAR from Multispectral Landsat-8 Data Using the Invertible Forest Reflectance Model INFORM. Yuan, HL; Ma, RH; Atzberger, C; Li, F; Loiselle, SA; Luo, JH. *Remote Sensing* 7, 7425-7446 (2015).
431. Evaluation of carbonic anhydrase IX as a therapeutic target for inhibition of breast cancer invasion and metastasis using a series of in vitro breast cancer models. Ward, C; Meehan, J; Mullen, P; Supuran, C; Dixon, JM; Thomas, JS; Winum, JY; Lambin, P; Dubois, L; Pavathaneni, NK; Jarman, EJ; Renshaw, L; Um, I; Kay, C; Harrison, DJ; Kunkler, IH; Langdon, SP. *Oncotarget* 6, 24856-24870 (2015).
432. Evidence of oleuropein degradation by olive leaf protein extract. De Leonardis, A; Macciola, V; Cuomo, F; Lopez, F. *Food Chemistry* 175, 568-574 (2015).
433. Experiments on and Numerical Modeling of the Capture and Concentration of Transcription-Translation Machinery inside Vesicles. Mavelli, F; Stano, P. *Artificial Life* 21, 445-463 (2015).
434. Exploration of anionic inhibition of the alpha-carbonic anhydrase from Thiomicrospira crunogena XCL-2 gammaproteobacterium: A potential bio-catalytic agent for industrial CO2 removal. Mahon, BP; Bhatt, A; Vullo, D; Supuran, CT; McKenna, R. *Chemical Engineering Science* 138, 575-580 (2015).
435. Exploring carbonic anhydrase inhibition with multimeric coumarins displayed on a fullerene scaffold. Abellan-Flos, M; Tanc, M; Supuran, CT; Vincent, SP. *Organic & Biomolecular Chemistry* 13, 7445-7451 (2015).
436. Exploring new Probenecid-based carbonic anhydrase inhibitors: Synthesis, biological evaluation and docking studies. Mollica, A; Costante, R; Akdemir, A; Carradori, S; Stefanucci, A; Macedonio, G; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 5311-5318 (2015).
437. Exploring QSARs of some benzenesulfonamides incorporating cyanoacrylamide moieties as a carbonic anhydrase inhibitors (specifically against tumor-associated isoforms IX and XII). Alafeefy, AM; Abdel-Aziz, HA; Carta, F; Supuran, CT; Pathak, SK; Prasad, O; Sinha, L. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 519-523 (2015).
438. Extraction and GC-MS analysis of phthalate esters in food matrices: A review. Russo, MV; Avino, P; Perugini, L; Notardonato, I. *RSC Advances* 5, 37023-37043 (2015).
439. Fabrication, Physico-Chemical, and Pharmaceutical Characterization of Budesonide-Loaded Electrospun Fibers for Drug Targeting to the Colon. Bruni, G; Maggi, L; Tammaro, L; Canobbio, A; Di Lorenzo, R; D'Aniello, S; Domenighini, C; Berbenni, V; Milanese, C; Marini, A. *Journal Of Pharmaceutical Sciences* 104, 3798-3803 (2015).
440. Faceted phospholipid vesicles tailored for the delivery of Santolina insularis essential oil to the skin. Castangia, I; Manca, ML; Caddeo, C; Maxia, A; Murgia, S; Pons, R; Demurtas, D; Pando, D; Falconieri, D; Peris, JE; Fadda, AM; Manconi, M. *Colloids And Surfaces B-Biointerfaces* 132, 185-193 (2015).

441. Filling station short-range impact on the surrounding area: A novel methodology for environmental monitoring based on the shadows study. Vitale, S; Zappalà, G; Tuccitto, N. *Environmental Technology and Innovation* 4, 210-217 (2015).
442. Fine tuning of metal-specific activity in the Mn-like group of cambialistic superoxide dismutases. Russo Krauss, I; Merlino, A; Pica, A; Rullo, R; Bertoni, A; Capasso, A; Amato, M; Riccitiello, F; De Vendittis, E; Sica, F. *RSC Advances* 5, 87876-87887 (2015).
443. Fluorescent Silica Nanoparticles with Multivalent Inhibitory Effects towards Carbonic Anhydrases. Touisni, N; Kanfar, N; Ulrich, S; Dumy, P; Supuran, CT; Mehdi, A; Winum, JY. *Chemistry-A European Journal* 21, 10306-10309 (2015).
444. Fluorinated pyrrolidines and piperidines incorporating tertiary benzenesulfonamide moieties are selective carbonic anhydrase II inhibitors. Le Darz, A; Mingot, A; Bouazza, F; Castelli, U; Karam, O; Tanc, M; Supuran, CT; Thibaudeau, S. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 737-745 (2015).
445. Fourteen-Year Record (2000-2013) of the Spatial and Temporal Dynamics of Floating Algae Blooms in Lake Chaohu, Observed from Time Series of MODIS Images. Zhang, YC; Ma, RH; Zhang, M; Duan, HT; Loiselle, S; Xu, JD. *Remote Sensing* 7, 10523-10542 (2015).
446. Fractal Dimension as a New Tool to Analyze Optic Nerve Head Vasculature in Primary Open Angle Glaucoma. Ciancaglini, M; Guerra, G; Agnifili, L; Mastropasqua, R; Fasanella, V; Cinelli, M; Costagliola, C; Ambrosone, L. *In Vivo* 29, 273-279 (2015).
447. Fullerene-based inhibitors of HIV-1 protease. Strom, TA; Durdagi, S; Ersoz, SS; Salmas, RE; Supuran, CT; Barron, AR. *Journal Of Peptide Science* 21, 862-870 (2015).
448. Fusion of raft-like lipid bilayers operated by a membranotropic domain of the HSV-type I glycoprotein gH occurs through a cholesterol-dependent mechanism. Vitiello, G; Falanga, A; Petruk, AA; Merlino, A; Fragneto, G; Paduano, L; Galdiero, S; D'Errico, G. *Soft Matter* 11, 3003-3016 (2015).
449. General Approach to the Immobilization of Glycoenzyme Chains Inside Calcium Alginate Beads for Bioassay. Mallardi, A; Angarano, V; Magliulo, M; Torsi, L; Palazzo, G. *Analytical Chemistry* 87, 11337-11344 (2015).
450. Giant Vesicles as Micro-Sized Enzymatic Reactors: Perspectives and Recent Experimental Advancements. Altamura, E; Stano, P; Walde, P; Mavelli, F. *International Journal Of Unconventional Computing* 11, 5-21 (2015).
451. Glutathione, glutathione disulfide, and S-glutathionylated proteins in cell cultures. Giustarini, D; Galvagni, F; Tesei, A; Farolfi, A; Zanoni, M; Pignatta, S; Milzani, A; Marone, IM; Dalle-Donne, I; Nassini, R; Rossi, R. *Free Radical Biology And Medicine* 89, 972-981 (2015).
452. Gold nanostars co-coated with the Cu(II) complex of a tetraazamacrocyclic ligand. Pallavicini, P; Bernhard, C; Chirico, G; Dacarro, G; Denat, F; Dona, A; Milanese, C; Taglietti, A. *Dalton Transactions* 44, 5652-5661 (2015).
453. Gold nanostars coated with neutral and charged polyethylene glycols: A comparative study of in-vitro biocompatibility and of their interaction with SH-SY5Y neuroblastoma cells. Pallavicini, P; Cabrini, E; Cavallaro, G; Chirico, G; Collini, M; D'Alfonso, L; Dacarro, G; Dona, A; Marchesi, N; Milanese, C; Pascale, A; Sironi, L; Taglietti, A. *Journal Of Inorganic Biochemistry* 151, 123-131 (2015).
454. Graphene and Selected Derivatives as Negative Electrodes in Sodium- and Lithium-Ion Batteries. Pramudita, JC; Pontiroli, D; Magnani, G; Gaboardi, M; Ricco, M; Milanese, C; Brand, HEA; Sharma, N. *Chemelectrochem* 2, 600-610 (2015).
455. Graphene oxide/plasmon nanoparticles bilayers for optimized SERS detection. Banchelli, M; de Angelis, M; Pini, R; Tiribilli, B; Caminati, G; Matteini, P. *Frontiers in Biological Detection: From Nanosensors to Systems VIII, edited by Benjamin L. Miller, Brian T. Cunningham. Proc. of SPIE*, 9725-97250Q (2015).
456. Graphene oxide/silver nanocube composites for SERS detection of biomolecules. Banchelli, M; Caminati, G; Tiribilli, B; Pini, R; Matteini, P. *BioPhotonics* (2015).
457. Highly stable ionic liquid-in-water emulsions as a new class of fluorescent sensors for metal ions: the case study of Fe3+ sensing. Bettoschi, A; Bencini, A; Berti, D; Caltagirone, C; Conti, L; Demurtas, D; Giorgi, C; Isaia, F; Lippolis, V; Mamusa, M; Murgia, S. *Rsc Advances* 5, 37385-37391 (2015).
458. Hit Recycling: Discovery of a Potent Carbonic Anhydrase Inhibitor by in Silico Target Fishing. Mori, M; Cau, Y; Vignaroli, G; Laurenzana, I; Caivano, A; Vullo, D; Supuran, CT; Botta, M. *Acs Chemical Biology* 10, 1964-1969 (2015).
459. Hofmeister effect of anions on calcium translocation by sarcoplasmic reticulum Ca2+-ATPase. Tadini-Buoninsegni, F; Moncelli, MR; Peruzzi, N; Ninham, BW; Dei, LG; Lo Nostro, P. *Scientific Reports* 5 (2015).
460. Hofmeister Phenomena in Bioelectrochemistry: The Supporting Electrolyte Affects the Response of Glucose Electrodes. Carucci, C; Haltenort, P; Salazar, M; Salis, A; Magner, E. *Chemelectrochem* 2, 659-663 (2015).

461. HoLaMa: A Klenow sub-fragment lacking the 3 '-5 ' exonuclease domain. Martina, CE; Lapenta, F; Silva, AM; Hochkoeppler, A. *Archives Of Biochemistry And Biophysics* 575, 46-53 (2015).
462. How hydrophobically modified chitosans are stabilized by biocompatible lipid aggregates. Ruocco, N; Frielinghaus, H; Vitiello, G; D'Errico, G; Leal, LG; Richter, D; Ortona, O; Paduano, L. *Journal Of Colloid And Interface Science* 452, 160-168 (2015).
463. Hybrid TiO2-acetylacetonate amorphous gel-derived material with stably adsorbed superoxide radical active in oxidative degradation of organic pollutants. Sannino, F; Pernice, P; Imparato, C; Aronne, A; D'Errico, G; Minieri, L; Perfetti, M; Pirozzi, D. *Rsc Advances* 5, 93831-93839 (2015).
464. Hydroxylamine-O-sulfonamide is a versatile lead compound for the development of carbonic anhydrase inhibitors. Di Fiore, A; Vergara, A; Caterino, M; Alterio, V; Monti, SM; Ombouma, J; Dumy, P; Vullo, D; Supuran, CT; Winum, JY; De Simone, G. *Chemical Communications* 51, 11519-11522 (2015).
465. Hypoxia induced CA9 targeting via different alternative approches including sulfonamide derivative compounds in human brain cancer in vitro. Said, HM; Soysal, Y; Harmanc, D; Hagemann, C; Carta, F; Katzer, A; Flentje, M; Supuran, CT. *Febs Journal* 282, 252-253 (2015).
466. Impact of the Competitive Adsorption of Ions at Surface Sites on Surface Free Energies and Surface Forces. Parsons, DF; Salis, A . *Journal of Chemical Physics* 142, 134707 (2015).
467. Improvement of the dissolution behavior of gliclazide, a slightly soluble drug using solid dispersions. Maggi, L; Canobbio, A; Bruni, G; Musitelli, G; Conte U. *Journal of Drug Delivery Science and Technology* 26, 17-23 (2015).
468. Improvement of thermal stability and reduction of $LiBH_4$/polymer host interaction of nanoconfined LiBH4 for reversible hydrogen storage. Plerdsranoy, P; Wiset, N; Milanese, C; Laipple, D; Marini, A; Klassen, T; Dornheim, M; Utike, RG. *International Journal Of Hydrogen Energy* 40, 392-402 (2015).
469. In Situ Neutron Powder Diffraction of Li_6C_{60} for Hydrogen Storage. Gaboardi, M; Duyker, S; Milanese, C; Magnani, G; Peterson, VK; Pontiroli, D; Sharma, N; Ricco, M. *Journal Of Physical Chemistry C* 119, 19715-19721 (2015).
470. Influence of hydrothermal synthesis conditions on size, morphology and colloidal properties of hematite nanoparticles. Colombo, C; Palumbo, G; Di Iorio, E; Song, X; Jiang, Z; Liu, Q; Angelico, R. *Nano-Structures & Nano-Objects* 2, 19-27 (2015).
471. Influence of milling parameters on the sorption properties of the LiH-MgB_2 system doped with $TiCl_3$. Busch, N; Jepsen, J; Pistidda, C; Puszkiel, JA; Karimi, F; Milanese, C; Tolkiehn, M; Chaudhary, AL; Klassen, T; Dornheim, M. *Journal Of Alloys And Compounds* 645, S299-S303 (2015).
472. Inhibition of beta-carbonic anhydrases from Brucella suis with C-cinnamoyl glycosides incorporating the phenol moiety. Riafrecha, LE; Vullo, D; Ouahrani-Bettache, S; Kohler, S; Dumy, P; Winum, JY; Supuran, CT; Colinas, PA. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 1017-1020 (2015).
473. Inhibition of carbonic anhydrase isoforms I, II, IX and XII with Schiff's bases incorporating iminoureido moieties. Singasane, N; Kharkar, PS; Ceruso, M; Supuran, CT; Toraskar, MP. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 901-907 (2015).
474. Inhibition of hERG potassium channel by the antiarrhythmic agent mexiletine and its metabolite m-hydroxymexiletine. Gualdani, R; Tadini-Buoninsegni, F; Roselli, M; Defrenza, I; Contino, M; Colabufo, NA; Lentini, G. *Pharmacology Research & Perspectives* 3, e00160 (2015).
475. Inhibition of human carbonic anhydrase isozymes I, II, IX and XII with a new series of sulfonamides incorporating aroylhydrazone-, [1,2,4]triazolo[3,4-b][1,3,4]thiadiazinyl- or 2-(cyanophenylmethylene)-1,3,4-thiadiazol-3(2H)-yl moieties. Alafeefy, AM; Abdel-Aziz, HA; Vullo, D; Al-Tamimi, AMS; Awaad, AS; Mohamed, MA; Capasso, C; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 52-56 (2015).
476. Inhibition of mammalian carbonic anhydrase isoforms I-XIV with a series of phenolic acid esters. Maresca, A; Akyuz, G; Osman, SM; AlOthman, Z; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 7181-7188 (2015).
477. Inhibition studies of bacterial, fungal and protozoan beta-class carbonic anhydrases with Schiff bases incorporating sulfonamide moieties. Ceruso, M; Carta, F; Osman, SM; Alothman, Z; Monti, SM; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 4181-4187 (2015).
478. Inhibition studies of quinazoline-sulfonamide derivatives against the gamma-CA (PgiCA) from the pathogenic bacterium, Porphyromonas gingivalis. Alafeefy, AM; Ceruso, M; Al-Tamimi, AMS; Del Prete, S; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 592-596 (2015).
479. Insights on Molecular Determinants of hERG K+ Channel Inhibition: Design, Synthesis, and Biological Evaluation of Lubeluzole Derivatives. Gualdani, R; Cavalluzzi, MM; Tadini-Buoninsegni, F; Moncelli, MR; Lentini, G. *Biophysical Journal* 108, 582A-582A (2015).

480. Insulin administration: present strategies and future directions for a noninvasive (possibly more physiological) delivery. Matteucci, E; Giampietro, O; Covolan, V; Giustarini, D; Fanti, P; Rossi, R. *Drug Design Development And Therapy* 9, 3109-3118 (2015).
481. Interaction of anticancer Ru(III) complexes with single stranded and duplex DNA model systems. Musumeci, D; Rozza, L; Merlino, A; Paduano, L; Marzo, T; Massai, L; Messori, L; Montesarchio, D. *Dalton Transactions* 44, 13914-13925 (2015).
482. Interaction of carbonic anhydrase isozymes I, II, and IX with some pyridine and phenol hydrazinecarbothioamide derivatives. Isik, S; Vullo, D; Durdagi, S; Ekinci, D; Senturk, M; Cetin, A; Senturk, E; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 5636-5641 (2015).
483. Interaction of the Belousov-Zhabotinsky Reaction with Phospholipid Engineered Membranes. Torbensen, K; Rossi, F; Pantani, OL; Ristori, S; Abou-Hassan, A. *J. Phys. Chem. B* 119, 10224-30 (2015).
484. Investigating nanoparticles properties in plasmonic nanoarchitectures with DNA by Surface Plasmon Resonance imaging. Mariani, S; Scarano, S; Ermini, ML; Bonini, M; Minunni, M. *Chem. Comm.* 51, 6587-6590 (2015).
485. Investigation of arenesulfonyl-2-imidazolidinones as potent carbonic anhydrase inhibitors. Abdel-Aziz, AAM; El-Azab, AS; Ekinci, D; Senturk, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 81-84 (2015).
486. Investigation of Ether-Based Ionic Liquid Electrolytes for Lithium-O2 Batteries. Ferrari, S; Quartarone, E; Tomasi, C; Bini, M; Galinetto, P; Fagnoni, M; Mustarelli, PJ. *Electrochem. Soc.* 162, A3001-A3006 (2015).
487. Investigation on hydration kinetics and structural properties of MgO-based eco-sustainable cements. Ridi, F; Tonelli, M; Fratini, E; Baglioni, P; Borsacchi, S; Martini, F; Calucci, L; Geppi, M. *Proceedings 14th International Congress on the Chemistry of Cement, 13-16 October 2015, Beijing, China* (2015).
488. Ionic Liquids Modify the AOT Interfacial Curvature and Self-Assembly. Murgia, S; Lampis, S; Mamusa, M; Palazzo, G. *Ionic liquid-based surfactant science: formulation, characterization and applications; Paul, B. K., Moulik, S. P., Eds.; John Wiley & Sons Inc.: Hoboken*, 1-22 (2015).
489. Isatin-pyrazole benzenesulfonamide hybrids potently inhibit tumor-associated carbonic anhydrase isoforms IX and XII. Ibrahim, HS; Abou-Seri, SM; Tanc, M; Elaasser, MM; Abdel-Aziz, HA; Supuran, CT. *European Journal Of Medicinal Chemistry* 103, 583-593 (2015).
490. Isolation and characterization of the alkaloid Nitidine responsible for the traditional use of Phyllanthus muellerianus (Kuntze) Excell stem bark against bacterial infections. Cesari, I; Grisoli, P; Paolillo, M; Milanese, C; Massolini, G; Brusotti, G. *Journal Of Pharmaceutical And Biomedical Analysis* 105, 115-120 (2015).
491. Kinetic characterization of 4,4 '-biphenylsulfonamides as selective non-zinc binding MMP inhibitors. Santamaria, S; Nuti, E; Cercignani, G; La Regina, G; Silvestri, R; Supuran, CT; Rossello, A. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 947-954 (2015).
492. Kinetic improvement on the CaH_2-catalyzed $Mg(NH_2)_2$+2LiH system. Torre, F; Valentoni, A; Milanese, C; Pistidda, C; Marini, A; Dornheim, M; Enzo, S; Mulas, G; Garroni, S. *Journal Of Alloys And Compounds* 645, S284-S287 (2015).
493. LCA of Arundo donax L. lignocellulosic feedstock production under Mediterranean conditions. Forte, A; Zucaro, A; Fagnano, M; Bastianoni, S; Basosi, R; Fierro, A. *Biomass & Bioenergy* 73, 32-47 (2015).
494. Life cycle assessment of high-protective clothing for complex emergency operations. Fatarella, E; Parisi, ML; Varheenmaa, M; Talvenmaa, P. *Journal Of The Textile Institute* 106, 1226-1238 (2015).
495. Lipoic-based TRPA1/TRPV1 antagonist to treat orofacial pain. Gualdani, R; Ceruti, S; Magni, G; Merli, D; Di Cesare Mannelli, L; Francesconi, O; Richichi, B; la Marca, G; Ghelardini, C; Moncelli, MR; Nativi, C. *ACS Chemical Neuroscience* 6, 380-385 (2015).
496. Lithium-Air batteries based on carbon nanomaterials. Capsoni, D; Bini, M; Ferrari, S; Mustarelli, P. *in "Carbon Nanomaterials for Advanced Energy Systems", Edited by W.Lu, J-B. Baek, L. Dai, Wiley*, 385-405 (2015).
497. Magnetocubosomes for the delivery and controlled release of therapeutics. Montis, C; Castroflorio, B; Mendozza, M; Salvatore, A; Berti, D; Baglioni, P. *Journal Of Colloid And Interface Science* 449, 317-326 (2015).
498. Mapping Selective Inhibition of the Cancer-Related Carbonic Anhydrase IX Using Structure-Activity Relationships of Glucosyl-Based Sulfamates. Mahon, BP; Lomelino, CL; Ladwig, J; Rankin, GM; Driscoll, JM; Salguero, AL; Pinard, MA; Vullo, D; Supuran, CT; Poulsen, SA; McKenna, R. *Journal Of Medicinal Chemistry* 58, 6630-6638 (2015).
499. Mechanical activation of the solid-phase reaction between bismuth citrate and iron(II) oxalate dihydrate to yield $BiFeO_3$. Berbenni, V; Milanese, C; Bruni, G; Girella, A; Marini, A. *Ceramics International* 41, 7216-7220 (2015).

500. Media effects in modulating the conformational equilibrium of a model compound for Tumor Necrosis factor converting enzyme inhibition. Banchelli, M; Guardiani, C; Sandberg, R; Menichetti, S; Procacci, P; Caminati G. *J.Mol. Struct.* 1091, 65-73 (2015).
501. Missing gold atoms in lysozyme crystals used to grow gold nanoparticles. Merlino, A; Caterino, M; Russo Krauss, I; Vergara, A. *Nature Nanotechnology* 10, 285-285 (2015).
502. Mixed zirconia calcium phosphate coatings for zirconia dental implants: Tailoring coating stability and bioactivity potential. Pardun, K; Treccani, L; Volkmann, E; Streckbein, P; Heiss, C; Li Destri, G; Marletta, G; Rezwan, K. *Mater. Sci. Engin. C* 48, 337-346 (2015).
503. Molecular interactions mediated by nucleo-base functionalized lipids. Cuomo, F; Lopez, F; Angelico, R; Ambrosone, L; De Socio, P; Ceglie, A . *Journal of Surface Science and Technology* 31, 59-68 (2015).
504. Monoolein-based cubosomes affect lipid profile in HeLa cells. Rosa, A; Murgia, S; Putzu, D; Meli, V; Falchi, AM. *Chemistry And Physics Of Lipids* 191, 96-105 (2015).
505. N-Acylsulfonamides strongly inhibit human carbonic anhydrase isoenzymes I and II. Yildirim, A; Atmaca, U; Keskin, A; Topal, M; Celik, M; Gulcin, I; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 2598-2605 (2015).
506. N-glycosyl-N-hydroxysulfamides as potent inhibitors of Brucella suis carbonic anhydrases. Ombouma, J; Vullo, D; Kohler, S; Dumy, P; Supuran, CT; Winum, JY. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 1010-1012 (2015).
507. Nanocomposites composed of HEUR polymer and magnetite iron oxide nanoparticles: Structure and magnetic response of the hydrogel and dried state. Campanella, A; Di, Z; Luchini, A; Paduano, L; Klapper, A; Herlitschke, M; Petracic, O; Appavou, MS; Muller-Buschbaum, P; Frielinghaus, H; Richter, D. *Polymer* 60, 176-185 (2015).
508. Nanomaterials in art conservation. Baglioni, P; Carretti, E; Chelazzi, D. *Nature Nanotechnology* 10, 287-290 (2015).
509. Nanoparticles for controlled release of anti-biofilm agents WO2014130994 (A1): a patent evaluation. Supuran, CT. *Expert Opinion On Therapeutic Patents* 25, 945-948 (2015).
510. Nanotechnologies in the Conservation of Cultural Heritage - A compendium of materials and techniques. Baglioni, P; Chelazzi, D; Giorgi, R. *Springer, Heidelberg* (2015).
511. Natural radioactivity as an easy and quick parameter for describing the dynamic of the Planetary Boundary Layer. Avino, P; Manigrasso, M; Cuomo, F. *Rsc Advances* 5, 57538-57549 (2015).
512. New 4-[(3-cyclohexyl-4-aryl-2,3-dihydro-1,3-thiazol-2-ylidene)amino]benzene-1-sulfonamides, synthesis and inhibitory activity toward carbonic anhydrase I, II, IX, XII. Meleddu, R; Maccioni, E; Distinto, S; Bianco, G; Melis, C; Alcaro, S; Cottiglia, F; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 3281-3284 (2015).
513. New amide derivatives of Probenecid as selective inhibitors of carbonic anhydrase IX and XII: Biological evaluation and molecular modelling studies. Carradori, S; Mollica, A; Ceruso, M; D'Ascenzio, M; De Monte, C; Chimenti, P; Sabia, R; Akdemir, A; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 2975-2981 (2015).
514. New approaches to the synthesis of sildenafil analogues and their enzyme inhibitory activity. Mojzych, M; Karczmarzyk, Z; Wysocki, W; Ceruso, M; Supuran, CT; Krystof, V; Urbanczyk-Lipkowska, Z; Kalicki, P. *Bioorganic & Medicinal Chemistry* 23, 1421-1429 (2015).
515. New natural product carbonic anhydrase inhibitors incorporating phenol moieties. Karioti, A; Ceruso, M; Carta, F; Bilia, AR; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 7219-7225 (2015).
516. New pyrazolo[4,3-e][1,2,4]triazine sulfonamides as carbonic anhydrase inhibitors. Mojzych, M; Ceruso, M; Bielawska, A; Bielawski, K; Fornal, E; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 3674-3680 (2015).
517. New series of sulfonamides containing amino acid moiety act as effective and selective inhibitors of tumor-associated carbonic anhydrase XII. Ceruso, M; Bragagni, M; AlOthman, Z; Osman, SM; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 430-434 (2015).
518. Nitric oxide assisted C60 secondary ion mass spectrometry for molecular depth profiling of polyelectrolyte multilayers. Zappalà, G; Motta, V; Tuccitto, N; Vitale, S; Torrisi, A; Licciardello, A. *Rapid Communications in Mass Spectrometry* 29, 2204-2210 (2015).
519. Nitric Oxide Donors and Selective Carbonic Anhydrase Inhibitors: A Dual Pharmacological Approach for the Treatment of Glaucoma, Cancer and Osteoporosis. Carradori, S; Mollica, A; De Monte, C; Granese, A; Supuran, CT. *Molecules* 20, 5667-5679 (2015).
520. NMR of liquid crystals and micellar solutions. D'Errico, G; Paduano, L. *Nuclear Magnetic Resonance Volume* 44, 456-506 (2015).
521. Non-conventional routes to Silver nanoantimicrobials. Technological issues, Bioactivity, Applications. Pollini, M; Paladini, F; Sannino, A; Picca, RA; Sportelli, MC; Cioffi, N; Nitti, M; Valentini, M. *Chapter n.6 in Nanotechnology in Diagnosis, Treatment and Prophylaxis of Infectious Diseases, K. Kon and M. Rai Eds., Elsevier Publisher*, 87-106 (2015).

522. Nucleation and growth of Au and Au-Pd nanoparticles at the beginning of electrochemical deposition. Fratini, E; Girella, A; Saldan, I; Milanese, C; Dobrovetska, O; Sus, L; Okhremchuk, Y; Kuntyi, O; Reshetnyak, O. *Materials Letters* 161, 263-266 (2015).
523. Nucleolipid-based Ru(III) complexes as new anticancer agents. Capuozzo, A; Piccolo, M; Misso, G; Caraglia, M; D'Errico, G; Montesarchio, D; Paduano, L; Irace, C; Santamaria, R. *Febs Journal* 282, 242-242 (2015).
524. Oligonucleotide biofunctionalization enhances endothelial progenitor cell adhesion on Cobalt-Chromium stents. Barsotti, MC; Al Kayal, T; Tedeschi, L; Dinucci, D; Losi, P; Sbrana, S; Briganti, E; Giorgi, R; Chiellini, F; Di Stefano, R; Soldani, G. *Journal of Biomedical Materials Research: Part A* 103, 3284-3292 (2015).
525. On the formation of dendrimer/nucleolipids surface films for directed self-assembly. Arteta, MY; Berti, D; Montis, C; Campbell, RA; Eriksson, C; Clifton, LA; Skoda, MWA; Soltwedel, O; Koutsioubas, A; Baglioni, P; Nylander, T. *Soft Matter* 11, 1973-1990 (2015).
526. Optical cell communication in fibroblasts. Prasad, A; Rossi, C; Lamponi, S; Bonechi, C; Pospíšil, P. *Physical Biology* peer reviewing (2015).
527. Organogel formulations for the cleaning of easel paintings. Baglioni, P; Bonelli, N; Chelazzi, D; Chevalier, A; Dei, LG; Domingues, J; Fratini, E; Giorgi, R; Martin, M. *Applied Physics A-Materials Science & Processing* 121, 857-868 (2015).
528. Origin and Electronic Features of Reactive Oxygen Species at Hybrid Zirconia-Acetylacetonate Interfaces. Munoz-Garcia, AB; Sannino, F; Vitiello, G; Pirozzi, D; Minieri, L; Aronne, A; Pernice, P; Pavone, M; D'Errico, G. *Acs Applied Materials & Interfaces* 7, 21662-21667 (2015).
529. Out of the active site binding pocket for carbonic anhydrase inhibitors. D'Ambrosio, K; Carradori, S; Monti, SM; Buonanno, M; Secci, D; Vullo, D; Supuran, CT; De Simone, G. *Chemical Communications* 51, 302-305 (2015).
530. Palmitoylethanolamide, a Natural Retinoprotectant: Its Putative Relevance for the Treatment of Glaucoma and Diabetic Retinopathy. Hesselink, JMK; Costagliola, C; Fakhry, J; Kopsky, DJ. *Journal Of Ophthalmology* (2015).
531. Penetration Enhancer-Containing Vesicles: Does the Penetration Enhancer Structure Affect Topical Drug Delivery?. Caddeo, C; Manconi, M; Sinico, C; Valenti, D; Celia, C; Monduzzi, M; Fadda, AM. *Current Drug Targets* 16, 1438-1447 (2015).
532. Peptidomimetics as protein arginine deiminase 4 (PAD4) inhibitors. Trabocchi, A; Pala, N; Krimmelbein, I; Menchi, G; Guarna, A; Sechi, M; Dreker, T; Scozzafava, A; Supuran, CT; Carta, F. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 466-471 (2015).
533. Performance Assessment in Fingerprinting and Multi Component Quantitative NMR Analyses. Gallo, V; Intini, N; Mastrorilli, P; Latronico, M; Scapicchio, P; Triggiani, M; Bevilacqua, V; Fanizzi, P; Acquotti, D; Airoldi, C; Arnesano, F; Assfalg, M; Benevelli, F; Bertelli, D; Cagliani, LR; Casadei, L; Marincola, FC; Colafemmina, G; Consonni, R; Cosentino, C; Davalli, S; De Pascali, SA; D'Aiuto, V; Faccini, A; Gobetto, R; Lamanna, R; Liguori, F; Longobardi, F; Mallamace, D; Mazzei, P; Menegazzo, I; Milone, S; Mucci, A; Napoli, C; Pertinhez, T; Rizzuti, A; Rocchigiani, L; Schievano, E; Sciubba, F; Sobolev, A; Tenon, L; Valerio, M. *Analytical Chemistry* 87, 6709-6717 (2015).
534. Pharmacokinetic and Pharmacodynamic Properties of Anti-VEGF Drugs After Intravitreal Injection. Semeraro, F; Morescalchi, F; Duse, S; Gambicorti, E; Cancarini, A; Costagliola, C. *Current Drug Metabolism* 16, 572-584 (2015).
535. Phase-selective Route to V-O Film Formation: A Systematic MOCVD Study Into the Effects of Deposition Temperature on Structure and Morphology. Spano, SF; Toro, RG; Condorelli, GG; Messina, GML; Marletta, G; Malandrino, G. *Chem. Vap. Deposition* 21, 319-32 (2015).
536. Phosphate Chemical Probes Designed for Location Specific Inhibition of Intracellular Carbonic Anhydrases. Rankin, GM; Vullo, D; Supuran, CT; Poulsen, SA. *Journal Of Medicinal Chemistry* 58, 7580-7590 (2015).
537. Physical routes to primitive cells: An experimental model based on the spontaneous entrapment of enzymes inside Micrometer-Sized liposomes. D'Aguanno E; Altamura E; Mavelli F; Fahr A; Stano P; Luisi PL. *Life* 5, 969-996 (2015).
538. Physico-chemical properties of Gemini micelles studied by X-Ray Scattering and ESR spectroscopy. Falsini, S; Arcangeli, A; Di Cola, E; Spinozzi, F; Ristori, S. *Coll. and Surf. A: Physicochemical and Engineering Aspects* 472, 101-8 (2015).
539. Plasmonic Particles that Hit Hypoxic Cells. Ratto, F; Witort, E; Tatini, F; Centi, S; Lazzeri, L; Carta, F; Lulli, M; Vullo, D; Fusi, F; Supuran, CT; Scozzafava, A; Capaccioli, S; Pini, R. *Advanced Functional Materials* 25, 316-323 (2015).
540. Platinated oligomers of bovine pancreatic ribonuclease: Structure and stability. Picone, D; Donnarumma, F; Ferraro, G; Russo Krauss, I; Fagagnini, A; Gotte, G; Merlino, A. *Journal Of Inorganic Biochemistry* 146, 37-43 (2015).
541. Pluronic/gelatin composites for controlled release of actives. Tatini, D; Tempesti, P; Ridi, F; Fratini, E; Bonini, M; Baglioni, P. *Colloids And Surfaces B-Biointerfaces* 135, 400-407 (2015).

542. Pluronic/gelatin composites for controlled release of actives. Tatini, D; Tempesti, P; Ridi, F; Fratini, E; Bonini, M; Baglioni, P. *Colloids And Surfaces B-Biointerfaces* 135, 400-407 (2015).
543. Poly(amidoamine) dendrimers show carbonic anhydrase inhibitory activity against alpha-, beta-, gamma- and eta-class enzymes. Carta, F; Osman, SM; Vullo, D; AlOthman, Z; Del Prete, S; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 6794-6798 (2015).
544. Poly(amidoamine) Dendrimers with Carbonic Anhydrase Inhibitory Activity and Antiglaucoma Action. Carta, F; Osman, SM; Vullo, D; Gullotto, A; Winum, JY; AlOthman, Z; Masini, E; Supuran, CT. *Journal Of Medicinal Chemistry* 58, 4039-4045 (2015).
545. Polybenzofulvene derivatives bearing dynamic binding sites as potential anticancer drug delivery systems. Cappelli, A; Grisci, G; Paolino, M; Razzano, V; Giuliani, G; Donati, A; Bonechi, C; Mendichi, R; Boccia, AC; Licciardi, M; Scialabba, C; Giammona, G; Vomero, S. *Journal Of Materials Chemistry B* 3, 361-374 (2015).
546. Polymer Films Removed from Solid Surfaces by Nanostructured Fluids: Microscopic Mechanism and Implications for the Conservation of Cultural Heritage. Raudino, M; Selvolini, G; Montis, C; Baglioni, M; Bonini, M; Berti, D; Baglioni, P. *Acs Applied Materials & Interfaces* 7, 6244-6253 (2015).
547. Printable Bioelectronics To Investigate Functional Biological Interfaces. Manoli, K; Magliulo, M; Mulla, MY; Singh, M; Sabbatini, L; Palazzo, G; Torsi, L. *Angewandte Chemie-International Edition* 54, 12562-12576 (2015).
548. Probing the 'bipolar' nature of the carbonic anhydrase active site: Aromatic sulfonamides containing 1,3-oxazol-5-yl moiety as picomolar inhibitors of cytosolic CA I and CA II isoforms. Krasavin, M; Korsakov, M; Dorogov, M; Tuccinardi, T; Dedeoglu, N; Supuran, CT. *European Journal Of Medicinal Chemistry* 101, 334-347 (2015).
549. Production of an enzymatic protein hydrolyzate from defatted sunflower seed meal for potential application as a plant biostimulant. Ugolini, L; Cinti, S; Righetti, L; Stefan, A; Matteo, R; D'Avino, L; Lazzeri, L. *Industrial Crops And Products* 75, 15-23 (2015).
550. Production of sulfonated polyetheretherketone/polypropylene fibers for photoactive textiles. Myllari, V; Fatarella, E; Ruzzante, M; Pogni, R; Baratto, MC; Skrifvars, M; Syrjala, S; Jarvela, P. *Journal Of Applied Polymer Science* 132 (2015).
551. Programmable 3D silk bone marrow niche for platelet generation ex vivo and modeling of megakaryopoiesis pathologies. Di Buduo, CA; Wray, LS; Tozzi, L; Malara, A; Chen, Y; Ghezzi, CE; Smoot, D; Sfara, C; Antonelli, A; Spedden, E; Bruni, G; Staii, C; De Marco, L; Magnani, M; Kaplan, DL; Balduini, A. *Blood* 125, 2254-2264 (2015).
552. Protonography, a new technique for the analysis of carbonic anhydrase activity. De Luca, V; Del Prete, S; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 277-282 (2015).
553. Protonography, a powerful tool for analyzing the activity and the oligomeric state of the gamma-carbonic anhydrase identified in the genome of Porphyromonas gingivalis. Del Prete, S; De Luca, V; Iandolo, E; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry* 23, 3747-3750 (2015).
554. Protonography, a technique applicable for the analysis of eta-carbonic anhydrase activity. Del Prete, S; De Luca, V; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 920-924 (2015).
555. Quantification of phytoplankton bloom dynamics by citizen scientists in urban and peri-urban environments. Castilla, EP; Cunha, DGF; Lee, FWF; Loiselle, S; Ho, KC; Hall, C. *Environmental monitoring and assessment* 187, 1-11 (2015).
556. Reaction kinetics and targeting to cellular glutathione S-transferase of the glutathione peroxidase mimetic PhSeZnCl and its D,L-polylactide microparticle formulation. Bartolini, D; Piroddi, M; Tidei, C; Giovagnoli, S; Pietrella, D; Manevich, Y; Tew, KD; Giustarini, D; Rossi, R; Townsend, DM; Santi, C; Galli, F. *Free Radical Biology And Medicine* 78, 56-65 (2015).
557. Recent advances in the discovery of zinc-binding motifs for the development of carbonic anhydrase inhibitors. Winum, JY; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 321-324 (2015).
558. Recent Biophysical Issues About the Preparation of Solute-Filled Lipid Vesicles. Stano, P; de Souza, TP; Carrara, P; Altamura, E; D'Aguanno, E; Caputo, M; Luisi, PL; Mavelli, F. *Mechanics Of Advanced Materials And Structures* 22, 748-759 (2015).
559. Recent trends in the electrochemical synthesis of zinc oxide nano-colloids. Sportelli, MC; Scarabino, S; Picca, RA; Cioffi, N. *book chapter, "CRC Concise Encyclopedia of Nanotechnology, 1st Edition, B. I. Kharisov Ed. ISBN: 9781466580343* (2015).
560. Rechargeable lithium batteries: key scientific and technological challenges. Bini, M; Capsoni, D; Ferrari, S; Quartarone, E; Mustarelli, P. *in "Rechargeable Lithium Batteries. From Fundamentals to Applications", Edited by A.A. Franco, Woodhead Publishing, Elsevier*, 1-17 (2015).
561. Redox-Active Sites in Auricularia auricula-judae Dye-Decolorizing Peroxidase and Several Directed Variants: A Multifrequency EPR Study. Baratto, MC; Sinicropi, A; Linde, D; Saez-Jimenez, V;

Sorace, L; Ruiz-Duenas, FJ; Martinez, AT; Basosi, R; Pogni, R. *Journal Of Physical Chemistry B* 119, 13583-13592 (2015).
562. Release of small hydrophilic molecules from polyelectrolyte capsules: Effect of the wall thickness. Cuomo, F; Lopez, F; Piludu, M; Miguel, MG; Lindman, B; Ceglie, A. *Journal Of Colloid And Interface Science* 447, 211-216 (2015).
563. Remote sensing of particulate organic carbon dynamics in a eutrophic lake (Taihu Lake, China). Jiang, GJ; Ma, RH; Loiselle, SA; Duan, HT; Su, W; Cai, WX; Huang, CG; Yang, J; Yu, W. *Science Of The Total Environment* 532, 245-254 (2015).
564. Restoration of foveal thickness and architecture after macula-off retinal detachment repair. Dell'Omo, R; Filippelli, M; Giorgio, D; Di Iorio, R; dell'Omo, E; Costagliola, C. *Investigative Ophthalmology & Visual Science* 56, 1040-1050 (2015).
565. Saccharin: A lead compound for structure-based drug design of carbonic anhydrase IX inhibitors. Mahon, BP; Hendon, AM; Driscoll, JM; Rankin, GM; Poulsen, SA; Supuran, CT; McKenna, R. *Bioorganic & Medicinal Chemistry* 23, 849-854 (2015).
566. Scanning Electrochemical Microscopy of Belousov-Zhabotinsky reaction: how confined oscillations reveal short lived radicals and auto-catalytic species. Stockmann, TJ; Noel, JM; Ristori, S; Combellas, C; Abou-Hassan, A; Rossi, F; Kanoufi, F. *Anal. Chem.* 87, 9621-30 (2015).
567. Self-Powered Microneedle-Based Biosensors for Pain-Free High-Accuracy Measurement of Glycaemia in Interstitial Fluid. Strambini, LM; Longo, A; Scarano, S; Prescimone, T; Palchetti, I; Minunni, M; Giannessi, D; Barillaro, G. *Biosens. Bioelectron.* 66, 162-168 (2015).
568. Shape-control by microwave-assisted hydrothermal method for the synthesis of magnetite nanoparticles using organic additives. Rizzuti, A; Dassisti, M; Mastrorilli, P; Sportelli, MC; Cioffi, N; Picca, RA; Agostinelli, E; Varvaro, G; Caliandro, R. *Journal Of Nanoparticle Research* 17 (2015).
569. Silane-coated magnetic nanoparticles with surface thiol functions for conjugation with gold nanostars. Pallavicini, P; Cabrini, E; Casu, A; Dacarro, G; Diaz-Fernandez, YA; Falqui, A; Milanese, C; Vita, F. *Dalton Transactions* 44, 21088-21098 (2015).
570. Silver Enhancement for Transmission Electron Microscopy Imaging of Antibody Fragment-Gold Nanoparticles Conjugates Immobilized on Ordered Mesoporous Silica. Piludu, M; Medda, L; Cugia, F; Monduzzi, M; Salis, A. *Langmuir* 31, 9458-9463 (2015).
571. Simultaneous ternary extension of DNA catalyzed by a trimeric replicase assembled in vivo. Silva, AM; Lapenta, F; Stefan, A; Dal Piaz, F; Ceccarelli, A; Perrone, A; Hochkoeppler, A. *Biochemical And Biophysical Research Communications* 462, 14-20 (2015).
572. Single-step Label-free Hepatitis B virus Detection by Piezoelectric Biosensor. Giamblanco, N; Conoci, S; Russo, D; Marletta, G. *RSC Advances* 5, 38152-38158 (2015).
573. Sn-deficiency in the electrodeposited ternary CuxSnySz thin films by ECALE. Caporali, S; Tolstogouzov, A; Teodoro, OMND; Innocenti, M; Di Benedetto, F; Cinotti, S; Picca, RA; Sportelli, MC; Cioffi, N. *Solar Energy Materials And Solar Cells* 138, 9-16 (2015).
574. Solid-state of captopril and metoprolol tartrate binary system. Marinescu, DC; Pincu, E; Oancea, P; Bruni, G; Marini, A; Meltzer, V. *Journal of Thermal Analysis and Calorimetry* 120, 829-837 (2015).
575. Solvatochromic fluorescent BODIPY derivative as imaging agent in camptothecin loaded hexosomes for possible theranostic applications. Caltagirone, C; Arca, M; Falchi, AM; Lippolis, V; Meli, V; Monduzzi, M; Nylander, T; Rosa, A; Schmidt, J; Talmon, Y; Murgia, S. *Rsc Advances* 5, 23443-23449 (2015).
576. Sources of protons involved in horizontal cell to cone feedback. Warren, T; Supuran, C; Thoreson, WB. *Investigative Ophthalmology & Visual Science* 56 (2015).
577. Specific anion effects in Artemia salina. Lo Nostro, P; Ninham, BW; Carretti, E; Dei, LG; Baglioni, P. *Chemosphere* 135, 335-340 (2015).
578. Spectroscopic and computational characterization of laccases and their substrate radical intermediates. Pogni, R; Baratto, MC; Sinicropi, A; Basosi, R. *Cellular And Molecular Life Sciences* 72, 885-896 (2015).
579. Spontaneous aggregation of humic acid observed with AFM at different pH. Colombo, C; Palumbo, G; Angelico, R; Cho, HG; Francioso, O; Ertani, A; Nardi, S. *Chemosphere* 138, 821-828 (2015).
580. SPR-based affinity biosensors as innovative analytical devices. Scarano, S; Mariani, S; Minunni, M. *Issue of the IEEE/OSA Journal of Lightwave Technology on Biomedical Applications of Lightwave Technologies, Guest Editors X. Wang, Br. Cunningham, A. Cusano, D. Sampson, J. Lightwave Tech.* 33, 3374-3384 (2015).
581. Stability evaluation of ivermectin loaded biodegradable microspheres. Dorati, R; Genta I; Colzani, B; Modena T; Bruni, G; Tripodo G; Conti, B. *AAPS PharmSciTech* 16, 1129-1139 (2015).
582. Structural and kinetic investigation of the hydride composite $Ca(BH_4)_2$ + MgH_2 system doped with NbF5 for solid-state hydrogen storage. Karimi, F; Pranzas, PK; Pistidda, C; Puszkiel, JA; Milanese, C; Vainio, U; Paskevicius, M; Emmler, T; Santoru, A; Utke, R; Tolkiehn, M; Minella, CB;

Chaudhary, AL; Boerries, S; Buckley, CE; Enzo, S; Schreyer, A; Klassen, T; Dornheim, M. *Physical Chemistry Chemical Physics* 17, 27328-27342 (2015).

583. Structural Basis for the Inhibition of Helicobacter pylori alpha-Carbonic Anhydrase by Sulfonamides. Modakh, JK; Liu, YC; Machuca, MA; Supuran, CT; Roujeinikova, A. *Plos One* 10, (2015).
584. Structure and inhibition studies of a type II beta-carbonic anhydrase psCA3 from Pseudomonas aeruginosa. Pinard, MA; Lotlikar, SR; Boone, CD; Vullo, D; Supuran, CT; Patrauchan, MA; McKenna, R. *Bioorganic & Medicinal Chemistry* 23, 4831-4838 (2015).
585. Structure of Escherichia coli dGTP Triphosphohydrolase a hexameric enzyme with dna effector molecules. Singh, D; Gawel, D; Itsko, M; Hochkoeppler, A; Krahn, JM; London, RE; Schaaper, RM. *Journal Of Biological Chemistry* 290, 10418-10429 (2015).
586. Sulfonamide bearing pyrazolylpyrazolines as potent inhibitors of carbonic anhydrase isoforms I, II, IX and XII. Khloya, P; Ceruso, M; Ram, S; Supuran, CT; Sharma, PK. *Bioorganic & Medicinal Chemistry Letters* 25, 3208-3212 (2015).
587. Sulfonamide inhibition studies of the eta-class carbonic anhydrase from the malaria pathogen Plasmodium falciparum. Vullo, D; Del Prete, S; Fisher, GM; Andrews, KT; Poulsen, SA; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 526-531 (2015).
588. Sulfonamide inhibition studies of the gamma-carbonic anhydrase from the Antarctic bacterium Pseudoalteromonas haloplanktis. Vullo, D; De Luca, V; Del Prete, S; Carginale, V; Scozzafava, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 3550-3555 (2015).
589. Sulfonamide inhibition studies of the gamma-carbonic anhydrase from the Antarctic cyanobacterium Nostoc commune. Vullo, D; De Luca, V; Del Prete, S; Carginale, V; Scozzafava, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 1728-1734 (2015).
590. Sulfonamide inhibition study of the beta-class carbonic anhydrase from the caries producing pathogen Streptococcus mutans. Dedeoglu, N; DeLuca, V; Isik, S; Yildirim, H; Kockar, F; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 2291-2297 (2015).
591. Sulfonated Polyetheretherketone/Polypropylene Polymer Blends for the Production of Photoactive Materials. Fatarella, E; Myllari, V; Ruzzante, M; Pogni, R; Baratto, MC; Skrifvars, M; Syrjala, S; Jarvela, P. *Journal Of Applied Polymer Science* 132 (2015).
592. Surface Charge and Coating of CoFe2O4 Nanoparticles: Evidence of Preserved Magnetic and Electronic Properties. Nappini, S; Magnano, E; Bondino, F; Pis, I; Barla, A; Fantechi, E; Pineider, F; Sangregorio, C; Vaccari, L; Venturelli, L; Baglioni, P. *Journal Of Physical Chemistry C* 119, 25529-25541 (2015).
593. Surface chemical and biological characterization of flax fabrics modified with silver nanoparticles for biomedical applications. Paladini, F; Picca, RA; Sportelli, MC; Cioffi, N; Sannino, A; Pollini, M. *Materials Science & Engineering C-Materials For Biological Applications* 52, 1-10 (2015).
594. Sustainable binder from high amount of gibbsite associated with kaolinitic clay. Njiomou Djangang, C; Kamseu, E; Tchamo Leussa, CC; Capsoni, D; Elimbi, A; Njopwouo, D. *Ann. Chim. Sci. Mat.* 39, 75-91 (2015).
595. Sustainable Process for Production of Azelaic Acid Through Oxidative Cleavage of Oleic Acid. Benessere, V; Cucciolito, ME; De Santis, A; Di Serio, M; Esposito, R; Ruffo, F; Turco, R. *JAOCS* 92, 1701-1707 (2015).
596. Synthesis and biological activity of novel thiourea derivatives as carbonic anhydrase inhibitors. Korkmaz, N; Obaidi, OA; Senturk, M; Astley, D; Ekinci, D; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 75-80 (2015).
597. Synthesis and carbonic anhydrase I, II, IX and XII inhibitory activity of sulfamates incorporating piperazinyl-ureido moieties. Congiu, C; Onnis, V; Deplano, A; Balboni, G; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 5619-5625 (2015).
598. Synthesis and Carbonic Anhydrase Isoenzymes I, II, IX, and XII Inhibitory Effects of Dimethoxybromophenol Derivatives Incorporating Cyclopropane Moieties. Boztas, M; Cetinkaya, Y; Topal, M; Gulcin, I; Menzek, A; Sahin, E; Tanc, M; Supuran, CT. *Journal Of Medicinal Chemistry* 58, 640-650 (2015).
599. Synthesis of 3,4-dihydroxypyrrolidine-2,5-dione and 3,5-dihydroxybenzoic acid derivatives and evaluation of the carbonic anhydrase I and II inhibition. Arslan, M; Senturk, M; Fidan, I; Talaz, O; Ekinci, D; Cosgun, S; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 896-900 (2015).
600. Synthesis of 6-aryl-substituted sulfocoumarins and investigation of their carbonic anhydrase inhibitory action. Grandane, A; Tanc, M; Zalubovskis, R; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 1430-1436 (2015).
601. Synthesis of a new series of dithiocarbamates with effective human carbonic anhydrase inhibitory activity and antiglaucoma action. Bozdag, M; Carta, F; Vullo, D; Akdemir, A; Isik, S; Lanzi, C; Scozzafava, A; Masini, E; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 2368-2376 (2015).

602. Synthesis of a novel affinity gel for the purification of carbonic anhydrases. Bozdag, M; Isik, S; Beyaztas, S; Arslan, O; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 240-244 (2015).
603. Synthesis of calcium metastannate ($CaSnO_3$) by solid state reactions in mechanically activated mixtures calcium citrate tetra hydrate [$Ca_3(C_6H_5O_7)_2 \cdot 4H_2O$] - tin(II) oxalate ($SnC_2O_4$). Berbenni, V; Milanese, C; Bruni, G; Girella, A; Marini, A. *Thermochimica Acta* 608, 59-64 (2015).
604. Synthesis of Enantiomeric Aminoalkylcarbamoylphosphonates and Their Evaluation as Dual-Action Anticancer MMP and Carbonic Anhydrase Inhibitors. Veerendhar, A; Cohen, S; Frant, J; Supuran, CT; Reich, R; Breuer, E. *Heteroatom Chemistry* 26, 257-269 (2015).
605. Synthesis of novel acridine bis-sulfonamides with effective inhibitory activity against the carbonic anhydrase isoforms I, II, IX and XII. Esirden, I; Ulus, R; Aday, B; Tanc, M; Supuran, CT; Kaya, M. *Bioorganic & Medicinal Chemistry* 23, 6573-6580 (2015).
606. Synthesis of pro-apoptotic indapamide derivatives as anticancer agents. Yilmaz, O; Turan, SO; Akbuga, J; Tiber, PM; Orun, O; Supuran, CT; Kucukguzel, SG. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 967-980 (2015).
607. Synthesis of Schiff base derivatives of 4-(2-aminoethyl)-benzenesulfonamide with inhibitory activity against carbonic anhydrase isoforms I, II, IX and XII. Durgun, M; Turkmen, H; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 2377-2381 (2015).
608. Synthesis of sulfonamide conjugates of Cu(II), Ga(III), In(III), Re(V) and Zn(II) complexes: carbonic anhydrase inhibition studies and cellular imaging investigations. Dilworth, JR; Pascu, SI; Waghorn, PA; Vullo, D; Bayly, SR; Christlieb, M; Suna, X; Supuranc, CT. *Dalton Transactions* 44, 4859-4873 (2015).
609. Synthesis of sulfonamides incorporating piperazinyl-ureido moieties and their carbonic anhydrase I, II, IX and XII inhibitory activity. Congiu, C; Onnis, V; Deplano, A; Balboni, G; Dedeoglu, N; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 3850-3853 (2015).
610. Synthesis, carbonic anhydrase inhibition and cytotoxic activity of novel chromone-based sulfonamide derivatives. Awadallah, FM; El-Waei, TA; Hanna, MM; Abbas, SE; Ceruso, M; Oz, BE; Guler, OO; Supuran, CT. *European Journal Of Medicinal Chemistry* 96, 425-435 (2015).
611. Tailoring Functional Interlayers in Organic Field-Effect Transistor Biosensors. Magliulo, M; Manoli, K; Macchia, E; Palazzo, G; Torsi, L. *Advanced Materials* 27, 7528-7551 (2015).
612. Targeting divalent metal cations with Re(I) tetrazolato complexes. Fiorini, V; Ranieri, AM; Muzzioli, S; Magee, KDM; Zacchini, S; Akabar, N; Stefan, A; Ogden, MI; Massi, M; Stagni, S. *Dalton Transactions* 44, 20597-20608 (2015).
613. Targeting tumour hypoxia to prevent cancer metastasis. From biology, biosensing and technology to drug development: the METOXIA consortium. Pettersen, EO; Ebbesen, P; Gieling, RG; Williams, KJ; Dubois, L; Lambin, P; Ward, C; Meehan, J; Kunkler, IH; Langdon, SP; Ree, AH; Flatmark, K; Lyng, H; Calzada, MJ; del Peso, L; Landazuri, MO; Gorlach, A; Flamm, H; Kieninger, J; Urban, G; Weltin, A; Singleton, DC; Haider, S; Buffa, FM; Harris, AL; Scozzafava, A; Supuran, CT; Moser, I; Jobst, G; Busk, M; Toustrup, K; Overgaard, J; Alsner, J; Pouyssegur, J; Chiche, J; Mazure, N; Marchiq, I; Parks, S; Ahmed, A; Ashcroft, M; Pastorekova, S; Cao, Y; Rouschop, KM; Wouters, BG; Koritzinsky, M; Mujcic, H; Cojocari, D. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 689-721 (2015).
614. The 2015 Countershock and the Prospects for a Low-carbon Energy Transition. Basosi, D; Basosi, R. *Iaee Energy Forum* Third Quarter, 37-40 (2015).
615. The beta-carbonic anhydrase from the malaria mosquito Anopheles gambiae is highly inhibited by sulfonamides. Syrjanen, L; Kuuslahti, M; Tolvanen, M; Vullo, D; Parkkila, S; Supuran, CT. *Bioorganic & Medicinal Chemistry* 23, 2303-2309 (2015).
616. The effect of charge on the release kinetics from polysaccharide-nanoclay composites. Del Buffa, S; Grifoni, E; Ridi, F; Baglioni, P. *Journal Of Nanoparticle Research* 17 (2015).
617. The eta-class carbonic anhydrases as drug targets for antimalarial agents. Supuran, CT; Capasso, C. *Expert Opinion On Therapeutic Targets* 19, 551-563 (2015).
618. The Glycan Role in the Glycopeptide Immunogenicity Revealed by Atomistic Simulations and Spectroscopic Experiments on the Multiple Sclerosis Biomarker CSF114(Glc). Bruno, A; Scrima, M; Novellino, E; D'Errico, G; D'Ursi, AM; Limongelli, V. *Scientific Reports* 5 (2015).
619. The impact of hydroquinone on acetylcholine esterase and certain human carbonic anhydrase isoenzymes (hCA I, II, IX, and XII). Scozzafava, A; Kalin, P; Supuran, CT; Gulcin, I; Alwasel, SH. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 30, 941-946 (2015).
620. The impact of the competitive adsorption of ions at surface sites on surface free energies and surface forces. Parsons, DF; Salis, A. *Journal Of Chemical Physics* 142, - (2015).
621. The molecular motion of bovine serum albumin under physiological conditions is ion specific. Medda, L; Monduzzi, M; Salis, A. *Chemical Communications* 51, 6663-6666 (2015).
622. The Multifaceted Benefits of Protein Co-expression in Escherichia coli. Stefan, A; Ceccarelli, A; Conte, E; Silva, AM; Hochkoeppler, A. *Jove-Journal Of Visualized Experiments* (2015).

623. The Phospholipidomic Signatures of Human Blood Microparticles, Platelets and Platelet-Derived Microparticles: a Comparative HILIC-ESI-MS Investigation. Losito, I; Conte, E; Cataldi, T; Cioffi, N; Megli, F; Palmisano, F. *Lipids* 50, 71-84 (2015).
624. The Solvation of Anions in Propylene Carbonate. Peruzzi, N; Lo Nostro, P; Ninham, BW; Baglioni, P. *Journal Of Solution Chemistry* 44, 1224-1239 (2015).
625. The use of CA-IX as a diagnostic method for oral leukoplakia. Perez-Sayans, M; Suarez-Penaranda, JM; Torres-Lopez, M; Supuran, CT; Gandara-Vila, P; Gayoso-Diz, P; Barros-Angueira, F; Gallas-Torreira, M; Garcia-Garcia, A. *Biotechnic & Histochemistry* 90, 124-131 (2015).
626. The use of the wheeler - widom model to compute the spinodal curve of the system water-1-hexanol-1-propanol. Sartorio, R; Mangiapia, G. *Romanian Reports In Physics* 67, 915-932 (2015).
627. The zinc coordination pattern in the eta-carbonic anhydrase from Plasmodium falciparum is different from all other carbonic anhydrase genetic families. De Simone, G; Di Fiore, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 25, 1385-1389 (2015).
628. Thermal and Chemical Stability of Thiol Bonding on Gold Nanostars. Borzenkov, M; Chirico, G; D'Alfonso, L; Sironi, L; Collini, M; Cahrini, E; Dacarro, G; Milanese, C; Pallavicini, P; Taglietti, A; Bernhard, C; Denat, F. *Langmuir* 31, 8081-8091 (2015).
629. Thiazolo[5,4-d]thiazole-based organic sensitizers with strong visible light absorption for transparent, efficient and stable dye-sensitized solar cells. Dessi, A; Calamante, M; Mordini, A; Peruzzini, M; Sinicropi, A; Basosi, R; de Biani, FF; Taddei, M; Colonna, D; di Carlo, A; Reginato, G; Zani, L. *Rsc Advances* 5, 32657-32668 (2015).
630. Titania as a driving agent for DHICA polymerization: a novel strategy for the design of bioinspired antimicrobial nanomaterials. Vitiello, G; Pezzella, A; Zanfardino, A; Varcamonti, M; Silvestri, B; Costantini, A; Branda, F; Luciani, G. *Journal Of Materials Chemistry B* 3, 2808-2815 (2015).
631. Towards a controlled fabrication of graphene oxide/silver nanocubes bilayer assemblies for optimized SERS detection. Banchelli, M; Tiribilli, B; Pini, R; Caminati, G; Matteini, P. *ChemPlusChem* (2015).
632. Translational and rotational dynamics of water contained in aged Portland cement pastes studied by quasi-elastic neutron scattering. Li, H; Zhang, LL; Yi, Z; Fratini, E; Baglioni, P; Chen, SH. *Journal Of Colloid And Interface Science* 452, 2-7 (2015).
633. Treatment of exudative age-related macular degeneration with ranibizumab combined with ketorolac eyedrops or photodynamic therapy. Semeraro, F; Russo, A; Delcassi, L; Romano, MR; Rinaldi, M; Chiosi, F; Costagliola, C. *Retina-The Journal Of Retinal And Vitreous Diseases* 35, 1547-1554 (2015).
634. Trimeric Radiofluorinated Sulfonamide Derivatives to Achieve In Vivo Selectivity for Carbonic Anhydrase IX-Targeted PET Imaging. Lau, J; Liu, ZB; Lin, KS; Pan, JH; Zhang, ZX; Vullo, D; Supuran, CT; Perrin, DM; Benard, F. *Journal Of Nuclear Medicine* 56, 1434-1440 (2015).
635. Two New Dyes with Carboxypyridinium Regioisomers as Anchoring Groups for Dye-Sensitized Solar Cells. Franchi, D; Calamante, M; Reginato, G; Zani, L; Peruzzini, M; Taddei, M; de Biani, FF; Basosi, R; Sinicropi, A; Colonna, D; Di Carlo, A; Mordini, A. *Synlett* 26, 2389-2394 (2015).
636. Urea vs. carbamate groups: a comparative study in a chiral C-2 symmetric organogelator. Lascialfari, L; Pescitelli, G; Brandi, A; Mannini, M; Berti, D; Cicchi, S. *Soft Matter* 11, 8333-8341 (2015).
637. Vasorelaxation induced by dodoneine is mediated by calcium channels blockade and carbonic anhydrase inhibition on vascular smooth muscle cells. Carre, G; Ouedraogo, M; Magaud, C; Carreyre, H; Becq, F; Bois, P; Supuran, CT; Thibaudeau, S; Vandebrouck, C; Bescond, J. *Journal Of Ethnopharmacology* 169, 8-17 (2015).
638. Visible Light Caffeic Acid Degradation by Carbon-Doped Titanium Dioxide. Venditti, F; Cuomo, F; Ceglie, A; Avino, P; Russo, MV; Lopez, F. *Langmuir* 31, 3627-3634 (2015).
639. X-ray crystallographic and kinetic investigations of 6-sulfamoyl-saccharin as a carbonic anhydrase inhibitor. Alterio, V; Tanc, M; Ivanova, J; Zalubovskis, R; Vozny, I; Monti, SM; Di Fiore, A; De Simone, G; Supuran, CT. *Organic & Biomolecular Chemistry* 13, 4064-4069 (2015).
640. X-ray crystallography-promoted drug design of carbonic anhydrase inhibitors. Ivanova, J; Leitans, J; Tanc, M; Kazaks, A; Zalubovskis, R; Supuran, CT; Tars, K. *Chemical Communications* 51, 7108-7111 (2015).
641. 1:1 and 1:2 Inclusion Complexes of Di-tert-butyl l-tartrate with alpha-Cyclodextrin: A Diffusion Study. Mangiapia, G; Sartorio, R. *Journal Of Solution Chemistry* 43, 186-205 (2014).
642. $2LiBH_4$-MgH_2-$0.13TiCl_4$ confined in nanoporous structure of carbon aerogel scaffold for reversible hydrogen storage. Gosalawit-Utke, R; Milanese, C; Javadian, P; Girella, A; Laipple, D; Puszkiel, J; Cattaneo, AS; Ferrara, C; Wittayakhun, J; Skibsted, J; Jensen, TR; Marini, A; Klassen, T; Dornheim, M. *Journal Of Alloys And Compounds* 599, 78-86 (2014).
643. 3D-QSAR CoMFA studies on sulfonamide inhibitors of the Rv3588c beta-carbonic anhydrase from Mycobacterium tuberculosis and design of not yet synthesized new molecules. Singh, S; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 449-455 (2014).

644. 4-Functionalized 1,3-diarylpyrazoles bearing 6-aminosulfonylbenzothiazole moiety as potent inhibitors of carbonic anhydrase isoforms hCA I, II, IX and XII. SitaRam; Ceruso, M; Khloya, P; Supuran, CT; Sharma, PK. *Bioorganic & Medicinal Chemistry* 22, 6945-6952 (2014).
645. 4-Functionalized 1,3-diarylpyrazoles bearing benzenesulfonamide moiety as selective potent inhibitors of the tumor associated carbonic anhydrase isoforms IX and XII. Khloya, P; Celik, G; SitaRam; Vullo, D; Supuran, CT; Sharma, PK. *European Journal Of Medicinal Chemistry* 76, 284-290 (2014).
646. 6-Triazolyl-substituted sulfocoumarins are potent, selective inhibitors of the tumor-associated carbonic anhydrases IX and XII. Grandane, A; Tanc, M; Zalubovskis, R; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 1256-1260 (2014).
647. A Class of 4-Sulfamoylphenyl-omega-aminoalkyl Ethers with Effective Carbonic Anhydrase Inhibitory Action and Antiglaucoma Effects. Bozdag, M; Pinard, M; Carta, F; Masini, E; Scozzafava, A; McKenna, R; Supuran, CT. *Journal Of Medicinal Chemistry* 57, 9673-9686 (2014).
648. A comparative study of chromatographic matrices for affinity chromatography of the diphtheria toxin variant Cross-Reacting Material 197. Stefan, A; Boiani, M; Longanesi, L; Hochkoeppler, A. *New Biotechnology* 31, S119-S119 (2014).
649. A comparison of carboxypyridine isomers as sensitizers for dye-sensitized solar cells: assessment of device efficiency and stability. Franchi, D; Calamante, M; Reginato, G; Zani, L; Peruzzini, M; Taddei, M; de Biani, FF; Basosi, R; Sinicropi, A; Colonna, D; Di Carlo, A; Mordini, A. *Tetrahedron* 70, 6285-6295 (2014).
650. A functionalized, ethynyl-decorated, tetracobalt(III) cubane molecular catalyst for photoinduced water oxidation. La Ganga, G; Nardo, VM; Cordaro, M; Natali, M; Vitale, S; Licciardello, A; Nastasi, F; Campagna, S. *Dalton Transactions* 43, 14926-14930 (2014).
651. A Novel Algorithm to Estimate Algal Bloom Coverage to Subpixel Resolution in Lake Taihu. Zhang, YC; Ma, RH; Duan, HT; Loiselle, SA; Xu, JD; Ma, MX. *Ieee Journal Of Selected Topics In Applied Earth Observations And Remote Sensing* 7, 3060-3068 (2014).
652. A pheromone analogue affects the evaporation rate of (+)- disparlure in Lymantria dispar(+). Sollai, G; Murgia, S; Secci, F; Frongia, A; Cerboneschi, A; Masala, C; Liscia, A; Crnjar, R; Solari, P. *Pest Management Science* 70, 674-681 (2014).
653. A regular thymine tetrad and a peculiar supramolecular assembly in the first crystal structure of an all-LNA G-quadruplex. Russo Krauss, I; Parkinson, GN; Merlino, A; Mattia, CA; Randazzo, A; Novellino, E; Mazzarella, L; Sica, F. *Acta Crystallographica Section D-Biological Crystallography* 70, 362-370 (2014).
654. A Small-Molecule Drug Conjugate for the Treatment of Carbonic Anhydrase IX Expressing Tumors. Krall, N; Pretto, F; Decurtins, W; Bernardes, GJL; Supuran, CT; Neri, D. *Angewandte Chemie-International Edition* 53, 4231-4235 (2014).
655. A Spectral Decomposition Algorithm for Estimating Chlorophyll-a Concentrations in Lake Taihu, China. Zhang, YC; Ma, RH; Duan, HT; Loiselle, S; Xu, JD. *Remote Sensing* 6, 5090-5106 (2014).
656. A synthetic biology approach to bio-chem-ICT: first moves towards chemical communication between synthetic and natural cells. Rampioni, G; Mavelli, F; Damiano, L; D'Angelo, F; Messina, M; Leoni, L; Stano, P. *Natural Computing* 13, 333-349 (2014).
657. Addition of transition metals to lithium intercalated fullerides enhances hydrogen storage properties. Aramini, M; Milanese, C; Pontiroli, D; Gaboardi, M; Girella, A; Bertoni, G; Ricco, M. *International Journal Of Hydrogen Energy* 39, 2124-2131 (2014).
658. Adsorption of Lysozyme on Hyaluronic Acid Functionalized SBA-15 Mesoporous Silica: A Possible Bioadhesive Depot System. Medda, L; Casula, MF; Monduzzi, M; Salis, A. *Langmuir* 30, 12996-13004 (2014).
659. Advances in Lipid-Based Platforms for RNAi Therapeutics. Falsini, S; Ciani, L; Ristori, S; Fortunato, A; Arcangeli, A. *J. Med. Chem.* 57, 1138-46 (2014).
660. Anethole dithiolethione lowers the homocysteine and raises the glutathione levels in solid tissues and plasma of rats: A novel non-vitamin homocysteine-lowering agent. Giustarini, D; Fanti, P; Sparatore, A; Matteucci, E; Rossi, R. *Biochemical Pharmacology* 89, 246-254 (2014).
661. Anion inhibition studies of two alpha-carbonic anhydrases from Lotus japonicus, LjCAA1 and LjCAA2. Vullo, D; Flemetakis, E; Scozzafava, A; Capasso, C; Supuran, CT. *Journal Of Inorganic Biochemistry* 136, 67-72 (2014).
662. Anion inhibition studies of two new beta-carbonic anhydrases from the bacterial pathogen Legionella pneumophila. Nishimori, I; Vullo, D; Minakuchi, T; Scozzafava, A; Osman, SM; AlOthman, Z; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 1127-1132 (2014).
663. Anion inhibition study of the beta-carbonic anhydrase (CahB1) from the cyanobacterium Coleofasciculus chthonoplastes (ex-Microcoleus chthonoplastes). Vullo, D; Kupriyanova, EV; Scozzafava, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 1667-1671 (2014).

664. Anion inhibition study of the beta-class carbonic anhydrase (PgiCAb) from the oral pathogen Porphyromonas gingivalis. Vullo, D; Del Prete, S; Osman, SM; Scozzafava, A; Alothman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry Letters* 24, 4402-4406 (2014).
665. Anti-TNF therapy for juvenile idiopathic arthritis-related uveitis. Semeraro, F; Arcidiacono, B; Nascimbeni, G; Angi, M; Parolini, B; Costagliola, C. *Drug Design Development And Therapy* 8, 341-348 (2014).
666. Antibacterial activity of silver nanoparticles grafted on stone surface. Bellissima, F; Bonini, M; Giorgi, R; Baglioni, P; Barresi, G; Mastromei, G; Perito, B. *Environmental Science And Pollution Research* 21, 13278-13286 (2014).
667. Anticancer Ruthenium(III) Complex KP1019 Interferes with ATP-Dependent Ca2+ Translocation by Sarco-Endoplasmic Reticulum Ca2+-ATPase (SERCA). Sadafi, FZ; Massai, L; Bartolommei, G; Moncelli, MR; Messori, L; Tadini-Buoninsegni, F. *Chemmedchem* 9, 1660-1664 (2014).
668. Approccio chimico-fisico alla sistematizzazione del fattore di scala nell'analisi del ciclo di vita. Maranghi, S; Parisi, ML; Busi, E; Basosi, R. *In Atti del VIII Convegno della Rete Italiana LCA - I nuovi orizzonti dell'LCA: verso un approccio sistemico e integrato alla progettazione di prodotti, processi e servizi*, 23-30 (2014).
669. Aragonite Crystals Grown on Bones by Reaction of CO2 with Nanostructured Ca(OH)(2) in the Presence of Collagen. Implications in Archaeology and Paleontology. Natali, I; Tempesti, P; Carretti, E; Potenza, M; Sansoni, S; Baglioni, P; Dei, L. *Langmuir* 30, 660-668 (2014).
670. Are algal blooms occurring later in Lake Taihu? Climate local effects outcompete mitigation prevention. Duan, HT; Ma, RH; Zhang, YC; Loiselle, SA. *Journal Of Plankton Research* 36, 866-871 (2014).
671. Artificial Biomelanin: Highly Light-Absorbing Nano-Sized Eumelanin by Biomimetic Synthesis in Chicken Egg White. della Vecchia, NF; Cerruti, P; Gentile, G; Errico, ME; Ambrogi, V; D'Errico, G; Longobardi, S; Napolitano, A; Paduano, L; Carfagna, C; d'Ischia, M. *Biomacromolecules* 15, 3811-3816 (2014).
672. Arylamino bisphosphonates: Potent and selective inhibitors of the tumor-associated carbonic anhydrase XII. Tauro, M; Loiodice, F; Ceruso, M; Supuran, CT; Tortorella, P. *Bioorganic & Medicinal Chemistry Letters* 24, 1941-1943 (2014).
673. Assimilation of MODIS Chlorophyll-a Data Into a Coupled Hydrodynamic-Biological Model of Taihu Lake. Qi, L; Ma, RH; Hu, WP; Loiselle, SA. *Ieee Journal Of Selected Topics In Applied Earth Observations And Remote Sensing* 7, 1623-1631 (2014).
674. Attachment of carbohydrates to methoxyaryl moieties leads to highly selective inhibitors of the cancer associated carbonic anhydrase isoforms IX and XII. Riafrecha, LE; Rodriguez, OM; Vullo, D; Supuran, CT; Colinas, PA. *Bioorganic & Medicinal Chemistry* 22, 5308-5314 (2014).
675. Benzenesulfonamide bearing 1,2,4-triazole scaffolds as potent inhibitors of tumor associated carbonic anhydrase isoforms hCA IX and hCA XII. SitaRam; Celik, G; Khloya, P; Vullo, D; Supuran, CT; Sharma, PK. *Bioorganic & Medicinal Chemistry* 22, 1873-1882 (2014).
676. Binding of a Monoclonal Antibody to the Phospholamban Cytoplasmic Domain Interferes with the Channel Activity of Phospholamban Reconstituted in a Tethered Bilayer Lipid Membrane. Smeazzetto, S; Sacconi, A; Schwan, AL; Margheri, G; Tadini-Buoninsegni, F. *Langmuir* 30, 10384-10388 (2014).
677. Bio-sorbable, liquid electrolyte gated thin-film transistor based on a solution-processed zinc oxide layer. Singh, M; Palazzo, G; Romanazzi, G; Suranna, GP; Ditaranto, N; Di Franco, C; Santacroce, MV; Mulla, MY; Magliulo, M; Manoli, K; Torsi, L. *Faraday Discussions* 174, 383-398 (2014).
678. Bioanalytical approaches for the detection of single nucleotide polymorphisms by surface plasmon resonance biosensors Ermini, ML; Scarano, S; Mariani, S; Minunni, M. *Biosens. Bioelectron.* 61, 28-37 (2014).
679. Biochemical characterization of P-type copper ATPases. Inesi, G; Pilankatta, R; Tadini-Buoninsegni, F. *Biochemical Journal* 463, 167-176 (2014).
680. Biochemical characterization of the chloroplastic beta-carbonic anhydrase from Flaveria bidentis (L.) "Kuntze". Dathan, NA; Alterio, V; Troiano, E; Vullo, D; Ludwig, M; De Simone, G; Supuran, CT; Monti, SM. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 500-504 (2014).
681. Biochemical characterization of the delta-carbonic anhydrase from the marine diatom Thalassiosira weissflogii, TweCA. Del Prete, S; Vullo, D; De Luca, V; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 906-911 (2014).
682. Biochemical characterization of the gamma-carbonic anhydrase from the oral pathogen Porphyromonas gingivalis, PgiCA. Del Prete, S; De Luca, V; Vullo, D; Scozzafava, A; Carginale, V; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 532-537 (2014).
683. Biochemical properties of a new alpha-carbonic anhydrase from the human pathogenic bacterium, Vibrio cholerae. Del Prete, S; De Luca, V; Scozzafava, A; Carginale, V; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 23-27 (2014).

684. Biocompatible cationic lipids for the formulation of liposomal DNA vectors. Montis, C; Sostegni, S; Milani, S; Baglioni, P; Berti, D. *Soft Matter* 10, 4287-4297 (2014).
685. Biomimetic CO2 capture using a highly thermostable bacterial alpha-carbonic anhydrase immobilized on a polyurethane foam. Migliardini, F; De Luca, V; Carginale, V; Rossi, M; Corbo, P; Supuran, CT; Capasso, C. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 146-150 (2014).
686. Biopolymers and Biomacromolecules Solvent Dynamics. Rossi, C; Bonechi, C; Foletti, A; Magnani, A; Martini, S. *Macromolecular Symposia* 335, 78-85 (2014).
687. Biosynthesis of ethyl butyrate with immobilized Candida rugosa lipase onto modified Eupergit C. Spinelli, D; Coppi, S; Basosi, R; Pogni, R. *Biocatalysis* 1, 1-12 (2014).
688. Boron concentration measurements by alpha spectrometry and quantitative neutron autoradiography in cells and tissues treated with different boronated formulations and administration protocols. Bortolussi, S; Ciani, L; Postuma, I; Protti, N; Reversi, L; Bruschi, P; Ferrari, C; Cansolino, L; Panza, L; Ristori, S; Altieri, S. *Appl. Rad. and Isotopes* 88, 78-80 (2014).
689. Ca2+/H+ exchange, lumenal Ca2+ release and Ca2+/ATP coupling ratios in the sarcoplasmic reticulum ATPase. Inesi, G; Tadini-Buoninsegni, F. *Journal Of Cell Communication And Signaling* 8, 5-11 (2014).
690. Calcium hydroxide nanoparticles for the conservation of cultural heritage: new formulations for the deacidification of cellulose-based artifacts. Poggi, G; Toccafondi, N; Melita, LN; Knowles, JC; Bozec, L; Giorgi, R; Baglioni, P. *Applied Physics A-Materials Science & Processing* 114, 685-693 (2014).
691. Cancer-Cell-Targeted Theranostic Cubosomes. Caltagirone, C; Falchi, AM; Lampis, S; Lippolis, V; Meli, V; Monduzzi, M; Prodi, L; Schmidt, J; Sgarzi, M; Talmon, Y; Bizzarri, R; Murgia, S. *Langmuir* 30, 6228-6236 (2014).
692. Carbonic Anhydrase Inhibition with Benzenesulfonamides and Tetrafluorobenzenesulfonamides Obtained via Click Chemistry. Pala, N; Micheletto, L; Sechi, M; Aggarwal, M; Carta, F; McKenna, R; Supuran, CT. *Acs Medicinal Chemistry Letters* 5, 927-930 (2014).
693. Carbonic Anhydrase Inhibitors: Design, Synthesis, and Biological Evaluation of Novel Sulfonyl Sennicarbazide Derivatives. Pichake, J; Kharkar, PS; Ceruso, M; Supuran, CT; Toraskar, MP. *Acs Medicinal Chemistry Letters* 5, 793-796 (2014).
694. Carbonic anhydrase inhibitors: Synthesis and inhibition of the human carbonic anhydrase isoforms I, II, IX and XII with benzene sulfonamides incorporating 4-and 3-nitrophthalimide moieties. Sethi, KK; Verma, SM; Tanc, M; Purper, G; Calafato, G; Carta, F; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 1586-1595 (2014).
695. Carbonic anhydrase inhibitors: Synthesis, molecular docking, cytotoxic and inhibition of the human carbonic anhydrase isoforms I, II, IX, XII with novel benzenesulfonamides incorporating pyrrole, pyrrolopyrimidine and fused pyrrolopyrimidine moieties. Ghorab, MM; Alsaid, MS; Ceruso, M; Nissan, YM; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 3684-3695 (2014).
696. Carbonic anhydrase inhibitors. Inhibition of human cytosolic isoforms I and II with (reduced) Schiff's bases incorporating sulfonamide, carboxylate and carboxymethyl moieties. Nasr, G; Cristian, A; Barboiu, M; Vullo, D; Winum, JY; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 2867-2874 (2014).
697. Carbonic anhydrase inhibitors. Phenols incorporating 2-or 3-pyridyl-ethenylcarbonyl and tertiary amine moieties strongly inhibit Saccharomyces cerevisiae beta-carbonic anhydrase. Bilginer, S; Unluer, E; Gul, HI; Mete, E; Isik, S; Vullo, D; Ozensoy-Guler, O; Beyaztas, S; Capasso, C; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 495-499 (2014).
698. Carbonic anhydrase inhibitors. Synthesis of a novel series of 5-substituted 2,4-dichlorobenzenesulfonamides and their inhibition of human cytosolic isozymes I and II and the transmembrane tumor-associated isozymes IX and XII. Slawinski, J; Pogorzelska, A; Zolnowska, B; Brozewicz, K; Vullo, D; Supuran, CT. *European Journal Of Medicinal Chemistry* 82, 47-55 (2014).
699. Carbonic anhydrase inhibitors. Synthesis, and molecular structure of novel series N-substituted N '-(2-arylmethylthio-4-chloro-5-methylbenzenesulfonyl)guanidines and their inhibition of human cytosolic isozymes I and II and the transmembrane tumor-associated isozymes IX and XII. Zolnowska, B; Slawinski, J; Pogorzelska, A; Chojnacki, J; Vullo, D; Supuran, CT. *European Journal Of Medicinal Chemistry* 71, 135-147 (2014).
700. Carbonic anhydrase inhibitory activity of sulfonamides and carboxylic acids incorporating cyclic imide scaffolds. Abdel-Aziz, AAM; El-Azab, AS; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 5185-5189 (2014).
701. Carbonic anhydrase inhibitory properties of novel sulfonamide derivatives of aminoindanes and aminotetralins. Akbaba, Y; Akincioglu, A; Gocer, H; Goksu, S; Gulcin, I; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 35-42 (2014).

702. Characterization and degradation of poly(vinyl acetate)-based adhesives for canvas paintings. Chelazzi, D; Chevalier, A; Pizzorusso, G; Giorgi, R; Menu, M; Baglioni, P. *Polymer Degradation And Stability* 107, 314-320 (2014).
703. Characterization of carbonic anhydrase from Turkish native "Gerze" chicken and influences of metal ions on enzyme activity. Mercan, L; Ekinci, D; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 773-776 (2014).
704. Chemical communication between liposomes encapsulating a chemical oscillatory reaction. Tomasi, R; Noël, JM; Zenati, A; Ristori, S; Rossi, F; Cabuil, V; Kanoufi, F; Abou-Hassan, A. *Chem. Sci.* 5, 1854-59 (2014).
705. Chemical semi-IPN hydrogels for the removal of adhesives from canvas paintings. Domingues, J; Bonelli, N; Giorgi, R; Baglioni, P. *Applied Physics A-Materials Science & Processing* 114, 705-710 (2014).
706. Chemometric modeling of breast cancer associated carbonic anhydrase IX inhibitors belonging to the ureido-substituted benzene sulfonamide class. Singh, S; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 877-883 (2014).
707. Chiral/ring closed vs. achiral/open chain triazine-based organogelators: induction and amplification of supramolecular chirality in organic gels. Lascialfari, L; Berti, D; Brandi, A; Cicchi, S; Mannini, M; Pescitelli, G; Procacci, P. *Soft Matter* 10, 3762-3770 (2014).
708. Chitosan Nanoparticles for Topical Co-Administration of the Antioxidants Glutathione and Idebenone: Characterization and In Vitro Release. Montenegro, L; Trapani, A; Fini, P; Mandracchia, D; Latrofa, A; Cioffi, N; Chiarantini, L; Piccieri, GG; Puglisi, G. *British Journal of Pharmaceutical Research* 4, 2387-2406 (2014).
709. Cigarette smoke induces alterations in the drug binding properties of human serum albumin. Clerici, M; Colombo, G; Secundo, F; Gagliano, N; Colombo, R; Portinaro, N; Giustarini, D; Milzani, A; Rossi, R; Dalle-Donne, I. *Blood Cells Molecules And Diseases* 53, 149-156 (2014).
710. Cloning, characterization and anion inhibition study of the delta-class carbonic anhydrase (TweCA) from the marine diatom Thalassiosira weissflogii. Del Prete, S; Vullo, D; Scozzafava, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 531-537 (2014).
711. Combining the tail and the ring approaches for obtaining potent and isoform-selective carbonic anhydrase inhibitors: Solution and X-ray crystallographic studies. Bozdag, M; Ferraroni, M; Nuti, E; Vullo, D; Rossello, A; Carta, F; Scozzafava, A; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 334-340 (2014).
712. Commercial Ca(OH)(2) nanoparticles for the consolidation of immovable works of art. Baglioni, P; Chelazzi, D; Giorgi, R; Carretti, E; Toccafondi, N; Jaidar, Y. *Applied Physics A-Materials Science & Processing* 114, 723-732 (2014).
713. Copper-induced structural propensities of the amyloidogenic region of human prion protein. Migliorini, C; Sinicropi, A; Kozlowski, H; Luczkowski, M; Valensin, D. *Journal Of Biological Inorganic Chemistry* 19, 635-645 (2014).
714. Corneal epithelial wound healing promoted by verbascoside-based liposomal eyedrops. Ambrosone, L; Guerra, G; Cinelli, M; Filippelli, M; Mosca, M; Vizzarri, F; Giorgio, D; Costagliola, C. *Biomed Research International* 2014, 471642-471642 (2014).
715. Covalently linked hopanoid-lipid A improves outer-membrane resistance of a Bradyrhizobium symbiont of legumes. Silipo, A; Vitiello, G; Gully, D; Sturiale, L; Chaintreuil, C; Fardoux, J; Gargani, D; Lee, HI; Kulkarni, G; Busset, N; Marchetti, R; Palmigiano, A; Moll, H; Engel, R; Lanzetta, R; Paduano, L; Parrilli, M; Chang, WS; Holst, O; Newman, DK; Garozzo, D; D'Errico, G; Giraud, E; Molinaro, A. *Nature Communications* 5 (2014).
716. Crystal structures of two tetrameric beta-carbonic anhydrases from the filamentous ascomycete Sordaria macrospora. Lehneck, R; Neumann, P; Vullo, D; Elleuche, S; Supuran, CT; Ficner, R; Poggeler, S. *Febs Journal* 281, 1759-1772 (2014).
717. Cyclic Secondary Sulfonamides: Unusually Good Inhibitors of Cancer-Related Carbonic Anhydrase Enzymes. Moeker, J; Peat, TS; Bornaghi, LF; Vullo, D; Supuran, CT; Poulsen, SA. *Journal Of Medicinal Chemistry* 57, 3522-3531 (2014).
718. Cyclic tertiary sulfamates: Selective inhibition of the tumor-associated carbonic anhydrases IX and XII by N- and O-substituted acesulfame derivatives. De Monte, C; Carradori, S; Secci, D; D'Ascenzio, M; Vullo, D; Ceruso, M; Supuran, CT. *European Journal Of Medicinal Chemistry* 84, 240-246 (2014).
719. Damage assessment of parchment at the collagen fibril level using atomic force microscopy and mechanical testing at the macro level. Odlyha, M; Bozec, L; Bartoletti, A; Noor Melita, L; Larsen, R; Axelsson, KM; Dahlin, E; Grontoft, T; Baglioni, P; Giorgi, R; Chelazzi, D. *ICOM-CC 17th Triennal Conference Preprints, Melbourne, 15-19 September 2014, ed. J. Bridgland, Paris: International Council of Museums, August 2014*, art 0607, 7 pp. (2014).

720. Decadal Trends and Common Dynamics of the Bio-Optical and Thermal Characteristics of the African Great Lakes. Loiselle, S; Cozar, A; Adgo, E; Ballatore, T; Chavula, G; Descy, JP; Harper, DM; Kansiime, F; Kimirei, I; Langenberg, V; Ma, RH; Sarmento, H; Odada, E. *Plos One* 9 (2014).
721. Design of 3d-scaffolds for tissue engineering testing a tough polylactide-based graft copolymer. Dorati, R; Colonna, C; Tomasi, C; Genta, I; Bruni, G; Conti, B. *Material Science and Engineering:C* 34, 130-139 (2014).
722. Design of novel indium oxide supported gold nanocatalysts and their application in homocoupling of arylboronic acids. Monopoli, A; Afzal, A; di Franco, C; Ditaranto, N; Cioffi, N; Nacci, A; Cotugno, P; Torsi, L. *Journal Of Molecular Catalysis A-Chemical* 386, 101-107 (2014).
723. Design, synthesis and evaluation of N-substituted saccharin derivatives as selective inhibitors of tumor-associated carbonic anhydrase XII. D'Ascenzio, M; Carradori, S; De Monte, C; Secci, D; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 1821-1831 (2014).
724. Design, Synthesis, and Evaluation of Hydroxamic Acid Derivatives as Promising Agents for the Management of Chagas Disease. Rodrigues, GC; Feijo, DF; Bozza, MT; Pan, PW; Vullo, D; Parkkila, S; Supuran, CT; Capasso, C; Aguiar, AP; Vermelho, AB. *Journal Of Medicinal Chemistry* 57, 298-308 (2014).
725. Designing functionalized gold surfaces and nanostructures for Laser Desorption Ionisation Mass Spectrometry. Pilolli, R; Ditaranto, N; Monopoli, A; Nacci, A; Palmisano, F; Sabbatini, L; Cioffi, N. *Vacuum* 100, 78-83 (2014).
726. Destabilization of $LiBH_4$ by nanoconfinement in PMMA-co-BM polymer matrix for reversible hydrogen storage. Gosalawit-Utke, R; Meethom, S; Pistidda, C; Milanese, C; Laipple, D; Saisopa, T; Marini, A; Klassen, T; Dornheim, M. *International Journal Of Hydrogen Energy* 39, 5019-5029 (2014).
727. Detection of Hg2+ insertion into cysteine pairs within protein single crystals via Raman microscopy. Caterino, M; Merlino, A; Balsamo, A; Russo Krauss, I; Parisi, S; Vergara A. *Journal of Solution Chemistry* 43, 135-143 (2014).
728. Determination of phthalate esters at trace levels in light alcoholic drinks and soft drinks by XAD-2 adsorbent and gas chromatography coupled with ion trap-mass spectrometry detection. Russo, MV; Notardonato, I; Avino, P; Cinelli, G. *Analytical Methods* 6, 7030-7037 (2014).
729. Development and biological evaluation of Tc-99m-sulfonamide derivatives for in vivo visualization of CA IX as surrogate tumor hypoxia markers. Akurathi, V; Dubois, L; Celen, S; Lieuwes, NG; Chitneni, SK; Cleynhens, BJ; Innocenti, A; Supuran, CT; Verbruggen, AM; Lambin, P; Bormans, GM. *European Journal Of Medicinal Chemistry* 71, 374-384 (2014).
730. Diameters and Wall-to-Lumen Ratio of Retinal Arterioles in Patients with Retinal Vein Occlusion Before and After Treatment with Dexamethasone Intravitreal Implants. Semeraro, F; Russo, A; Rizzoni, D; Danzi, P; Morescalchi, F; Costagliola, C. *Journal Of Ocular Pharmacology And Therapeutics* 30, 573-579 (2014).
731. Diastereoselective self-assembly of clofarabine lipids. Sandin, P; Bombelli, FB; Castroflorio, B; Muller, C; Obermeier, J; Karlsson, G; Edwards, K; Baglioni, P; Berti, D. *New Journal Of Chemistry* 38, 5247-5253 (2014).
732. Dielectric response of shelled toroidal particles carrying localized surface charge distributions. The effect of concentric and confocal shells. Di Biasio, A; Ambrosone, L; Cametti, C. *Bioelectrochemistry* 98, 76-86 (2014).
733. Diffusion Properties of the Ternary System Human Serum Albumin-Sodium Cholate-Water. D'Errico, G; Ortona, O; Paduano, L; Sartorio, R. *Journal Of Solution Chemistry* 43, 893-915 (2014).
734. Direct electronic probing of biological complexes formation. Macchia, E; Magliulo, M; Manoli, K; Giordano, F; Palazzo, G; Torsi, L. *Organic Light Emitting Materials And Devices Xviii* 9183 (2014).
735. Discovery of a new family of carbonic anhydrases in the malaria pathogen Plasmodium falciparum-The eta-carbonic anhydrases. Del Prete, S; Vullo, D; Fisher, GM; Andrews, KT; Poulsen, SA; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 4389-4396 (2014).
736. Disentangling spatial and non-spatial effects in real complex networks. Squartini, T; Picciolo, F; Ruzzenenti, F; Basosi, R; Garlaschelli, D. *In: Hocine Cherifi. Complex networks and their applications* (2014).
737. Dominant behaviours in the expression of human carbonic anhydrase hCA I activity. Abdelrahim, MYM; Tanc, M; Winum, JY; Supuran, CT; Barboiu, M. *Chemical Communications* 50, 8043-8046 (2014).
738. Driving h-osteoblast adhesion and proliferation on titania- peptide hydrogels decorated with growth factors and adhesive conjugates. Dettin, M; Zamuner, A; Iucci, G; Messina, GML; Battocchio, C; Picariello, G; Gallina, G; Marletta, G; Castagliuolo, I; Brun, P. *Journal of Peptide Science* 20, 585-594 (2014).
739. Dual carbonic anhydrase/matrix metalloproteinase inhibitors incorporating bisphosphonic acid moieties targeting bone tumors. Tauro, M; Loiodice, F; Ceruso, M; Supuran, CT; Tortorella, P. *Bioorganic & Medicinal Chemistry Letters* 24, 2617-2620 (2014).

740. Effect of intravitreal bevacizumab on serum, aqueous, and vitreous humor levels of erythropoietin in patients with proliferative diabetic retinopathy. Cancarini, A; Costagliola, C; Dell'omo, R; Romano, MR; Morescalchi, F; Agnifili, L; Ruggeri, G; Semeraro, F. *Minerva Endocrinologica* 39, 305-311 (2014).
741. Effect of Palmitoylethanolamide on Visual Field Damage Progression in Normal Tension Glaucoma Patients: Results of an Open-Label Six-Month Follow-Up. Costagliola, C; Romano, MR; dell'Omo, R; Russo, A; Mastropasqua, R; Semeraro, F. *Journal Of Medicinal Food* 17, 949-954 (2014).
742. Effect of powder characteristics for a magnesium based metal hydride store. Bennett, CMJ; Patman, AJ; Milanese, C; Eastwick, CN; Walker, GS. *International Journal Of Hydrogen Energy* 39, 19646-19655 (2014).
743. Effect of the Alkyl Chains and of the Headgroups on the Thermal Behavior of Ascorbic Acid Surfactants Mixtures. Venturini, C; Pomposi, C; Ambrosi, M; Carretti, E; Fratini, E; Lo Nostro, P; Baglioni, P. *Journal Of Physical Chemistry B* 118, 3053-3062 (2014).
744. Effect of the Partial Replacement of CaH_2 with CaF_2 in the Mixed System $CaH_2 + MgB_2$. Pistidda, C; Karimi, F; Garroni, S; Rzeszutek, A; Minella, CB; Milanese, C; Le, TT; Rude, LH; Skibsted, J; Jensen, TR; Horstmann, C; Gundlach, C; Tolkiehn, M; Pranzas, PK; Schreyer, A; Klassen, T; Dornheim, M. *Journal Of Physical Chemistry C* 118, 28409-28417 (2014).
745. Effective mutations in a high redox potential laccase from Pleurotus ostreatus. Macellaro, G; Baratto, MC; Piscitelli, A; Pezzella, C; de Biani, FF; Palmese, A; Piumi, F; Record, E; Basosi, R; Sannia, G. *Applied Microbiology And Biotechnology* 98, 4949-4961 (2014).
746. Effects of Salts on the Micellization of a Short-Tailed Nonionic Ethoxylated Surfactant: An Intradiffusion Study. Imperatore, R; Vitiello, G; Ciccarelli, D; D'Errico, G. *Journal Of Solution Chemistry* 43, 227-239 (2014).
747. Efficient Nonequilibrium Method for Binding Free Energy Calculations in Molecular Dynamics Simulations. Sandberg, R; Banchelli, M; Guardiani, C; Menichetti, S; Caminati, G; Procacci, P. *J. Chem. Theory Comput.* 11, 423-435 (2014).
748. Electrochemistry of orthosilicate-based lithium battery cathodes: a perspective. Ferrari, S; Capsoni, D; Casino, S; Destro, M; Gerbaldi, C; Bini, M. *Phys. Chem. Chem. Phys.* 16, 10353-10366 (2014).
749. Electronic Transduction of Proton Translocations in Nanoassembled Lamellae of Bacteriorhodopsin. Palazzo, G; Magliulo, M; Mallardi, A; Angione, MD; Gobeljic, D; Scamarcio, G; Fratini, E; Ridi, F; Torsi, L. *Acs Nano* 8, 7834-7845 (2014).
750. Emergent properties arising from the assembly of amphiphiles. Artificial vesicle membranes as reaction promoters and regulators. Walde, P; Umakoshi, H; Stano, P; Mavelli, F. *Chemical Communications* 50, 10177-10197 (2014).
751. Energy efficiency in dyes production: bio-synthetic pathway versus chemical process. Parisi, ML; Spinelli, D; Pogni, R; Basosi, R. *In Atti del VIII Congresso Nazionale dell'AIGE -Associazione Italiana Gestione Energia*, 43-49 (2014).
752. Enhancement of the Uptake and Cytotoxic Activity of Doxorubicin in Cancer Cells by Novel cRGD-Semipeptide-Anchoring Liposomes. Battistini, L; Burreddu, P; Sartori, A; Arosio, D; Manzoni, L; Paduano, L; D'Errico, G; Sala, R; Reia, L; Bonomini, S; Rassu, G; Zanardi, F. *Molecular Pharmaceutics* 11, 2280-2293 (2014).
753. Environmental impact of electricity from selected geothermal power plants in Italy. Bravi, M; Basosi, R. *Journal Of Cleaner Production* 66, 301-308 (2014).
754. Enzyme-containing paints inhibit the growth of marine microorganisms. Panizza, L; Frisenda, P; Stefan, A; Francese, M; Madeo, A; Martelli E; Hochkoeppler, A. *Journal of Chemistry and Chemical Engineering* 8, 151-156 (2014).
755. Ethylene bis-imidazoles are highly potent and selective activators for isozymes VA and VII of carbonic anhydrase, with a potential nootropic effect. Draghici, B; Vullo, D; Akocak, S; Walker, EA; Supuran, CT; Ilies, MA. *Chemical Communications* 50, 5980-5983 (2014).
756. Evaluation of capillary chromatographic supports for immobilized human purine nucleoside phosphorylase in frontal affinity chromatography studies. de Moraes, MC; Temporini, C; Calleri, E; Bruni, G; Ducati RG; Santos, DS; Cardoso, CL; Cass, QB; Massolini G. *Journal of Chromatography A* 1338, 77-84 (2014).
757. Evaluation of the environmental sustainability of a micro CHP system fueled by low-temperature geothermal and solar energy. Ruzzenenti, F; Bravi, M; Tempesti, D; Salvatici, E; Manfrida, G; Basosi, R. *Energy Conversion And Management* 78, 611-616 (2014).
758. Excited State Geometries and Vertical Emission Energies of Solvated Dyes for DSSC: A PCM/TD-DFT Benchmark Study. Bernini, C; Zani, L; Calamante, M; Reginato, G; Mordini, A; Taddei, M; Basosi, R; Sinicropi, A. *Journal Of Chemical Theory And Computation* 10, 3925-3933 (2014).
759. Expression of CA IX in dysplasia adjacent to surgical resection margins of oral squamous cell carcinoma. Perez-Sayans, M; Suerez-Penaranda, JM; Torres-Lopez, M; Supuran, CT; Gandara-Vila, P; Gayoso-Diz, P; Barros-Angueira, F; Blanco-Carrion, A; Gandara-Rey, JM; Garcia-Garcia, A. *Biotechnic & Histochemistry* 89, 91-97 (2014).

760. Fabrication and electrochemical characterization of amorphous lithium iron silicate thin films as positive electrodes for lithium batteries. Quinzeni, I; Ferrari, S; Quartarone, E; Capsoni, D; Caputo, M; Goldoni, A; Mustarelli, P; Bini, M. *J. Power Sources* 266, 179-185 (2014).
761. Facilitation by intracellular carbonic anhydrase of Na+-HCO3- co-transport but not Na+/H+ exchange activity in the mammalian ventricular myocyte. Villafuerte, FC; Swietach, P; Youm, JB; Ford, K; Cardenas, R; Supuran, CT; Cobden, PM; Rohling, M; Vaughan-Jones, RD. *Journal Of Physiology-London* 592, 991-1007 (2014).
762. Fast determination of phthalate ester residues in soft drinks and light alcoholic beverages by ultrasound/vortex assisted dispersive liquid-liquid microextraction followed by gas chromatographyion trap mass spectrometry. Russo, MV; Notardonato, I; Avino, P; Cinelli, G. *Rsc Advances* 4, 59655-59663 (2014).
763. Ferrier sulfamidoglycosylation of glycals catalyzed by nitrosonium tetrafluoroborate: Towards new carbonic anhydrase glycoinhibitors. Ombouma, J; Vullo, D; Supuran, CT; Winum, JY. *Bioorganic & Medicinal Chemistry* 22, 6353-6359 (2014).
764. Flow synthesis and biological activity of aryl sulfonamides as selective carbonic anhydrase IX and XII inhibitors. Rosatelli, E; Carotti, A; Ceruso, M; Supuran, CT; Gioiello, A. *Bioorganic & Medicinal Chemistry Letters* 24, 3422-3425 (2014).
765. From self-assembly fundamental knowledge to nanomedicine developments. Monduzzi, M; Lampis, S; Murgia, S; Salis, A. *Advances In Colloid And Interface Science* 205, 48-67 (2014).
766. Functional potential of sulfonamide derivative compounds in the regulation of hypoxia induced carbonic anhydrase 9 (CA9) in human brain cancer. Said, HM; Hagemann, C; Carta, F; Katzer, A; Flentje, M; Supuran, CT. *Febs Journal* 281, 467-467 (2014).
767. Functionalized clay micro-particles as catalysts for chemical oscillators. Rossi, F; Ristori, S; Marchettini, N; Pantani, OL. *J. Phys. Chem. C* 118, 24389-96 (2014).
768. Furazan and furoxan sulfonamides are strong alpha-carbonic anhydrase inhibitors and potential antiglaucoma agents. Chegaev, K; Lazzarato, L; Tamboli, Y; Boschi, D; Blangetti, M; Scozzafava, A; Carta, F; Masini, E; Fruttero, R; Supuran, CT; Gasco, A. *Bioorganic & Medicinal Chemistry* 22, 3913-3921 (2014).
769. Heavy Silicone Oil and Intraocular Inflammation. Morescalchi, F; Costagliola, C; Duse, S; Gambicorti, E; Parolini, B; Arcidiacono, B; Romano, MR; Semeraro, F. *Biomed Research International* (2014).
770. High-performance and anti-stain coating for porcelain stoneware tiles based on nanostructured zirconium compounds. Ambrosi, M; Santoni, S; Giorgi, R; Fratini, E; Toccafondi, N; Baglioni, P. *Journal Of Colloid And Interface Science* 432, 117-127 (2014).
771. HPLC-DAD-ESI/MSn characterization of environmentally friendly polyphenolic extract from Raphanus sativus L. var. "Cherry Belle" skin and stability of its red components. Papetti, A; Milanese, C; Zanchi, C; Gazzani, G. *Food Research International* 65, 238-246 (2014).
772. Human neutrophil peptide 1 variants bearing arginine modified cationic side chains: Effects on membrane partitioning. Bonucci, A; Balducci, E; Martinelli, M; Pogni, R. *Biophysical Chemistry* 190, 32-40 (2014).
773. Hydration-dependent dynamic crossover phenomenon in protein hydration water. Wang, Z; Fratini, E; Li, MD; Le, PS; Mamontov, E; Baglioni, P; Chen, SH. *Physical Review E* 90, 42705 (2014).
774. Hydrogen storage systems from waste Mg alloys. Pistidda, C; Bergemann, N; Wurr, J; Rzeszutek, A; Moller, KT; Hansen, BRS; Garroni, S; Horstmann, C; Milanese, C; Girella, A; Metz, O; Taube, K; Jensen, TR; Thomas, D; Liermann, HP; Klassen, T; Dornheim, M. *Journal Of Power Sources* 270, 554-563 (2014).
775. Hydrophobic Substituents of the Phenylmethylsulfamide Moiety Can Be Used for the Development of New Selective Carbonic Anhydrase Inhibitors. De Simone, G; Pizika, G; Monti, SM; Di Fiore, A; Ivanova, J; Vozny, I; Trapencieris, P; Zalubovskis, R; Supuran, CT; Alterio, V. *Biomed Research International* (2014).
776. Impact of selective fibronectin nanoconfinement on human dental pulp stem cells. Karakeçili, A; Messina, GML; Yurtsever, MC; Gümüşderelioğlu, M; Marletta, G. *Colloids and Surfaces B: Biointerfaces* 123, 39-48 (2014).
777. Improvement of quercetin protective effect against oxidative stress skin damages by incorporation in nanovesicles. Manca, ML; Castangia, I; Caddeo, C; Pando, D; Escribano, E; Valenti, D; Lampis, S; Zaru, M; Fadda, AM; Manconi, M. *Colloids And Surfaces B-Biointerfaces* 123, 566-574 (2014).
778. Improving impedimetric nucleic acid detection by using enzyme-decorated liposomes and nanostructured screen-printed electrodes. Voccia, D; Bettazzi, F; Fratini, E; Berti, D; Palchetti, I. *Analytical and Bioanalytical Chemistry* 408, 7271-7281 (2016).
779. In Silico Spectroscopy of Tryptophan and Tyrosine Radicals Involved in the Long-Range Electron Transfer of Cytochrome c Peroxidase. Bernini, C; Arezzini, E; Basosi, R; Sinicropi, A. *Journal Of Physical Chemistry B* 118, 9525-9537 (2014).

780. In vitro and ex vivo retina angiogenesis assays. Rezzola, S; Belleri, M; Gariano, G; Ribatti, D; Costagliola, C; Semeraro, F; Presta, M. *Angiogenesis* 17, 429-442 (2014).
781. Incoherent Quasielastic Neutron Scattering Study of the Relaxation Dynamics in Molybdenum-Oxide Keplerate-Type Nanocages. Faraone, A; Fratini, E; Garai, S; Muller, A; Tyagi, M; Jenkins, T; Mamontov, E; Paul, RL; Copley, JRD; Baglioni, P. *Journal Of Physical Chemistry C* 118, 13300-13312 (2014).
782. Inflammaging: should this term be suitable for age related macular degeneration too? Gallenga, CE; Parmeggiani, F; Costagliola, C; Sebastiani, A; Gallenga, PE. *Inflammation Research* 63, 105-107 (2014).
783. Inhibiting carbonic anhydrase IX targets hypoxic small cell lung cancer cells. Bryant, JL; Meredith, SL; Gieling, RG; Telfer, BA; Babur, M; Supuran, CT; Williams, KJ; White, A. *Cancer Research* 74, (2014).
784. Inhibition of carbonic anhydrase isoforms I, II, IX and XII with novel Schiff bases: Identification of selective inhibitors for the tumor-associated isoforms over the cytosolic ones. Sarikaya, B; Ceruso, M; Carta, F; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 5883-5890 (2014).
785. Inhibition of carbonic anhydrases from the extremophilic bacteria Sulfurihydrogenibium yellostonense (SspCA) and S. azorense (SazCA) with a new series of sulfonamides incorporating aroylhydrazone-, [1,2,4]triazolo[3,4-b][1,3,4]thiadiazinyl- or 2-(cyanophenylmethylene)-1,3,4-thiadiazol-3(2H)-yl moieties. Alafeefy, AM; Abdel-Aziz, HA; Vullo, D; Al-Tamimi, AMS; Al-Jaber, NA; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 141-147 (2014).
786. Inhibition of mammalian carbonic anhydrases I-XIV with grayanotoxin III: solution and in silico studies. Durdagi, S; Scozzafava, G; Vullo, D; Sahin, H; Kolayli, S; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 469-475 (2014).
787. Inhibition studies of new ureido-substituted sulfonamides incorporating a GABA moiety against human carbonic anhydrase isoforms I-XIV. Ceruso, M; Antel, S; Vullo, D; Scozzafava, A; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 6768-6775 (2014).
788. Inhibitory targeting of CA9 by two different sulfonamide derivative compounds including acetazolamide in human brain cancer. Said, HM; Hagemann, C; Carta, F; Katzer, A; Scozzafava, A; Flentje, M; Supuran, CT. *International Journal Of Molecular Medicine* 34, S90-S90 (2014).
789. Interaction of nanoparticles with lipid membranes: a multiscale perspective. Montis, C; Maiolo, D; Alessandri, I; Bergese, P; Berti, D. *Nanoscale* 6, 6452-6457 (2014).
790. Interactions between Anticancer trans-Platinum Compounds and Proteins: Crystal Structures and ESI-MS Spectra of Two Protein Adducts of trans-(Dimethylamino)(methylamino)dichloridoplatinum(II). Messori, L; Marzo, T; Michelucci, E; Russo Krauss, I; Navarro-Ranninger, C; Quiroga, AG; Merlino, A. *Inorganic Chemistry* 53, 7806-7808 (2014).
791. Interactions of gold-based drugs with proteins: crystal structure of the adduct formed between ribonuclease A and a cytotoxic gold(III) compound. Messori, L; Scaletti, F; Massai, L; Cinellu, MA; Russo Krauss, I; di Martino, G; Vergara, A; Paduano, L; Merlino, A. *Metallomics* 6, 233-236 (2014).
792. Interactions of gold-based drugs with proteins: the structure and stability of the adduct formed in the reaction between lysozyme and the cytotoxic gold(III) compound Auoxo3. Russo Krauss, I; Messori, L; Cinellu, MA; Marasco, D; Sirignano, R; Merlino, A. *Dalton Transactions* 43, 17483-17488 (2014).
793. Interplay of crystallography, Raman microspectroscopy and electrospray mass spectrometry for studying the reaction between ruthenium complexes and proteins. Vergara, A; Messori, L; Montesarchio, D; Paduano, L; Marzo, T; Sanches, RNF; Ur-Rehman, H; Silva, DD; Krauss, IR; Caterino, M; Merlino, A. *Febs Journal* 281, 626-626 (2014).
794. Investigation on the influence of (Z)-3-(2-(3-chlorophenyl)hydrazono)-5,6-dihydroxyindolin-2-one (PT2) on beta-amyloid(1-40) aggregation and toxicity. Catto, M; Arnesano, F; Palazzo, G; De Stradis, A; Calo, V; Losacco, M; Purgatorio, R; Campagna, F. *Archives Of Biochemistry And Biophysics* 560, 73-82 (2014).
795. Ion Beam Sputtering Deposition and Characterization of ZnO-Fluoropolymer Nano-Antimicrobials. Sportelli, MC; Nitti, MA; Valentini, M; Picca, RA; Bonerba, E; Sabbatini, L; Tantillo, G; Cioffi, N; Valentini, A. *Science Of Advanced Materials* 6, 1019-1025 (2014).
796. Kinetic modeling of partial oxidation of benzyl alcohol in water by means of Fe(III)/O-2/UV-solar simulated process. Spasiano, D; Marotta, R; Gargano, I; Di Somma, I; Vitiello, G; D'Errico, G; Andreozzi, R. *Chemical Engineering Journal* 249, 130-142 (2014).
797. Laser Removal of Mold Growth from Paper. Rosati, C; Ciofini, D; Osticioli, I; Giorgi, R; Tegli, S; Siano, S. *Applied Physics A* 117, 253-259 (2014).
798. Latest treatment option and technology advancement in corneal and ocular surface disease. Costagliola, C; Batterbury, M; Dua, HS; Mastropasqua, L. *Biomed Research International* 2014, 203868-203868 (2014).

799. Lattice Corneal Dystrophy: a report of two cases in twin sisters due to 3 mutations (T1620C, C1416T, A1924G) in the TGFBI (BIGH3) gene. Costagliola, C; Romano, V; Cifariello, F; Aceto, F; Porcellini, A. *La Clinica Terapeutica* 165, e73-5 (2014).
800. $Li_{12}C_{60}$: A lithium clusters intercalated fulleride. Giglio, F; Pontiroli, D; Gaboardi, M; Aramini, M; Cavallari, C; Brunelli, M; Galinetto, P; Milanese, C; Ricco, M. *Chemical Physics Letters* 609, 155-160 (2014).
801. Lipophilic nucleic acids - A flexible construction kit for organization and functionalization of surfaces. Schade, M; Berti, D; Huster, D; Herrmann, A; Arbuzova, A. *Advances In Colloid And Interface Science* 208, 235-251 (2014).
802. Loading and Protection of Hydrophilic Molecules into Liposome-Templated Polyelectrolyte Nanocapsules. Cuomo, F; Ceglie, A; Piludu, M; Miguel, MG; Lindman, B; Lopez, F. *Langmuir* 30, 7993-7999 (2014).
803. Low-voltage solid electrolyte-gated OFETs for gas sensing applications. Dumitru, LM; Manoli, K; Magliulo, M; Palazzo, G; Torsi, L. *Microelectronics Journal* 45, 1679-1683 (2014).
804. Macular hypotrophy after internal limiting membrane removal for diabetic macular edema. Romano, MR; Romano, V; Vallejo-Garcia, JL; Vinciguerra, R; Romano, M; Cereda, M; Angi, M; Valldeperas, X; Costagliola, C; Vinciguerra, P. *Retina-The Journal Of Retinal And Vitreous Diseases* 34, 1182-1189 (2014).
805. Magnetic nanoparticle clusters as actuators of ssDNA release. Banchelli, M; Nappini, S; Montis, C; Bonini, M; Canton, P; Berti, D; Baglioni, P. *Physical Chemistry Chemical Physics* 16, 10023-10031 (2014).
806. Magnetic polystyrene nanocomposites for the separation of oil and water. Tempesti, P; Bonini, M; Ridi, F; Baglioni, P. *Journal Of Materials Chemistry A* 2, 1980-1984 (2014).
807. Magneto-responsive nanocomposites: Preparation and integration of magnetic nanoparticles into films, capsules, and gels. Ridi, F; Bonini, M; Baglioni, P. *Advances In Colloid And Interface Science* 207, 3-13 (2014).
808. Mechanochemical Synthesis of Bumetanide-4-Aminobenzoic Acid Molecular Cocrystals: A Facile and Green Approach to Drug Optimization. Bruni, G; Maietta, M; Berbenni, V; Mustarelli, P; Ferrara, C; Freccero, M; Grande, V; Maggi, L; Milanese, C; Girella, A; Marini, A. *Journal Of Physical Chemistry B* 118, 9180-9190 (2014).
809. Mechanothermal Synthesis of $SrSnO_3$. Berbenni, V; Milanese, C; Bruni, G; Girella, A; Marini, A. *Zeitschrift Fur Naturforschung Section B-A Journal Of Chemical Sciences* 69, 313-320 (2014).
810. Micelle, microemulsions, and gels for the conservation of cultural heritage. Baglioni, P; Berti, D; Bonini, M; Carretti, E; Dei, L; Fratini, E; Giorgi, R. *Advances In Colloid And Interface Science* 205, 361-371 (2014).
811. Micro-layers of polystyrene film preventing metal oxidation: implications in cultural heritage conservation. Giambi, F; Carretti, E; Dei, L; Baglioni, P. *Applied Physics A-Materials Science & Processing* 117, 2025-2032 (2014).
812. Micro-method for the determination of glutathione in human blood. Giustarini, D; Fanti, P; Matteucci, E; Rossi, R. *Journal Of Chromatography B-Analytical Technologies In The Biomedical And Life Sciences* 964, 191-194 (2014).
813. Micro-patterned nanoscale Au films on PMMA: fabrication and effect of PMMA dewetting on Au patterning. Ruffino, F; Torrisi, V; Marletta, G; Grimaldi, MG. *J. Mater. Sci.: Materials in Electronics* 25, 1138-1147 (2014).
814. Mineral Nitrogen Fertilizers: Environmental Impact of Production and Use. Basosi, R; Spinelli, D; Fierro, A; Jez, S. *In "Fertilizer , Components, Uses in Agriculture and Environmental Impacts" (eds. F. Lopez-Valdez, F. Fernandez-Luqueño) Nova Science Publisher*, 3-43 (2014).
815. Modelling Lipid Competition Dynamics in Heterogeneous Protocell Populations. Shirt-Ediss, B; Ruiz-Mirazo, K; Mavelli, F; Sole, RV. *Scientific Reports* 4 (2014).
816. Models and mechanisms of Hofmeister effects in electrolyte solutions, and colloid and protein systems revisited. Salis, A; Ninham, BW. *Chemical Society Reviews* 43, 7358-7377 (2014).
817. Molecular arrangements and interconnected bilayer formation induced by alcohol or polyalcohol in phospholipid vesicles. Manca, ML; Castangia, I; Matricardi, P; Lampis, S; Fernandez-Busquets, X; Fadda, AM; Manconi, M. *Colloids And Surfaces B-Biointerfaces* 117, 360-367 (2014).
818. Molecular communication technology: General considerations on the use of synthetic cells and some hints from in silico modelling. Mavelli F; Rampioni G; Damiano L; Messina M; Leoni L; Stano P. *in Pizzuti C., Spezzano G. Eds.: "Advances in Artificial Life and Evolutionary Computation", in book series: Communications in Computer and Information Science* 445, 169-189 (2014).
819. Molecular recognition of nucleic acids by nucleolipid/dendrimer surface complexes. Arteta, MY; Berti, D; Montis, C; Campbell, RA; Clifton, LA; Skoda, MWA; Soltwedel, O; Baglioni, P; Nylander, T. *Soft Matter* 10, 8401-8405 (2014).
820. Monitoring the interaction of nucleolipoplexes with model membranes. Montis, C; Baglioni, P; Berti, D. *Soft Matter* 10, 39-43 (2014).

821. Mono- and di-halogenated histamine, histidine and carnosine derivatives are potent carbonic anhydrase I, II, VII, XII and XIV activators. Saada, MC; Vullo, D; Montero, JL; Scozzafava, A; Supuran, CT; Winum, JY. *Bioorganic & Medicinal Chemistry* 22, 4752-4758 (2014).
822. Monoclonal antibodies raised against 167-180 aa sequence of human carbonic anhydrase XII inhibit its enzymatic activity. Dekaminaviciute, D; Kairys, V; Zilnyte, M; Petrikaite, V; Jogaite, V; Matuliene, J; Gudleviciene, Z; Vullo, D; Supuran, CT; Zvirbliene, A. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 804-810 (2014).
823. Morphology of synthetic DOPA-eumelanin deposited on glass and mica substrates: An atomic force microscopy investigation. Perna, G; Lasalvia, M; D'Antonio, P; Mallardi, A; Palazzo, G; Fiocco, D; Gallone, A; Cicero, R; Capozzi, V. *Micron* 64, 28-33 (2014).
824. Mucoadhesive Properties and Interaction with P-Glycoprotein (P-gp) of Thiolated-Chitosans and -Glycol Chitosans and Corresponding Parent Polymers: A Comparative Study. Trapani, A; Palazzo, C; Contino, M; Perrone, MG; Cioffi, N; Ditaranto, N; Colabufo, NA; Conese, M; Trapani, G; Puglisi, G. *Biomacromolecules* 15, 882-893 (2014).
825. Multiscale structure of calcium- and magnesium-silicate-hydrate gels. Chiang, WS; Ferraro, G; Fratini, E; Ridi, F; Yeh, YQ; Jeng, US; Chen, SH; Baglioni, P. *Journal Of Materials Chemistry A* 2, 12991-12998 (2014).
826. Muon spin relaxation reveals the hydrogen storage mechanism in light alkali metal fullerides. Aramini, M; Gaboardi, M; Vlahopoulou, G; Pontiroli, D; Cavallari, C; Milanese, C; Ricco, M. *Carbon* 67, 92-97 (2014).
827. Myopia onset and progression: Can it be prevented? Russo, A; Semeraro, F; Romano, MR; Mastropasqua, R; Dell'Omo, R; Costagliola, C. *International Ophthalmology* 34, 693-705 (2014).
828. $NaAlH_4$ production from waste aluminum by reactive ball milling. Bergemann, N; Pistidda, C; Milanese, C; Girella, A; Hansen, BRS; Wurr, J; von Colbe, JMB; Jepsen, J; Jensen, TR; Marini, A; Klassen, T; Dornheim, M. *International Journal Of Hydrogen Energy* 39, 9877-9882 (2014).
829. Nano-antimicrobials based on metals. Sportelli, MC; Picca, RA; Cioffi, N. *in "Novel antimicrobial agents and strategies", chapter 8, Phoenix, Harris, Dennison, Eds., Wiley-VCH Verlag Publisher*, 181-218 (2014).
830. Nanoscale electrical investigation of layer-by-layer grown molecular wires, Musumeci, C; Zappalà, G; Martsinovich, N; Orgiu, E; Schuster, S; Quici, S; Zharnikov, M; Troisi, A; Licciardello, A; Samori, P. *Advanced Materials* 26, 1688-1693 (2014).
831. Nanostructured fluids from degradable nonionic surfactants for the cleaning of works of art from polymer contaminants. Baglioni, M; Raudino, M; Berti, D; Keiderling, U; Bordes, R; Holmberg, K; Baglioni, P. *Soft Matter* 10, 6798-6809 (2014).
832. Natural Product Polyamines That Inhibit Human Carbonic Anhydrases. Davis, RA; Vullo, D; Supuran, CT; Poulsen, SA. *Biomed Research International* (2014).
833. Neurotrophic Keratitis. Semeraro, F; Forbice, E; Romano, V; Angi, M; Romano, MR; Filippelli, ME; Di Iorio, R; Costagliola, C. *Ophthalmologica* 231, 191-197 (2014).
834. New Insight into Adiponectin Role in Obesity and Obesity-Related Diseases. Nigro, E; Scudiero, O; Monaco, ML; Palmieri, A; Mazzarella, G; Costagliola, C; Bianco, A; Daniele, A. *Biomed Research International* (2014).
835. NMR of liquid crystals and micellar solutions. D'Errico, G; Paduano, L. *Nuclear Magnetic Resonance Volume* 43, 457-494 (2014).
836. Novel coumarins and benzocoumarins acting as isoform-selective inhibitors against the tumor-associated carbonic anhydrase IX. Sharma, A; Tiwari, M; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 292-296 (2014).
837. Novel DFO-SAM on mesoporous silica for iron sensing. Part I. Synthesis optimization and characterization of the material. Biesuz, R; Emma, G; Milanese, C; Dacarro, G; Taglietti, A; Nurchi, VM; Alberti, G. *Analyst* 139, 3932-3939 (2014).
838. Novel inhibitory monoclonal antibodies against tumour-associated carbonic anhydrase XII. Dekaminaviciute, D; Kairys, V; Petrikaite, V; Matuliene, J; Supuran, CT; Zvirbliene, A. *Febs Journal* 281, 414-414 (2014).
839. Novel sulfonamides bearing pyrrole and pyrrolopyrimidine moieties as carbonic anhydrase inhibitors: Synthesis, cytotoxic activity and molecular modeling. Ghorab, MM; Ceruso, M; Alsaid, MS; Nissan, YM; Arafa, RK; Supuran, CT. *European Journal Of Medicinal Chemistry* 87, 186-196 (2014).
840. Nylon 6 film and nanofiber carriers: Preparation and laccase immobilization performance. Fatarella, E; Spinelli, D; Ruzzante, M; Pogni, R. *Journal Of Molecular Catalysis B-Enzymatic* 102, 41-47 (2014).
841. Ocular tissues and fluids oxidative stress in hares fed on verbascoside supplement. Mosca, M; Ambrosone, L; Semeraro, F; Casamassima, D; Vizzarri, F; Costagliola, C. *International Journal Of Food Sciences And Nutrition* 65, 235-240 (2014).

842. Old interventions and potential new treatments for Maya mural paintings in Tulum (Mexico). Meehan, P; Jáidar Benavides, Y; Giorgi, R; Baglioni, P. *ICOM-CC 17th Triennial Conference Preprints, Melbourne, 15–19 September 2014, ed. J. Bridgland*, *Paris: International Council of Museums*, art. 1106, 7 pp. (2014).
843. On the macromolecular cellulosic network of paper: changes induced by acid hydrolysis studied by NMR diffusometry and relaxometry. Conti, A; Poggi, G; Baglioni, P; De Luca, F. *Physical Chemistry Chemical Physics* 16, 8409-8417 (2014).
844. On-column refolding of diphtheria toxin variant CRM197 by different metal affinity chromatography matrices. Stefan A; Boiani M; Longanesi L; Hochkoeppler, A. *Journal of Chemistry and Chemical Engineering* 8, 1135-1141 (2014).
845. One role of hydration water in proteins: key to the "softening" of short time intraprotein collective vibrations of a specific length scale. Wang, Z; Chiang, WS; Le, PS; Fratini, E; Li, MD; Alatas, A; Baglioni, P; Chen, SH. *Soft Matter* 10, 4298-4303 (2014).
846. Optical characterization of black water blooms in eutrophic waters. Duan, HT; Ma, RH; Loiselle, SA; Shen, QS; Yin, HB; Zhang, YC. *Science Of The Total Environment* 482, 174-183 (2014).
847. Organic dyes with intense light absorption especially suitable for application in thin-layer dye-sensitized solar cells. Dessi, A; Calamante, M; Mordini, A; Peruzzini, M; Sinicropi, A; Basosi, R; de Biani, FF; Taddei, M; Colonna, D; Di Carlo, A; Reginato, G; Zani, L. *Chemical Communications* 50, 13952-13955 (2014).
848. Our Memories of Dr. Donald G. Miller. Sartorio, R; Paduano, L. *Journal Of Solution Chemistry* 43, 4-5 (2014).
849. Oxidation of cyanobenzocycloheptatrienes: Synthesis, photooxygenation reaction and carbonic anhydrase isoenzymes inhibition properties of some new benzotropone derivatives. Guney, M; Coskun, A; Topal, F; Dastan, A; Gulcin, I; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 3537-3543 (2014).
850. Oxidative degradation of phenanthrene in the absence of light irradiatiion by hybrid ZrO2-acetylacetonate gel-derived catalyst. Sannino, F; Pirozzi, D; Vitiello, G; D'errico, G; Aronne, A; Fanelli, E; Pernice, P. *Applied Catalysis B-Environmental* 156, 101-107 (2014).
851. Particle size, charge and colloidal stability of humic acids coprecipitated with Ferrihydrite. Angelico, R; Ceglie, A; He, JZ; Liu, YR; Palumbo, G; Colombo, C. *Chemosphere* 99, 239-247 (2014).
852. Pathophysiology of tobacco smoke exposure: recent insights from comparative and redox proteomics. Colombo, G; Clerici, M; Giustarini, D; Portinaro, NM; Aldini, G; Rossi, R; Milzani, A; Dalle-Donne, I. *Mass Spectrometry Reviews* 33, 183-218 (2014).
853. Phase behavior of the ternary aqueous mixtures of two polydisperse ethoxylated nonionic surfactants. Vitiello, G; Mangiapia, G; Romano, E; Lavorgna, M; Guido, S; Guida, V; Paduano, L; D'Errico, G. *Colloids And Surfaces A-Physicochemical And Engineering Aspects* 442, 16-24 (2014).
854. Physicochemical characterization of partially hydrolyzed poly(vinyl acetate)-borate aqueous dispersions. Carretti, E; Matarrese, C; Fratini, E; Baglioni, P; Dei, L. *Soft Matter* 10, 4443-4450 (2014).
855. Phyto-liposomes as nanoshuttles for water-insoluble silybin-phospholipid complex. Angelico, R; Ceglie, A; Sacco, P; Colafemmina, G; Ripoli, M; Mangia, A. *International Journal Of Pharmaceutics* 471, 173-181 (2014).
856. Prediction of hydrogen-bonding networks around tyrosyl radical in P. eryngii versatile peroxidase W164Y variants: a QM/MMMD study. Bernini, C; Pogni, R; Basosi, R; Sinicropi, A. *Molecular Simulation* 40, 485-490 (2014).
857. Preparation and characterization of an advanced medical device for bone regeneration. Dorati, R; Colonna, C; Genta, I; Bruni, G; Visai, L; Conti, B. *AAPS PharmSciTech* 15, 75-82 (2014).
858. Preventing corona effects: multi-phosphonic acid poly(ethylene glycol) copolymers for stable stealth iron oxide nanoparticles. Torrisi, V; Graillot, A; Vitorazi, L; Crouzet, Q; Marletta, G; Loubat, C; Berret, JF. *Biomacromolecules* 15, 3171-3179 (2014).
859. Pyrazolo[4,3-e][1,2,4]triazine sulfonamides as carbonic anhydrase inhibitors with antitumor activity. Mojzych, M; Bielawska, A; Bielawski, K; Ceruso, M; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 2643-2647 (2014).
860. Quality of vision in patients implanted with aspherical and spherical intraocular lens: Intraindividual comparison. Semeraro, F; Romano, MR; Duse, S; Costagliola, C. *Indian Journal Of Ophthalmology* 62, 461-463 (2014).
861. Quinazoline-sulfonamides with potent inhibitory activity against the alpha-carbonic anhydrase from Vibrio cholerae. Alafeefy, AM; Ceruso, M; Al-Tamimi, AMS; Del Prete, S; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 5133-5140 (2014).
862. Rapid and simple determination of acrylamide in conventional cereal-based foods and potato chips through conversion to 3-[bis(trifluoroethanoyl)amino]-3-oxopropyl trifluoroacetate by gas chromatography coupled with electron capture and ion trap mass spectrometry detectors. Russo, MV; Avino, P; Centola, A; Notardonato, I; Cinelli, G. *Food Chemistry* 146, 204-211 (2014).

863. Reaction of Hg2+ Insertion into Cysteine Pairs Within Bovine Insulin Crystals Followed via Raman Spectroscopy. Caterino, M; Merlino, A; Balsamo, A; Russo Krauss, I; Parisi, S; Vergara, A. *Journal Of Solution Chemistry* 43, 135-143 (2014).
864. Recent Theoretical Approaches to Minimal Artificial Cells. Mavelli, F; Altamura, E; Cassidei, L; Stano, P. *Entropy* 16, 2488-2511 (2014).
865. Red human hair pheomelanin is a potent pro-oxidant mediating UV-independent contributory mechanisms of melanomagenesis. Panzella, L; Leone, L; Greco, G; Vitiello, G; D'Errico, G; Napolitano, A; d'Ischia, M. *Pigment Cell & Melanoma Research* 27 (2014).
866. Reduction of spectral interferences using ultraclean gold nanowire arrays in the LDI-MS analysis of a model peptide. Colaianni, L; Kung, SC; Taggart, DK; Picca, RA; Greaves, J; Penner, RM; Cioffi, N. *Analytical And Bioanalytical Chemistry* 406, 4571-4583 (2014).
867. Remote determination of chromophoric dissolved organic matter in lakes, China. Jiang, GJ; Ma, RH; Duan, HT; Loiselle, SA; Xu, JP; Liu, DW. *International Journal Of Digital Earth* 7, 897-915 (2014).
868. Removal of EDDS and copper from waters by TiO2 photocatalysis under simulated UV-solar conditions. Satyro, S; Marotta, R; Clarizia, L; Di Somma, I; Vitiello, G; Dezotti, M; Pinto, G; Dantas, RF; Andreozzi, R. *Chemical Engineering Journal* 251, 257-268 (2014).
869. Residual Perfluorocarbon Liquid (PFCL) in Human Eyes. Romano, MR; Vallejo-Garcia, JL; Castellani, C; Costagliola, C; Vinciguerra, P. *Annals Academy Of Medicine Singapore* 43, 195-196 (2014).
870. Salinity stress constrains photosynthesis in Fraxinus ornus more when growing in partial shading than in full sunlight: consequences for the antioxidant defence system. Fini, A; Guidi, L; Giordano, C; Baratto, MC; Ferrini, F; Brunetti, C; Calamai, L; Tattini, M. *Annals Of Botany* 114, 525-538 (2014).
871. Schottky barrier height tuning by Hybrid organic-inorganic multilayers. Torrisi, V; Squillaci, MA; Ruffino, F; Crupi, I; Grimaldi, MG; Marletta, G. *MRS Proceedings* 1660, 396/1-396/6 (2014).
872. Selective and simultaneous determination of NSAIDs in equine plasma by high-performance liquid chromatography with molecularly imprinted solid-phase extraction. Meucci, V; Minunni, M; Vanni, M; Sgorbini, M; Corazza, M; Intorre, L. *Bioanalysis* 6, 2055-2066 (2014).
873. Selective inhibition of human carbonic anhydrases by novel amide derivatives of probenecid: Synthesis, biological evaluation and molecular modelling studies. D'Ascenzio, M; Carradori, S; Secci, D; Vullo, D; Ceruso, M; Akdemir, A; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 3982-3988 (2014).
874. Separation of Enantiomers of a Phospholipid in Langmuir Monolayers by a New Selector. Caminati, G; Cicchi, S; Lascialfari, L; Brandi, A. *Chirality* 27, 784-787 (2014).
875. Serum and intraocular concentrations of erythropoietin and vascular endothelial growth factor in patients with type 2 diabetes and proliferative retinopathy. Semeraro, F; Cancarini, A; Morescalchi, F; Romano, MR; dell'Omo, R; Ruggeri, G; Agnifili, L; Costagliola, C. *Diabetes & Metabolism* 40, 445-451 (2014).
876. Shadow ribbon: A detailed study of complex chemical plants with a simple integrated approach. Monitto, R; Tuccitto, N. *RSC Advances* 4, 32237-32240 (2014).
877. Simultaneous removal of N, N'-ethylenediamine-disuccinic acid (EDDS) and cupric ions from aqueous solution by TiO2 photocatalysis under simulated UV-solar conditions: kinetics, mechanism and ecotoxicity assessment. Satyro, S; Clarizia, L; Di Somma, I; Vitiello, G; Marotta, R; Pinto, G; Dantas, RF; Dezotti, M; Andreozzi, R. *Chemical Engineering Journal* 251, 257-268 (2014).
878. Some physicochemical remarks on spontaneous emulsification of vitreal tamponades. Costagliola, C; Semeraro, F; dell'Omo, R; Zeppa, L; Bufalo, G; Cardone, M; Romano, M; Ambrosone, L. *Biomed Research International* 2014, 243056-243056 (2014).
879. Spectroscopic characterization of 2,6-dimethoxyphenol radical intermediates in the Coriolopsis gallica laccase-mediator system. Martorana, A; Vazquez-Duhalt, R; Aguila, SA; Basosi, R; Baratto, MC. *Journal Of Molecular Catalysis B-Enzymatic* 107, 100-105 (2014).
880. Structural and denaturation studies of two mutants of a cold adapted superoxide dismutase point to the importance of electrostatic interactions in protein stability. Merlino, A; Russo Krauss, I; Castellano, I; Ruocco, MR; Capasso, A; De Vendittis, E; Rossi, B; Sica, F. *Biochimica Et Biophysica Acta-Proteins And Proteomics* 1844, 632-640 (2014).
881. Structural and Morphological Study of a Poly(3-hexylthiophene)/Streptavidin Multi layer Structure Serving as Active Layer in Ultra-Sensitive OFET Biosensors. Magliulo, M; Altamura, D; Di Franco, C; Santacroce, MV; Manoli, K; Mallardi, A; Palazzo, G; Scamarcio, G; Giannini, C; Torsi, L. *Journal Of Physical Chemistry C* 118, 15853-15862 (2014).
882. Structural evolution upon decomposition of the $LiAlH_4$ + $LiBH_4$ system. Soru, S; Taras, A; Pistidda, C; Milanese, C; Minella, CB; Masolo, E; Nolis, P; Baro, MD; Marini, A; Tolkiehn, M; Domheim, M; Enzo, S; Mulas, G; Garroni, S. *Journal Of Alloys And Compounds* 615, S693-S697 (2014).

883. Structural features of the C8 antiviral peptide in a membrane-mimicking environment. Scrima, M; Di Marino, S; Grimaldi, M; Campana, F; Vitiello, G; Piotto, SP; D'Errico, G; D'Ursi, AM. *Biochimica Et Biophysica Acta-Biomembranes* 1838, 1010-1018 (2014).
884. Structural Insights into Carbonic Anhydrase IX Isoform Specificity of Carbohydrate-Based Sulfamates. Moeker, J; Mahon, BP; Bornaghi, LF; Vullo, D; Supuran, CT; McKenna, R; Poulsen, SA. *Journal Of Medicinal Chemistry* 57, 8635-8645 (2014).
885. Structural Insights on Carbonic Anhydrase Inhibitory Action, Isoform Selectivity, and Potency of Sulfonamides and Coumarins Incorporating Arylsulfonylureido Groups. Bozdag, M; Ferraroni, M; Carta, F; Vullo, D; Lucarini, L; Orlandini, E; Rossello, A; Nuti, E; Scozzafava, A; Masini, E; Supuran, CT. *Journal Of Medicinal Chemistry* 57, 9152-9167 (2014).
886. Structural insights on nanoparticles containing gadolinium complexes as potential theranostic. Accardo, A; Ringhieri, P; Szekely, N; Pipich, V; Luchini, A; Paduano, L; Tesauro, D. *Colloid And Polymer Science* 292, 1121-1127 (2014).
887. Structure-based screening for the discovery of new carbonic anhydrase VII inhibitors. De Luca, L; Ferro, S; Damiano, FM; Supuran, CT; Vullo, D; Chimirri, A; Gitto, R. *European Journal Of Medicinal Chemistry* 71, 105-111 (2014).
888. Structure-rheology relationship in weakly amphiphilic block-copolymer Langmuir monolayers. Li Destri, G; Miano, F; Marletta, G. *Langmuir* 30, 3345-3353 (2014).
889. Study of XAD-2 adsorbent for the enrichment of trace levels of phthalate esters in hydroalcoholic food beverages and analysis by gas chromatography coupled with flame ionization and ion-trap mass spectrometry detectors. Cinelli, G; Avino, P; Notardonato, I; Centola, A; Russo, MV. *Food Chemistry* 146, 181-187 (2014).
890. Studying the Colline Metallifere mining area in Tuscany: an interdisciplinary approach. Benvenuti, M; Bianchi. G; Bruttini, J; Buonincontri, L; Chiarantini, L; Dallai, L; Di Pasquale, G; Donati, A; Grassi, F; Pescini, V. *IES Yearbook*, 261-287 (2014).
891. Substituted benzene sulfonamides incorporating 1,3,5-triazinyl moieties potently inhibit human carbonic anhydrases II, IX and XII. Saluja, AK; Tiwari, M; Vullo, D; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 1310-1314 (2014).
892. Sulfa and trimethoprim-like drugs - antimetabolites acting as carbonic anhydrase, dihydropteroate synthase and dihydrofolate reductase inhibitors. Capasso, C; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 379-387 (2014).
893. Sulfonamide inhibition studies of the beta carbonic anhydrase from Drosophila melanogaster. Syrjanen, L; Parkkila, S; Scozzafava, A; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 2797-2801 (2014).
894. Sulfonamide inhibition studies of the delta-carbonic anhydrase from the diatom Thalassiosira weissflogii. Vullo, D; Del Prete, S; Osman, SM; De Luca, V; Scozzafava, A; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry Letters* 24, 275-279 (2014).
895. Sulfonamide inhibition studies of the gamma-carbonic anhydrase from the oral pathogen Porphyromonas gingivalis. Vullo, D; Del Prete, S; Osman, SM; De Luca, V; Scozzafava, A; AlOthman, Z; Supuran, CT; Capasso, C. *Bioorganic & Medicinal Chemistry Letters* 24, 240-244 (2014).
896. Sulfonamide inhibition studies of two beta-carbonic anhydrases from the bacterial pathogen Legionella pneumophila. Nishimori, I; Vullo, D; Minakuchi, T; Scozzafava, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 2939-2946 (2014).
897. Sulfonamide inhibition study of the carbonic anhydrases from the bacterial pathogen Porphyromonas gingivalis: The beta-class (PgiCAb) versus the gamma-class (PgiCA) enzymes. Del Prete, S; Vullo, D; Osman, SM; Scozzafava, A; AlOthman, Z; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 4537-4543 (2014).
898. Sulfonamides and their isosters as carbonic anhydrase inhibitors. Carta, F; Supuran, CT; Scozzafava, A. *Future Medicinal Chemistry* 6, 1149-1165 (2014).
899. Sulfonamides incorporating fluorine and 1,3,5-triazine moieties are effective inhibitors of three beta-class carbonic anhydrases from Mycobacterium tuberculosis. Ceruso, M; Vullo, D; Scozzafava, A; Supuran, CT. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 686-689 (2014).
900. Sulfonamides with Potent Inhibitory Action and Selectivity against the alpha-Carbonic Anhydrase from Vibrio cholerae. Ceruso, M; Del Prete, S; Alothman, Z; Capasso, C; Supuran, CT. *Acs Medicinal Chemistry Letters* 5, 826-830 (2014).
901. Surface plasmon resonance applications in clinical analysis. Mariani, S; Minunni, M. *Analytical, Bioanalytical Chemistry* 406, 2303-2323 (2014).
902. Surfactant recovery from mesoporous metal-modified materials (Sn–, Y–, Ce–, Si–MCM-41), by ultrasound assisted ion-exchange extraction and its re-use for a microwave in situ cheap and eco-friendly MCM-41 synthesis. González-Rivera, J; Tovar-Rodríguez, J; Bramanti, E; Duce, C; Longo, I; Fratini, E; Galindo-Esquivel, IR; Ferrari, C. *Journal of Materials Chemistry A* 2, 7020 (2014).

903. Synthesis and carbonic anhydrase I, II, IX and XII inhibition studies of 4-N,N-disubstituted sulfanilamides incorporating 4,4,4-trifluoro-3-oxo-but-1-enyl, phenacylthiourea and imidazol-2(3H)-one/thione moieties. Congiu, C; Onnis, V; Balboni, G; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 1776-1779 (2014).
904. Synthesis and characterization of hybrid copper-chitosan nano-antimicrobials by femtosecond laser-ablation in liquids. Ancona, A; Sportelli, MC; Trapani, A; Picca, RA; Palazzo, C; Bonerba, E; Mezzapesa, FP; Tantillo, G; Trapani, G; Cioffi, N. *Materials Letters* 136, 397-400 (2014).
905. Synthesis and evaluation of F-18-labeled carbonic anhydrase IX inhibitors for imaging with positron emission tomography. Pan, JH; Lau, J; Mesak, F; Hundal, N; Pourghiasian, M; Liu, ZB; Benard, F; Dedhar, S; Supuran, CT; Lin, KS. *Journal Of Enzyme Inhibition And Medicinal Chemistry* 29, 249-255 (2014).
906. Synthesis of 6-tetrazolyl-substituted sulfocoumarins acting as highly potent and selective inhibitors of the tumor-associated carbonic anhydrase isoforms IX and XII. Grandane, A; Tanc, M; Zalubovskis, R; Supuran, CT. *Bioorganic & Medicinal Chemistry* 22, 1522-1528 (2014).
907. Synthesis of a new series of N-4-substituted 4-(2-aminoethyl) benzenesulfonamides and their inhibitory effect on human carbonic anhydrase cytosolic isozymes I and II and transmembrane tumor-associated isozymes IX and XII. Slawinski, J; Brzozowski, Z; Zolnowska, B; Szafranski, K; Pogorzelska, A; Vullo, D; Supuran, CT. *European Journal Of Medicinal Chemistry* 84, 59-67 (2014).
908. Synthesis of new biologically active isothiazolo[4,5-b]carbazole-type tetracyclic derivatives via an indole-2,3-quinodimethane approach. Miambo, RF; Laronze-Cochard, M; Lawson, AM; Guillot, R; Baldeyrou, B; Lansiaux, A; Supuran, CT; Sapi, J. *Tetrahedron* 70, 8286-8302 (2014).
909. Synthesis of sulfonamides with effective inhibitory action against Porphyromonas gingivalis gamma-carbonic anhydrase. Ceruso, M; Del Prete, S; AlOthman, Z; Osman, SM; Scozzafava, A; Capasso, C; Supuran, CT. *Bioorganic & Medicinal Chemistry Letters* 24, 4006-4010 (2014).
910. Systemic thromboembolic adverse events in patients treated with intravitreal anti-VEGF drugs for neovascular age-related macular degeneration: an overview. Semeraro, F; Morescalchi, F; Duse, S; Gambicorti, E; Romano, MR; Costagliola, C. *Expert Opinion On Drug Safety* 13, 785-802 (2014).
911. Tamponade or Filling Effect: Changes of Forces in Myopic Eyes. Semeraro, F; Morescalchi, F; Russo, A; Romano, MR; Costagliola, C. *Biomed Research International* (2014).
912. Templated globules - applications and perspectives. Cuomo, F; Lopez, F; Ceglie, A. *Advances In Colloid And Interface Science* 205, 124-133 (2014).
913. The binding of quinone to the photosynthetic reaction centers: kinetics and thermodynamics of reactions occurring at the Q(B)-site in zwitterionic and anionic liposomes. Mavelli, F; Trotta, M; Ciriaco, F; Agostiano, A; Giotta, L; Italiano, F; Milano, F. *European Biophysics Journal With Biophysics Letters* 43, 301-315 (2014).
914. The conservation of wall paintings: the conflictual relationship with water. Baglioni, P; Chelazzi, D; Giorgi, R. *Aqua Incognita: Why Ice Floats on Water, and Galileo 400 Years on, Lo Nostro, P; Ninham, BW Eds., Connor Court, Ballarat*, 18-33 (2014).
915. The evolution of the dye sensitized solar cells from Gratzel prototype to up-scaled solar applications: A life cycle assessment approach. Parisi, ML; Maranghi, S; Basosi, R. *Renewable & Sustainable Energy Reviews* 39, 124-138 (2014).
916. The influence of water on protein properties. Mallamace, F; Baglioni, P; Corsaro, C; Chen, SH; Mallamace, D; Vasi, C; Stanley, HE. *Journal Of Chemical Physics* 141 (2014).
917. The p85 regulatory subunit of PI3K mediates cAMP-PKA and insulin biological effects on MCF-7 cell growth and motility. Di Zazzo, E; Feola, A; Zuchegna, C; Romano, A; Donini, C F; Bartollino, S; Costagliola, C; Frunzio, R; Laccetti, P; Di Domenico, M; Porcellini, A. *The Scientific World Journal* 2014, 565839-565839 (2014).
918. The removal of aged acrylic coatings from wall paintings using microemulsions. Brajer, I; Fossé-Le Rouzic, M; Shashoua, Y; Taube, M; Chelazzi, D; Baglioni, M; Giorgi, R; Baglioni, P. *ICOM-CC 17th Triennial Conference Preprints, Melbourne, 15–19 September 2014, ed. J. Bridgland, Paris: International Council of Museums*, art. 1103, 8 pp. (2014).
919. The role of microemulsions in lipase-catalyzed hydrolysis reactions. Lopez, F; Cinelli, G; Colella, M; De Leonardis, A; Palazzo, G; Ambrosone, L. *Biotechnology Progress* 30, 360-366 (2014).
920. The Role Of Virgin Olive Oil In The Traditional Mediterranean Cuisine. De Leonardis, A; Macciola, V; Lopez, F. *In: Virgin Olive Oil: Production, Composition, Uses and Benefits for Man*, 258-281 (2014).
921. The Structural Comparison Between Membrane-Associated Human Carbonic Anhydrases Provides Insights into Drug Design of Selective Inhibitors. Alterio, V; Pan, P; Parkkila, S; Buonanno, M; Supuran, CT; Monti, SM; De Simone, G. *Biopolymers* 101, 769-778 (2014).
922. Therapeutic targeting of cancer cells in the hypoxic microenvironment using an orally bioavailable small molecule inhibitor of carbonic anhydrase IX. McDonald, PC; Sanghera, J; Singh, M; Lou, YM; Vallejo, M; Supuran, CT; Dedhar, S. *Cancer Research* 74 (2014).

923. Thermal analysis of milling products and its implications in self-ignition. Bufalo, G; Costagliola, C; Mosca, M; Ambrosone, L. *Journal Of Thermal Analysis And Calorimetry* 115, 1989-1998 (2014).
924. Three immobilized enzymes acting in series in layer by layer assemblies: Exploiting the trehalase-glucose oxidase-horseradish peroxidase cascade reactions for the optical determination of trehalose. Palazzo, G; Colafemmina, G; Iudice, CG; Mallardi, A. *Sensors And Actuators B-Chemical* 202, 217-223 (2014).
925. Time resolved SAXS to study the complexation of siRNA with cationic micelles of divalent surfactants. Falsini, S; Ristori, S; Ciani, L; Di Cola, E; Supuran, CT; Arcangeli, A; In, M. *Soft Matter* 10, 2226-2233 (2014).
926. TiO2/graphene-like photocatalysts for selective oxidation of 3-pyridine-methanol to vitamin B3 under UV/solar simulated radiation in aqueous solution at room conditions: The effect of morphology on catalyst performances. Alfe, M; Spasiano, D; Gargiulo, V; Vitiello, G; Di Capua, R; Marotta, R. *Applied Catalysis A-General* 487, 91-99 (2014).
927. Trace determination of acaricides in honey samples using XAD-2 adsorbent and gas chromatography coupled with an ion trap mass spectrometer detector. Notardonato, I; Avino, P; Cinelli, G; Russo, MV. *Rsc Advances* 4, 42424-42431 (2014).
928. Translocation of Platinum Anticancer Drugs by Human Copper ATPases ATP7A and ATP7B. Tadini-Buoninsegni, F; Bartolommei, G; Moncelli, MR; Inesi, G; Galliani, A; Sinisi, M; Losacco, M; Natile, G; Arnesano, F. *Angewandte Chemie-International Edition* 53, 1297-1301 (2014).
929. Tris Buffer Modulates Polydopamine Growth, Aggregation, and Paramagnetic Properties. Della Vecchia, NF; Luchini, A; Napolitano, A; D'Errico, G; Vitiello, G; Szekely, N; d'Ischia, M; Paduano, L. *Langmuir* 30, 9811-9818 (2014).
930. Tumor Microenvironment as Target in Cancer Therapy. Reich, R; Supuran, CT; Breuer, E. *Annual Reports In Medicinal Chemistry, Vol 49* 49, 269-284 (2014).
931. Tumor Microenvironmental Changes Induced by the Sulfamate Carbonic Anhydrase IX Inhibitor S4 in a Laryngeal Tumor Model. Meijer, TWH; Bussink, J; Zatovicova, M; Span, PN; Lok, J; Supuran, CT; Kaanders, JHAM. *Plos One* 9 (2014).
932. Ultrasound-vortex-assisted dispersive liquid-liquid microextraction coupled with gas chromatography with a nitrogen-phosphorus detector for simultaneous and rapid determination of organophosphorus pesticides and triazines in wine. Cinelli, G; Avino, P; Notardonato, I; Russo, MV. *Analytical Methods* 6, 782-790 (2014).
933. Understanding non-ideal voltage behaviour of cathodes for lithium-ion batteries. Kalantarian, MM; Oghbaei, M; Asgari, S; Ferrari, S; Capsoni, D; Mustarelli, PJ. *Mater Chem A* 2, 19451-19460 (2014).
934. Unveiling the artistic technique of the Florentine Codex: when the Old World and the New World met. Giorgi, R; Chelazzi, D; Magaloni Kerpel, D. *Science and Art - The Painted Surface Edited by A. Sgamellotti, B.G. Brunetti, C. Miliani, RSC publishing* (2014).
935. Using canalography to visualize the in vivo aqueous humor outflow conventional pathway in humans. Zeppa, L; Ambrosone, L; Guerra, G; Fortunato, M; Costagliola, C. *JAMA Ophthalmology* 132, 1281 (2014).
936. Variability of particulate organic carbon in inland waters observed from MODIS Aqua imagery. Duan, HT; Feng, L; Ma, RH; Zhang, YC; Loiselle, SA. *Environmental Research Letters* 9 (2014).
937. Water soluble trehalose-derived oligoamides. Oliva, R; Albanese, F; Cipriani, G; Ridi, F; Giomi, D; Malavolti, M; Bernini, L; Salvini, A. *Journal Of Polymer Research* 21 (2014).

Conferences 2014-2016

1. Altamura, E.; Milano, F.; Trotta, M.; Omar, O.H.; Stano, P.; Mavelli, F. XXIII Congresso Nazionale SIPBA, in Cortona (Italy), 18-21/09/2016. Oral presentation.
2. Altamura, E.; Milano, F.; Trotta, M.; Omar, O.H.; Stano, P.; Mavelli, F. Syschem 2016, Valtice Chateau (CZ), 08-12/05/2016. Oral presentation.
3. Ancona, A.; Sportelli, M.C.; Picca, R.A.; Izzi, M.; Di Maria, A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. EMRS2016 Spring Meeting, Lille (France), 01-06/05/2016, Symposium C. Oral communication.
4. Angelico, R.; Ceglie, A.; Sacco, P.; Ripoli, M. 30th Conference of the European Colloid and Interface Society (ECIS 2016), Roma (Italy), 04-09/09/2016. Poster.
5. Angelico, R.; Ceglie, A.; Sacco, P.; Ripoli, M. 30th Conference of the European Colloid and Interface Society (ECIS 2016), Roma (Italy), 04-09/09/2016. Poster.
6. Angelico, R.; Gentile, L.; Ranieri, G.A.; Oliviero Rossi, C. Organizing Molecular Matter - A Soft Matter Symposium, Lund (Sweden), 19-26/06/2016. Oral presentation.
7. Angelico, R.; Gentile, L.; Ranieri, G.A.; Oliviero Rossi, C. XLIV Congresso Nazionale della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
8. Angelico, R.; Oliviero Rossi, C.; Caputo, P.; Calandra, P.; Mezzi, A.; Teltayev, B. 30th Conference of the European Colloid and Interface Society (ECIS 2016), Roma (Italy), 04-09/09/2016. Poster.
9. Baglioni, P. 12th International Conference on Colloid and Surface Chemistry, Iasi (Romania), 16-18/05/2016. Invited lecture.
10. Baglioni, P. Annual Surface and Materials Chemistry Symposium 2016, Gothenburg (Svezia), 8-10/11/2016. Invited lecture.
11. Baglioni, P. Chemistry of Art Reconstruction, Accademia Reale Olandese, Van Arkel Award, Amsterdam (Olanda), 26/05/2016. Plenary lecture.
12. Baglioni, P. ECIS 2016, 30th International conference of the European Colloid and Interface Society, Rome, 04-09/09/2016. Overbeek award plenary lecture.
13. Baglioni, P. Formula VIII, Barcelona (Spagna), 04-07/07/2016. Plenary lecture.
14. Baglioni, P. Italy-Mexico, bilateral meeting on study, conservation and restoration of cultural and archeological heritage: research technologies and infrastructures for the science of cultural heritage, Mexico City, 02-03/02/2016. Invited lecture.
15. Baglioni, P. Italian National Conference on Materials Science and Technology, Catania, 12-16/12/2016. Invited lecture.
16. Baglioni, P. IV International workshop on research, conservation and valorization of architectural monuments: preservation of built heritage, Lima (Peru), 04-06/05/2016. Invited lecture.
17. Baglioni, P. La fisica incontra la città - Phisics meets the city, Università degli Studi Roma Tre, 9th March 2016. Public invited lecture.
18. Baglioni, P. Nano and advanced materials for cultural heritage, Bruxelles (Belgio), 24/05/2016. Invited lecture.
19. Baglioni, P. Nanoinnovation 2016, Rome, 20-23/09/2016. Invited lecture.
20. Baglioni, P. Nanotechitaly, Roma, 21/09/2016. Invited lecture.
21. Baglioni, P. Nanotechnology applied to conservation and restoration, Pinacoteca de Sao Paulo, Brasil, 07/04/2016. Invited lecture.
22. Baglioni, P. Our Past, your Future, Venezia, 29-30/10/2016. Invited lecture.
23. Baglioni, P. Second Riches Polymer Seminar – New horizons for cultural heritage, Bruxelles (Belgio), 23/05/2016. Invited lecture.
24. Baglioni, P. Third Riches Polymer Seminar – Networking session of EC-funded projects, Berlin, 22/11/2016. Invited lecture.
25. Baglioni, P.; Pensabene, L. 'Sette'-Magazine del Corriere della sera, 02/09/2016. "Il Picasso che non ti aspetti, ritrovato sotto una mano di bianco". Invited article and Youtube.
26. Baratto, M.C.; Al Khatib, M.; Harir, M; Pogni, R.; Basosi, R. Xth EFEPR Conference, Torino (Italy), 04-08/09/2016. Poster.
27. Basosi, R. Congresso ATI 15/09/2016. Plenary lecture.
28. Basosi, R. University of Beni Mellal (Morocco), 19/10/2016. Plenary lecture.
29. Basosi, R. University of Teheran 30/08/2016. Plenary lecture.
30. Berretti, E.; Di Benedetto, F.; Cioffi, N.; Capolupo, F.; Lavacchi, A.; Picca, R.A.; Comparini, A.; Passaponti, M.; Innocenti, M. Enerchem-1, Firenze, 18-20/02/2016. Poster.
31. Berti, D. 30th Conference of the European Colloid and Interaface Society, Rome, September 2016. Invited lecture.
32. Berti, D. Nanostructured materials meet lipid bilayer membranes: a colloidal perspective, Università di Tor Vergata, Dipartimento di Chimica, Roma (Italia), Aprile 2016. Invited presentation.
33. Bonechi, C.; Tamasi, G.; Donati, A.; Magnani, A Rossi, C. 13th Edition Emory-Unisi Summer School, Chemistry for Life and Environment, Siena, 27/05/2016-04/07/2016. Poster.

34. Byelyakova, A.; Tamasi, G.; Rossi, C. 13th Edition Emory-Unisi Summer School, Chemistry for Life and Environment, Siena, 27/05/2016-04/07/2016. Poster.
35. Caminati, G. 16th International Conference on Organized Molecular Films (ICOMF16)-LB16, Helsinki (Finland), 25-29/07/2016. Oral presentation.
36. Carretti, E.; Scarano, S.; Dei, L.; Minunni, M.; Baglioni, P. 251 American Chemical Society (ACS) Spring meeting, San Diego, CA, USA, 13-17/03/2016. Oral presentation.
37. Casiello, M.; Sikorski, W.; Cotugno, P.; Monopoli, A.; Ciminale, F.; Picca, R.; Cioffi, N.; Bellebuono, L.; Irrera, A.; Trusso, S.; Lo Faro, M.J.; Trzeciak, A.M.; Nacci, A. 12th Congress of the Interdivisional Group of Organometallic Chemistry Genoa, 05-08/06/2016. Poster.
38. Chaudhary, A.L.; Milanese, C.; Girella, A.; Bergemann, N.; Pistidda, C.; Klassen, T.; Dornheim, M. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken Switzerland, 07-12/08/2016. Oral presentation.
39. Cioffi, N. N&N 2016 - Nanoscience & Nanotechnology INFN Meeting 2016, INFN national laboratories, Frascati-Rome, 26-29/09/2016. Plenary lecture.
40. Cofrancesco, P.; Milanese, C.; Trojsi, G.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Frisetti A., XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
41. Cuomo, F.; Ceglie, A.; Caltagirone, C.; Murgia, S.; Lopez, F. 30th Conference of The European Colloid and Interface Society (ECIS), Rome (Italy), 04-09/09/2016. Poster.
42. Dallai, L.; Volpi. V.; Donati. A. CAA 2016 - The 44rd Computer Applications and Quantitative Methods in Archaeology 'Exploring Ocean's of data' Conference, Oslo, 29/03/2016-02/04/2016. Poster.
43. De Luca, A.; Giaccherini, A.; Comparini, A.; Pasquini, B.; Picca, R.A.; Cioffi, N.; Piciollo, E.; Furlanetto, S.; Di Benedetto, F.; Innocenti, M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Poster.
44. De Santis, A; Emendato, A; Russo Krauss, I; Picone, D; D'Errico, G; Pauanno, L. 6th EuCheMS Chemistry Congress, Seville (Spain), 11-15/09/16. Oral presentation.
45. De Santis, A; Russo Krauss, I; Marasco, D; D'Errico, G. XLIV Congresso della Divisione di Chimica Fisica della Società Chimica Italiana. Napoli (Italy), 20-23/09/2016. Poster.
46. Dilonardo, E.; Penza, M.; Alvisi, M.; Cassano, G.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium X. Poster.
47. Dilonardo, E.; Penza, M.; Alvisi, M.; Rossi, R.; Cassano, G.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium X. Oral communication.
48. Ditaranto, N.; Casiello, M.; Nacci, A.; Palmisano, F.; Sabbatini, L.; Torsi, L.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Invited oral communication.
49. Donati, A. Congresso I paesaggi dell'allume: archeologia della produzione ed economia di rete, Roma-Siena, 09-11/05/2016. Oral presentation.
50. Ferraro, G.; Fratini, E.; Rausa, R.; Baglioni P. ECIS Conference, Roma (Italy), 05-09/09/2016. Oral presentation.
51. Ferraro, G.; Fratini, E.; Rausa, R.; Baglioni P. EMRS Fall Meeting, Warsaw (Poland), 19-22/09/2016. Poster.
52. Franchini, C.; Cavalluzzi, M.M.; Gualdani, R.; Moncelli, M.R.; Lentini, G. XXIV National Meeting in Medicinal Chemistry, Perugia (Italy), 11-14/09/2016. Poster.
53. Gaboardi, M.; Milanese, C.; Magnani, G.; Mauron, P.; Duyker, S.; Peterson, V.K.; Saldan, I.; Pontiroli, D.; Galinetto, P.; Riccò, M. 10th International Symposium Hydrogen & Energy, Sendai (Japan), 21-26/02/2016. Oral presentation.
54. Galinetto P.; Albini, B.; Mozzati, M.C.; Bini, M.; Tondo, C.; Capsoni, D. CNISM-Materials 2016, Catania (Italia) 12-16/12/2016. Poster.
55. Giaccherini, A.; Giurlani, W.; Pasquini, B.; Capolupo, F.; Picca, R.A.; Felici, R.; Carlà, F.; Cioffi, N.; Furlanetto, S.; Lavacchi, A.; Di Benedetto, F.; Innocenti, M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
56. Giaccherini, A.; Picca, R.A.; Sportelli, M.C.; Capolupo, F.; Montegrossi, G.; Cioffi, N.; Felici, R.; Carlà, F.; Lavacchi, A.; Di Benedetto, F.; Innocenti, M. Enerchem-1, Firenze (Italy), 18-20/02/2016. Poster.
57. Giorgi, R. II Simposio Internacional Andrew W. Mellon: El esplendor del Pórtico de la Gloria: conservación, policromía y la transfiguración de la material, 07-08/07/2016. Oral presentation.
58. Giorgi, R. International Winter School Molecules@Surfaces, Societa' Chimica Italiana, 31/01-05/2/2016, Villaggio Olimpico di Bardonecchia. Oral presentation.
59. Giorgi, R. Meeting SSH 2016 Net4Society – SSH in H2020 Societal Challenge 6 and integration in other challenges, Bruxelles, 05/07/2016. Oral presentation.

60. Giorgi, R.; Baglioni, M.; Shashoua, Y.; Brajer, I.; Baglioni, P. XVI Congresso nazionale di Chimica dell'Ambiente e dei Beni Culturali - Dall'emergenza alla salvaguardia: la chimica per un nuovo modello di sviluppo, Lecce, 26-29/06/2016. Oral presentation.
61. Gualdani, R. Regional Biophysics Conference RBC2016, Trieste (Italy), 25-28/08/2016. Invited talk.
62. Gualdani, R.; Cavalluzzi, M.M.; Lentini, G. XXIII Congresso Nazionale SIBPA 2016, Cortona (Italy) 18-21/09/2016. Poster.
63. Gualdani, R.; Guerrini, A.; Fantechi, E.; Sangregorio, C.; Moncelli, M.R. 60th Biophysical Meeting, Los Angeles (USA), 27/02/2016-02/03/2016. Poster.
64. Harir, M.; Baratto, M.C.; Basosi, R.; Pogni, R. Oxizymes 2016, Wageningen, 03-06/07/2016. Poster.
65. Innocenti, M.; Di Benedetto, F.; Giaccherini, A.; Guerri, A.; Lavacchi, A.; Comparini, A.; Miller, H.; Carlà, F.; Felici, R.; Picca, R.A.; Cioffi, N.; Vizza, F. ECM6: 6th International symposium on Energy Challenges and Mechanics, Inverness (Scotland), 14-18/08/2016. Invited oral communication.
66. Innocenti, M.; Giaccherini, A.; Di Benedetto, F.; Lavacchi, A.; Miller, H.A.; Cioffi, N.; Picca, R.A.; Vizza, F. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
67. Licciardello, A. Workshop & reunion des utilisateurs francophones ToF-SIMS, Mons, 09-10/03/2016. "SIMS and chemistry: from surface engineering to sputtering of polymers". Invited oral presentation.
68. Lisi, S.; Ravelet, C.; Scarano, S.; M. Minunni, M.; Peyrin, E. Aptamers in Bordeaux, Bordeaux (France), June 2016. Poster.
69. Lisi, S.; Ravelet, C.; Scarano, S.; Minunni, M.; Peyrin, E. Biosensors 2016, Gothenburg (Sweden), 25-27/05/2016. Poster.
70. Lisi, S.; Scarano, S.; Fedeli, S.; Cicchi, S.; Ravelet, C.; Peyrin, E.; Minunni, M. Bioanalitica 2016, giornata scientifica "Chimica bioanalitica e nanotecnologie", Bologna, 04/07/2016. Oral presentation.
71. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni, M. Biosensors 2016, 25-27/05/2016, Gothenburg (Sweden). Poster.
72. Luchini A.; Gerelli Y.; Fragneto G.; Nylander T.; Paduano L. VI EuCheMS Chemistry Congress, Seville (Spain), 11-15/09/2016. Oral presentation.
73. Luchini, A.; Gerelli, Y.; Fragneto, G.; Nylander, T.; Paduano, L. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, 20-23/09/16. Poster presentation.
74. Maranghi, S.; Parisi, M.L; Sinicropi, A.; Basosi, R. 1° Congress of the Interdivisional Group of Chemistry for Renewable Energy of the Italian Chemical Society (ENERCHEM-1), Florence (FI), 18-20/02/2016. Poster.
75. Maranghi, S.; Parisi, M.L.; Basosi, R. IX Convegno della Rete Italiana LCA, Ravenna (RA), 23-24/06/2016. Poster.
76. Marletta, G. 8th International School on Organic Electronics: Nano-Organics and devices, Paris, France, 04-08/07/2016. Invited lecture.
77. Marletta, G. Symposium PM1 - Fall Meeting MRS, Boston 28/11-02/12/2016. Invited lecture.
78. Martina, M.R.; Baglioni, P.; Caminati, G. 16th International Conference on Organized Molecular Films (ICOMF16)-LB16, Helsinki (Finland), 25-29/07/2016. Oral presentation.
79. Mavelli, F. COMSOL Conference, Munich, Germany, 12-14/10/2016. Oral presentation.
80. Mavelli, F. International Workshop on Synthetic Approach to Origin of Life, Glasgow University, 29-30/09/2016. Invited oral presentation.
81. Mavelli, F. Wivace-Bionam 2016, Università di Salerno, Italy, 4-7/10/2016. Oral presentation.
82. Messina, G.M.L.; Marletta, G. E-MRS Spring Meeting, Lille (France), 02-06/05/2016. Oral presentation.
83. Messina, G.M.L.; Marletta, G. PEPMAT Peptide Materials for biomedicine and Nanotechnology, Barcelona (Spain), 13-17/03/2016. Invited lecture.
84. Messina, G.M.L.; Marletta, G. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, Italy, 20-23/09/2016. Oral presentation.
85. Messina, G.M.L.; Marletta, G.; De Zotti, M.; Formaggio, F. Materials.IT, Catania, Italy, 19-23/12/2016. Oral presentation.
86. Milanese, C.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Cofrancesco, P.; Marini, A.; Rueda Noriega, M.; Sanz-Moral, L.M.; Martin, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
87. Milanese, C.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Cofrancesco, P.; Marini, A.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Poster presentation.
88. Milanese, C.; Girella, A.; Valsecchi, G.; Marini, A.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M. E-MRS Fall Meeting 2016, Varsaw, Poland, 19-22/09/2016. Oral presentation.
89. Milanese, C.; Girella, A.; Valsecchi, G.; Saldan, I.; Gaboardi, M.; Pontiroli, D., Magnani, G.; Riccò, M.; Marini, A. International Symposium on Metal – Hydrogen Systems, MH 2016, Interlaken, Switzerland, 07-12/08/2016. Oral presentation.

90. Milanese, C.; Pontiroli, D.; D'Alessio, D.; Gaboardi, M.; Magnani, G.; Duyker, S.K.; Peterson, V.K.; Sharma, N.; Riccò, M. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken Switzerland, 07-12/08/2016. Poster presentation.
91. Milanese, C.; Saldan, I.; Girella, A.; Valsecchi, G.; Cofrancesco, P.; Marini, A.; Rueda Noriega, M.; Sanz-Moral, L.M.; Martin, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M. E-MRS Fall Meeting 2016, Varsaw, Poland, 19-22/09/2016. Oral presentation.
92. Milanese, C.; Saldan, I.;, Girella, A., Valsecchi, G.; Cabrini, E.; Pallavicini, P.; Galinetto, P.; Rueda Noriega, M.; Martin, A.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M.; Marini, A. 10th International Symposium Hydrogen & Energy, Sendai, Japan, 21-26/02/2016. Oral presentation.
93. Mozzachiodi, S.; Cardelli, L.; Stano, P.; Altamura, E.; Mavelli, F.; Marangoni, R. 13th Annual Meeting of the Bioinformatics Italian Society (BIT 2016), Università di Salerno (Italy), 15-17/06/2016. Poster.
94. Murgia, S. 2nd International Symposium on Nanoparticles/Nanomaterials and Applications, Caparica, Portogallo, 18-21/01/2016. Keynote lecture.
95. Murgia, S. Engineering Conference International, Hernstein, Austria, 10-14/07/2016. Invited speaker.
96. Murgia, S.; Meli, V.; Caltagirone, C.; Falchi, A.M.; Lippolis, V.; Hyde, S.T.; Monduzzi, M.; Obiols-Rabasa, M.; Rosa, A.; Schmidt, J.; Talmon, Y. 30th ECIS Conference, Rome, 04-09/09/2016. Poster.
97. Murgia. S. XLIV Congresso Divisione Chimica Fisica, Napoli, 20-23/09/2016. Oral presentation.
98. Nairi, V.; Salis, A.; Fanti, M; Medda, L; Cugia, F.; Piludu, M; Sogos, V.; Monduzzi M. 30th ECIS Conference, Roma (Italy), 04-09/09/2016. Poster.
99. Perfetti, M.; D'Errico, G.; Paduano L. 6th European Association of Chemical and Materials Societies (EuCheMs) International Congress Conference of the European Colloid and Interface Society, Siviglia (Spain), 11-15/09/2016. Poster.
100. Perfetti, M.; D'Errico, G.; Paduano L. XLIV Congresso della Divisione di Chimica Fisica della Società Chimica Italiana. Napoli (Italy), 20-23/09/2016. Oral presentation.
101. Perfetti, M.; Heenan, R.K.; D'Errico, G.; Paduano L. 30th Conference of the European Colloid and Interface Society, Roma (Italy), 04-09/09/2016. Poster.
102. Pica, A.; Russo Krauss, I.; Parente, V.; Sica, F. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli. Napoli (Italy), 20-23/09/16. Poster.
103. Picca, R.A.; Cinotti, S.; Giaccherini, A.; Sportelli, M.C.; Di Benedetto, F.; Innocenti, M.; Cioffi, N. Enerchem-1, Firenze, 18-20/02/2016. Oral communication.
104. Picca, R.A.; Giaccherini, A.; Di Benedetto, F.; Innocenti, M.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Oral communication.
105. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. EMN Croatia Meeting 2016 Dubrovnik, 04-07/05/2016. Invited communication.
106. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
107. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium L. Poster.
108. Picca, R.A.; Paladini, F.; Sportelli, M.C.; Pollini, M.; Giannossa, L.C.; Di Franco, C.; Mangone, A.; Valentini, A.; Sannino, A.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium S. Oral communication.
109. Picca, R.A.; Sportelli, M.C.; Ditaranto, N.; Giannossa, C.; Mangone, A.; Di Franco, C.; Paladini, F.; Pollini, M.; Sannino, A.; Tütüncü, E.; Kranz, C.; Mizaikoff, B.; Valentini, M.; Valentini, A.; Cioffi, N. EMN Energy Materials Nanotechnology, Cancun, Mexico, 04-09/06/2016. Invited oral communication.
110. Picca, R.A.; Sportelli, M.C.; Lopetuso, R.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium AA. Poster.
111. Picca, R.A.; Sportelli, M.C.; Lopetuso, R.; Villone, V.; Cioffi, N. 12th Congress of the Interdivisional Group of Organometallic Chemistry, Genoa, 05-08/06/2016. Poster.
112. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. Orbitaly 2016 Santa Cesarea, Lecce (Italy) 26-28/10/2016. Invited oral communication.
113. Picca, R.A.; Sportelli, M.C.; Quarto, R.; Ditaranto, N.; Valentini, A.; Cioffi, N. EMRS2016 Spring Meeting, Lille (France), 01-06/05/2016, Symposium Q. Poster.
114. Picca, R.A.; Sportelli, M.C.; Quarto, R.; Valentini, A.; Cioffi, N. 12th Congress of the Interdivisional Group of Organometallic Chemistry Genoa, 05-08/06/2016. Poster.
115. Picca, R.A.; Sportelli, M.C.; Villone, V.; Lopetuso, R.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Messina), 18-22/09/2016. Poster.
116. Pitzalis, F.; Salis, A.; Monduzzi, M. 30th ECIS Conference, Roma (Italy), 04-09/09/2016. Poster.

117. Pogni, R. Emory@Unisi, Siena, 21/06/2016. Invited lecture.
118. Pontiroli, D.; D'Alessio, D.; Gaboardi, M.; Magnani, G.; Riccò, G.; Milanese, C.; Duyker, S.G.; Peterson, V.K.; Sharma, N. E-MRS Fall Meeting 2016, Warsaw (Poland), 19-22/09/2016. Oral presentation.
119. Pontiroli, D.; Gaboardi, M.; Magnani, G.; Aramini, M.; Riccò, M.; Duyker, S.G.; Peterson, V.K.; Mauron, P.; Girella, A.; Milanese, C. Tematic Meeting "Materials for Energy", Roma, Università La Sapienza (Italy), 09/09/2016. Oral presentation.
120. Pontiroli, D.; Magnani, G.; Gaboardi, M.; Riccò, M.; Pramudita, J.C.; Sharma, N.; Milanese, C. 10th International Symposium Hydrogen & Energy, Sendai (Japan), 21-26/02/2016. Oral presentation.
121. Riccardi, C.; Musumeci, D.; Morvan, F.; Meyer, A.; Vasseur, J.J.; Russo Krauss, I.; Paduano, L., Montesarchio, D. 22th International Round Table on Nucleosides, Nucleotides and Nucleic Acids, Paris (France), 18-22/07/2016. Poster.
122. Ridi, F.; Tonelli, M.; Resta, C.; Baglioni, P. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, 20-23/09/2016. Poster.
123. Rossi, C.O.; Caputo, P.; Calandra, P.; Mezzi, A.; Teltayev, B; Angelico, R. 30th Conference of The European Colloid and Interface Society (ECIS), Rome (Italy), 04-09/09/2016. Poster.
124. Rueda Noriega, M.; Sanz-Moral, L.M.; Saldan, I.; Girella, A.; Milanese, C.; Martín, A. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken (Switzerland), 07-12/08/2016. Oral presentation.
125. Russo Krauss, I.; Napolitano, V.; Petraccone, L.; Mattia, C.A.; Sica, F. XLIV Congresso della Divisione di Chimica Fisica della SCI. Napoli (Italy), 20-23/09/16. Poster.
126. Russo Krauss, I.; Riccardi, C.; Montesarchio, D.; D'Errico, G.; Paduano, L. 30th Conference of the European Colloid and Interface Society, Roma (Italy), 05-09/09/16. Oral presentation
127. Salis, A.; Cugia, F.; Sedda, S.; Pitzalis, F.; Monduzzi, M. 30th ECIS Conference, Roma (Italy), 04-09/09/2016. Oral presentation.
128. Sarzi Amadè, N.; Sanna, S.; Carretta, P.; Riccò, M.; Pontiroli, D.; Gaboardi, M.; Magnani, G.; Milanese, C.; Girella, A. International Symposium on Metal – Hydrogen Systems MH 2016, Interlaken Switzerland, 07-12/08/2016. Oral presentation.
129. Scarano, S.; Berlangieri, C.; Carretti, E.; Dei, L.; Baglioni, P.; Minunni M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (ME), 18-22/09/2016. Poster.
130. Scarano, S.; Bonini, M.; Manera, M.G.; Colombelli, A.; Rella, R.; Minunni M. Plasmonica 2016, Genova, 14-16/09/2016. Poster.
131. Scarano, S.; Bonini, M.; Manera, M.G.; Rella, R.; Minunni, M. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Giardini Naxos (Italy), 18-22/09/2016. Oral presentation.
132. Scarano, S.; Carretti, E.; Baglioni, P.; Dei, L.; Minunni, M. Biosensors 2016, Gothenburg (Sweden), 25-27/05/2016. Poster.
133. Scarano, S.; Minunni, M. "Molecular diagnostic by optical based sensing", Warsaw (Polonia), 12-14/09/2016. Invited lecture.
134. Scarano, S.; Minunni, M. Acoustic and electrochemical methods in the study of affinity interactions at surfaces, AEMIS 2016, Bratislava (Slovakia), 20/06/2016. Oral presentation.
135. Scarano, S.; Minunni, M. Bioelectrochemistry and more…2016, Wiener Neustadt (Austria), 13-14/060/2016. Plenary invited presentation.
136. Sinicropi, A.; Parisi, M.L.; Basosi, R. XLIV Congresso della Divisione di Chimica Fisica, Napoli, 20-23/09/2016. Poster.
137. Sinicropi, A.; Parisi, M.L.; Reginato, G.; Zani, L.; Calamante, M.; Mordini, A.; Basosi, R.; Taddei, M. 1° Congress of the Interdivisional Group of Chemistry for Renewable Energy of the Italian Chemical Society (ENERCHEM-1), Florence (Italy), 18-20/02/2016. Poster.
138. Smeazzetto, S.; Young, H.S.; Trieber, C.A.; Moncelli M.R.; Tadini-Buoninsegni, F. 60th Biophysical Meeting, Los Angeles (USA), 27/02/2016-02/03/2016. Poster.
139. Spinelli, D.; Baratto, M.C.; Basosi, R.; Pogni, R. Oxizymes 2016, Wageningen, 03-06/07/2016. Poster.
140. Sportelli, M.C.; Ancona, A.; Picca, R.A.; Izzi, M.; Di Maria, A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. 12th Congress of the Interdivisional Group of Organometallic Chemistry Genoa, 05-08/06/2016. Oral communication.
141. Sportelli, M.C.; Ancona, A.; Picca, R.A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. XXVI Congresso della Divisione di Chimica Analitica della Società Chimica Italiana, Giardini Naxos (Italy), 18-22/09/2016. Oral communication.
142. Sportelli, M.C.; Tütüncü, E.; Picca, R.A.; Valentini, M.; Valentini, A.; Kranz, C.; Mizaikoff, B.; Cioffi, N. ISA2016 Matera, 29/05/2016-01/06/2016. Oral communication.
143. Sportelli, M.C.; Tütüncü, E.; Picca, R.A.; Valentini, M.; Valentini, A.; Kranz, C.; Mizaikoff, B.; Cioffi, N. EMRS2016 Spring Meeting, Lille, France, 01-06/05/2016, Symposium Q. Oral

communication.

144. Strambini, L.M.; Longo, A.; Scarano, S.; Prescimone, T.; Palchetti, I.; Minunni, M.; Giannessi, D.; Barillaro, G. Terzo Convegno Nazionale Sensori, Roma, 23-25/02/2016. Oral presentation.
145. Tadini-Buoninsegni, F.; Smeazzetto, S.; Moncelli, M.R.; Trieber, C.A.; Young, H.S. XXIII Congresso Nazionale SIBPA 2016, Cortona (Italy) 18-21/09/2016. Oral presentation.
146. Tamasi, G.; Bonechi, C.; Leone, G.; Donati, A.; Magnani, A.; Rossi, C. 13th Edition Emory-Unisi Summer School, Chemistry for Life and Environment, Siena, 27/05/2016-04/07/2016. Poster.
147. Tonelli, M.; Resta, C.; Ridi, F.; Baglioni, P. 6th EuCheMS Chemistry Congress, Sevilla (Spain), 12-16/09/2016. Poster.
148. Tonelli, M.; Ridi, F; Borsacchi, S.; Martini, F.; Calucci, L.; Geppi, M. 30th Conference of the European Colloid and Interface Society, Roma, 04-09/09/2016. Poster.
149. Tonelli, M.; Ridi, F.; Borsacchi, S.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Baglioni, P. 4th International Workshop on: Mechanisms and Modelling of Waste /Cement Interactions, Structural characterization of magnesium silicate hydrate: towards the design of eco-sustainable cements, 22-25/05/2016. Oral presentation.
150. Tonelli, M.; Ridi, F.; Borsacchi, S.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Baglioni, P. 4th International Workshop on: Mechanisms and Modelling of Waste /Cement Interactions, Structural characterization of magnesium silicate hydrate: towards the design of eco-sustainable cements, 22-25/05/2016. Poster.
151. Tovar Rodríguez, J.; Donato Moreno, J. E.; Galindo Esquivel, I.R.; Fratini, E.; Baglioni, P. Merck Young Chemists Symposium, MYCS 2016, Rimini (IT), 25-27/10/2016. Poster.
152. Tovar Rodríguez, J.; González Rivera, J.; Ferrari, C.; Longo, I; Fratini, E.; Baglioni, P. European Materials Research Society, EMRS Fall Meeting 2016, Warsaw (Poland), 19-22/09/2016. Oral presentation.
153. Troisi, R.; Russo Krauss, I.; Napolitano, V.; Sica, F. XLIV Congresso della Divisione di Chimica Fisica della SCI. Napoli (Italy), 20-23/09/16. Poster presentation.
154. Tuccitto, N.; Giamblanco, N.; Zappalà, G.; Licciardello, A.; Marletta, A. EMRS-Spring Meeting Lille (France), 2016. Oral presentation.
155. Tuccitto, N.; Marletta, G. Materials.IT, Catania (Italy), 19-23/12/2016. Oral presentation.
156. Tuccitto, N.; Sfuncia, G.; Marletta, G. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli (Italy), 20-23/09/2016. Oral presentation.
157. Tuccitto, N.; Vitale, S.; Zappalà, G.; Ronconi, F.; Licciardello, A. EMRS-Fall Meeting, Warsaw (Poland), 2016. Poster.
158. Tuccitto, N.; Zappalà, G.; Vitale, S.; Marletta, G.; Licciardello, A. EMRS-Fall Meeting, Warsaw (Poland), 2016. Invited keynote.
159. Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. SIMS Europe 2016, Münster (Germany), 18-20/09/2016. Oral presentation.
160. Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. SIMS Europe 2016, Münster (Germany), 18-20/09/2016. Poster.
161. Vitale, S.; Zappalà, G.; Santoni, M.P.; Tuccitto, N.; Hanan, G.; Campagna, S.; Licciardello, A. SIMS Europe 2016, Münster, Germany, 18-20/09/2016. Oral presentation.
162. Vitiello, G.; Silvestri, B.; Zanfardino, A.; Costantini, A.; Varcamonti, M.; D'Errico, G.; Branda, F.; Pezzella, A.; Luciani, G. XLIV Congresso Divisione Chimica-Fisica, Società Chimica Italiana (SCI), Napoli (Italy), 20-23/09/2016. Oral presentation.
163. Volpi, V; Donati, A; Dallai, L. Conference Precious metal in the medieval mediterranean, Aix-en-Provence (France), 06-08/10/2016. Oral presentation.
164. Weththimuni, M.L.; Capsoni, D.; Milenese, C.; Licchelli, M.; Malagodi, M. INART – 2nd International Conference on Innovation in Art Research and Technology, Ghent (Belgium), 21-25/03/2016. Oral presentation.
165. Altamura, E.; Cazzolla, F.; Palazzo, G.; Stano, P.; Mavelli, F. Wivace 2015 - Italian Workshop of artificial Life and Evolutionary Computing, Bari (Italy), 22-24/09/2015. Poster.
166. Altamura, E.; Regina, G.; Stano, P.; Mavelli, F. Wivace 2015 - Italian Workshop of artificial Life and Evolutionary Computing, Bari (Italy), 22-24/09/2015. Poster.
167. Altamura, E.; Stano, P.; Mavelli, F. Congresso Nazionale della Società Italiana di FotoBiologia (SIFB 2015), Università degli Studi di Bari (Italy), 11-13/06/2015. Oral presentation.
168. Altamura, E.; Stano, P.; Mavelli, F. Syschem 2015, Abdij Rolduc (the Netherlands), 19-22/05/2015. Oral presentation.
169. Altamura, E.; Stano, P.; Mavelli, F.; Milano, F.; Tangorra, R.R.; Omar, O.H.; Farinola, G.M.; Mavelli, F. Wivace 2015 - Italian Workshop of artificial Life and Evolutionary Computing, Bari (Italy), 22-24/09/2015. Oral presentation.
170. Altamura, E.; Vucojevic, V.; Mavelli, F. Working group meeting COST Action CM1304 - Biomimetic compartmentalized chemical systems, Università di Bari (Italy), 25-26/09/2015. "Characterizing giant vesicles composition by fluorescence correlation spectroscopy". Oral

presentation.

171. Ancona, A.; Picca, R.A.; Di Maria, A.; Říháková, L.; Volpe, A.; Sportelli, M-C; Lugarà, P.M.; Cioffi, N. 2015 MRS Fall Meeting & Exhibit, 29/11-04/12/2015, Boston, Massachusetts. Poster.
172. Ancona, A.; Picca, R.A.; Di Maria, A.; Říháková, L.; Volpe, A.; Sportelli, M.C.; Lugarà, P.M.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Poster.
173. Angelico, R.; Ceglie, A.; Sacco, P.; Ripoli, M.; Mangia, A. School of Nanomedicine, organizzata dal Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali (INSTM – Firenze) e dall'Istituto di Cristallografia CNR-IC, Bari (Italy), 02-04/12/2015. Poster.
174. Baglioni, M.; Bartoletti, A.; Bozec, L.; Chelazzi, D.; Giorgi, R.; Odlyha, M.; Pianorsi, D.; Baglioni, P. E-MRS - European Materials Research Society, Spring Meeting 2015, Lille (France), 11-13/05/2015. Oral presentation.
175. Baglioni, P. 1st European Conference on Physical and Theoretical Chemistry,Catania, 15-18/09/2015. Plenary lecture.
176. Baglioni, P. 2015 Materials Research Society Fall Meeting & Exibit, Boston (USA), 30/11-04/12/2015. Invited lecture.
177. Baglioni, P. Fifth International Colloids Conference: Colloid and Interface Sciences for a Brighter Future, Amsterdam (Olanda), 21-24/06/2015. Invited lecture.
178. Baglioni, P. Conservation of cultural heritage: challenges and reviews, Atene (Grecia), 25-29/05/2015. Invited lecture.
179. Baglioni, P. EuroNanoForum 2015, Riga (Lettonia), 10-12/06/2015. Invited lecture.
180. Baglioni, P. Future and Current Use of Neutron Spin-Echo Spectroscopy in Condensed Matter Research Workshop, Oak Ridge, USA, 12-16/05/2015. Invited lecture.
181. Baglioni, P. International workshop on the application of nano-lime for consolidation of weathered stones, Bath University, UK, 24th September 2015. Invited lecture.
182. Baglioni, P. Jülich Soft Matter Days 2015, Bad Honnef (Germany), 10-13/11/2015. Invited lecture.
183. Baglioni, P. NanotechItaly 2015, Bologna, 25-26/11/2015. Invited lecture.
184. Baglioni, P. Nanotechnologies for cultural conservation: current trends and practices, IDEAL Center for Innovation of Lafayette College, Allentow, Pennsylvania (USA), 30-31/10/2015. Plenary lecture.
185. Baglioni, P. National Congress of Italian Physical Society, Rome, Italy, 25th September 2015. Invited lecture.
186. Baglioni, P. Oorgandagarna 2015, Wisby Strand Sweden, Stoccolma (Svezia), 15-17/06/2015. Invited lecture.
187. Baglioni, P. RICHES – Renewal, Innovation and Change Heritage and European Society, Bruxelles, 19th October 2015. Oral presentation.
188. Baglioni, P. Science and Innovation for the study and conservation of works of art, Rio de Janeiro (Brazil), 4th December 2015. Invited lecture.
189. Bardi, A.; Dallai, L.; Donati. A.; Volpi. V. CAA 2015 - The 43rd Computer Applications and Quantitative Methods in Archaeology "Keep the revolution going" Conference, Siena, 30/03/2015-03/04/2015. Oral presentation.
190. Basosi, R. Biwaes, Stockholm, 04/05/2015. Plenary lecture.
191. Basosi, R. Jagellonian, University Krakow, 16/02/2015. Plenary lecture.
192. Bergemann, N.; Pistidda, C.; Karimi, F.; Gobetto, R.; Milanese, C.; Emmler, T.; Klassen, T.; Dornehim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
193. Berretti, E.; Cinotti, S.; Picca, R.A.; Di Benedetto, F.; Cioffi, N.; De Luca, A.; Lavacchi, A.; Innocenti, M. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Poster.
194. Berti, D. 15th Conference of the International Association of Colloid and Interface Scientists, Mainz (Germany), 24-29/05/2015. Invited keynote lecture.
195. Berti, D. 5th International Colloids Conference, Amsterdam, Netherlands, 21-24/06/2015. Invited keynote lecture.
196. Berti, D. Jülich Centre for Neutron Science Workshop, Tutzing (Germany), 05-08/10/2015. Invited lecture.
197. Berti, D. Hybrid Soft Nanostructured Architectures: Structural, Functional and Biophysical Aspects, Università di Salerno (Italia), Marzo 2015. Invited presentation.
198. Berti, D. Soft Matter for Biological Applications An Overview, CNR-ISMN, Bologna (Italia), Luglio 2015. Invited presentation.
199. Bonechi, C.; Tamasi, G.; Donati, A.; Magnani, A.; Rossi, C. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
200. Bonini, M.; Gelli, R.; Del Buffa, S.; Tempesti, P.; Ridi, F.; Baglioni, P. EMRS – Spring meeting, Lille, Marzo 2015. Oral presentation.
201. Borsacchi, S.; Martini, F.; Calucci, L.; Ridi, F.; Tonelli, M.; Fratini, E.; Baglioni, P. Geppi, M. XLIV National congress on magnetic resonance, Roma, 28-30/09/2015. Oral presentation.

202. Borsacchi, S.; Martini, F.; Geppi, M.; Fratini, E.; Ridi, F.; Tonelli, M.; Calucci, L. 9th Field-Cycling NMR conference, Aberdeen, 27-30/07/2015. Oral presentation.
203. Busi, E.; Maranghi, S.; Corsi, L.; Basosi, R. International conference on Life Cycle Assessment as reference methodology for assessing supply chains and supporting global sustainability challenges, Stresa and Milano, 06-08/10/2015. Poster.
204. Calvano, C.D.; Picca, R.A.; Bonerba, E.; Ditaranto, N.; Pellegrini, T.; Tantillo, G.; Cioffi, N.; Palmisano, F. 4th MS Food Day, 07-09/10/2015, Foggia (Italy). Poster.
205. Calvano, C.D.; Picca, R.A.; Bonerba, E.; Ditaranto, N.; Tantillo, G.; Cioffi, N.; Palmisano, F. XXV Congresso Nazionale di Chimica Analitica, Trieste, 13-17/09/2015. Poster.
206. Caminati, G. 14th European Conference on Organized films ECOF-14, Genova (Italy), 29/06-02/07/2015. Oral presentation.
207. Capurso, G.; Bellosta von Colbe, J.M.; Gupta, N.; Yigit, D.; Pendolino, F.; Melnichuk, M.; Milanese, C.; Girella, A.; Taube, K.; Klassen, T.; Dornheim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
208. Cofrancesco, P.; Frisetti, A.; Licchelli, M.; Milanese, C.; Trojsi, G. 1st International Conference on Metrology for Archaeology, Benevento (Italy), 22-23/10/2015. Oral presentation.
209. Cugia, F.; Monduzzi, M.; Salis, A. 1st European Conference on Physical and Theoretical Chemistry Catania (Italy), 14-18/09/2015. Poster.
210. Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman, B. 15th Conference of the International Association of Colloid and Interface Scientists. Mainz (Germany), 24-29/05/2015. Oral presentation.
211. Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman, B. 1st European Conference on Physical and Theoretical Chemistry and XLII annual meeting of the Physical Chemistry Division of SCI, Catania (Italy), 14-16/09/2015. Poster.
212. De Santis, A; Vitiello, G; D'Errico, G; Paduano, L. 1st European Conference on Physical and Theoretical Chemistry, Catania, 10-14/09/2015. Poster.
213. Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Oral communication.
214. Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Suriano, D.; Palmisano, F.; Torsi, L.; Cioffi, N. MRS2015 Spring Meeting, San Francisco, CA, (USA), 21-25/04/2015. Poster.
215. Dilonardo, E.; Penza, M.; Alvisi, M.; Difranco, C.; Palmisano, F.; Torsi, L.; Cioffi , N. MRS2015 Spring Meeting, San Francisco, CA, (USA), 21-25/04/2015. Oral communication.
216. Dilonardo, E.; Penza, M.; Alvisi, M.; Rossi, R.; Di Franco, C.; Torsi, L.; Cioffi, N. COST Action TD1105 EuNetAir 3rd International Workshop EuNetAir, Riga (Latvia), 26-27/03/2015. Oral communication.
217. Ditaranto, N.; Picca, R.A.; Sportelli, M.C.; Sabbatini, L.; Cioffi, N. 16th European Conference on Applications of Surface and Interface Analysis ECASIA'15, Granada (Spain) 28/09-01/10/2015. Oral communication.
218. Donati, A; Bardi, A.; Volpi, V.; Mencuccini, L.; Bianchi, G.;, Benvenuti, M.; Chiarantini, L.; Rossi, C.; Dallai, L. The 1st European Conference on Physical and Theoretical Chemistry and XLII Annual Meeting of the Physical Chemistry Division of SCI, Catania, 14-18/09/2015. Oral presentation.
219. Giaccherini, A.; Cinotti, S.; Picca, R.A.; Carlà, F.; Montegrossi, G.; Capolupo, F.; Felici, R.; Di Benedetto, F.; Furlanetto, S.; Cioffi, N.; Lavacchi, A.; Innocenti, M. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Oral communication.
220. Giorgi, R. Conference at Lafayette College 2015 Easton, PA (USA), 02/11/2015. Oral presentation.
221. Giorgi, R. Keynote at XV Congresso Nazionale Divisione Chimica dell'Ambiente e dei beni Culturali, Società Chimica Italiana, Bergamo, 14-18/06/2015. Oral presentation.
222. Giorgi, R. NanoItaly 2015, Roma University of Rome - La Sapienza, 21-24/09/2015. Oral presentation.
223. Giorgi, R.; Poggi, G.; Mirabile, A.; Hui Ping, X.; Baglioni, P. E-MRS - European Materials Research Society, Spring Meeting 2015, Lille (France), 11-13/05/2015. Oral presentation.
224. Gualdani, R.; di Cesare Mannelli, L.; Francesconi, O.; Ghelardini, C.; Moncelli M.R.; Richichi, B.; Nativi, C. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
225. Gualdani, R.; Guerrini, A.; Fantechi, E.; Moncelli, M.R.; Sangregorio, C. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
226. Lamberti, I.; Scarano, S.; Esposito, C.L.; Antoccia, A.; Antonini, G.; Tanzarella, C.; De Franciscis, V.; Minunni, M. XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI), Trieste, 13-17/09/2015. Poster.
227. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni M. Biaoanalitica 2015, Firenze, 26/06/2015. Poster.
228. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni, M. XXV Congresso della Divisione di Chimica

Analitica della Società Chimica Italiana (SCI), Trieste, 13-17/09/2015. Poster.

229. Lisi, S.; Scarano, S.; Ravelet, C.; Peyrin, E.; Minunni, M. XXXIV Congresso Interregionale delle Sezioni Toscana, Umbria, Marche e Abruzzo della Società Chimica Italiana - TUMA 34, 23-25/09/2015. Oral presentation.
230. Lopez, F.; Venditti, F.; Ambrosone, L.; Cuomo, F.; Ceglie, A. Workshop "Chimica, Ambiente e Territorio" organizzato dalla Società Chimica Italiana, Sezione Campania, e dal Dipartimento di Scienze e Tecnologie Ambientali, Biologiche e Farmaceutiche della Seconda Università di Napoli. Caserta (Italy), 30/09/2015. Oral presentation.
231. Lopez, F.; Venditti, F.; Cuomo, F.; Ceglie, A. 1st European Conference on Physical and Theoretical Chemistry and XLII annual meeting of the Physical Chemistry Division of SCI, Catania (Italy), 14-16/09/2015. Poster.
232. Luchini, A.; Gerelli, Y.; Fragneto, G.; Paduano, L. XXVI Congresso Annuale SISN – Italian Neutron Scattering Conference, Frascati-Roma, 01-03/07/2015. Oral presentation.
233. Luci, G.; Vanni, M.; Minunni, M.; Intorre, L.; Meucci V. Atti Sisvet LXVIII. Vol. LXIX, Perugia, 16-18/06/2015. Poster.
234. Martini, F.; Calucci, L.; Geppi, M.; Fratini, E.; Ridi, F.; Tonelli, M.; Baglioni P.; Borsacchi S. GIDRM 2015, Roma, 28-30/09/2015. Poster and oral presentation.
235. Martini, F.; Calucci, L.; Geppi, M.; Fratini, E.; Ridi, F.; Tonelli, M.; Baglioni, P.; Borsacchi, S. EUROMAR 2015, Praga, 05-10/07/2015. Oral presentation.
236. Mavelli, F.; Altamura, E.; Stano, P. Working group meeting COST Action CM1304 - Biomimetic compartmentalized chemical systems, Università di Bari (Italy), 25-26/09/2015. Oral presentation.
237. Mavelli, F.; Emiliano, A.; Stano, P. Syschem 2015, Abdij Rolduc, the Netherlands, 19-22/05/2015. Oral presentation.
238. Meli, V.; Murgia, S.; Caltagirone, C.; Falchi, A.M.; Monduzzi, M. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
239. Merlino, A.; Russo Krauss, I.; Caterino, M.; Vergara A. 29th Annual Symposium of The Protein Society, Barcelona (Spain), 22-25/07/2015. Poster.
240. Messina, G.M.L. BioEl 2015 – BioEl 2015 International Winterschool on Bioelectronics, Kirchberg in Tyrol (Austria), 28/02-07/03/2015. Poster.
241. Messina, G.M.L.; Karakeçili, A.; Yurtsever, M.; Gümüşderelioğlu, M.; Marletta, G. Euro Biomat, Weimar, Germany, 21-22/04/2015. Oral presentation.
242. Messina, G.M.L.; Marletta, G. E-MRS Spring Meeting, Lille, France, 11-15/05/2015. Oral presentation.
243. Messina, G.M.L.; Marletta, G. EuroPhysChem, Catania, Italy, 14-18/09/2015. Oral presentation.
244. Milanese, C.; Girella, A.; Saldan, I.; Marini, A.; Gaboardi, M.; Pontiroli, D., Magnani, G.; Riccò, M. 1st European Conference on Physical and theoretical chemistry, Catania (Italy), 14-18/09/2015. Oral presentation.
245. Milanese, C.; Girella, A.; Saldan, I.; Rueda Noriega, M.; Martin, A.; Marini, A. 1st European Conference on Physical and theoretical chemistry, Catania, (Italy) 14-18/09/2015. Poster.
246. Milanese, C.; Girella, A.; Saldan, I.; Valsecchi, G.; Gaboardi, M.; Pontiroli, D.; Magnani, G.; Riccò, M.; Marini, A. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
247. Murgia, S.; Meli, V.; Falchi, A.M.; Nylander, T.; Schillén, K.; Monduzzi, M.; Talmon, Y. 5th International Colloids Conference, Amsterdam (The Netherlands), 21-24/06/2015. Poster.
248. Picca, R.A.; Ditaranto, N.; Sportelli, M.C.; Pellegrini, T.; Valentini, A.; Cioffi, N. 2015 Materials Research Society Fall Meeting & Exhibit, 29/11-04/12/2015, Boston, Massachusetts. Poster.
249. Picca, R.A.; Fazio, B.; Calvano, C.D.; Lo Faro, M.J.; Sportelli, M.C.; D'Andrea, C.; Irrera, A.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Poster.
250. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. 2015 Materials Research Society Fall Meeting & Exhibit, 29/11-04/12/2015, Boston, Massachusetts. Poster.
251. Picca, R.A.; Lo Faro, M.J.; Calvano, C.D.; Fazio, B.; Sportelli, M.C.; Trusso, S.; Ossi, P.M.; Neri, F.; D'Andrea, C.; Irrera, A.; Cioffi, N. 4th MS Food Day, 07-09/10/2015, Foggia (Italy). Oral communication.
252. Picca, R.A.; Manoli, K.; Sportelli, M.C.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. 2015 Materials Research Society Fall Meeting & Exhibit, 29/11-04/2015, Boston, Massachusetts. Oral communication.
253. Picca, R.A.; Paladini, F.; Sportelli, M.C.; Pollini, M.; Giannossa, L.C.; Di Franco, C.; Mangone, A.; Valentini, A.; Sannino, A.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Keynote.
254. Picca, R.A.; Sportelli, M.C.; Calvano, C.D.; Ditaranto, N.; Cioffi, N. EMN Energy Materials Nanotechnology, Cancun (Mexico), 07-11/06/2015. Invited oral communication.

255. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Cioffi, N. Materials Research Society 2015 Spring Meeting, San Francisco, CA (USA), 21-25/04/2015. Poster.
256. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. GEI – Giornate dell'Elettrochimica Italiana 2015, Bertinoro, 20-24/09/2015. Oral communication.
257. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. International Workshop on the Electrochemistry of Electroactive Materials WEEM – 2015 Bad Herrenalb (Germany), 31/05-05/06/2015. Invited oral communication.
258. Picca, R.A.; Sportelli, M.C.; Luciano, A.; Manoli, K.; Magliulo, M.; Palazzo, G.; Torsi, L.; Cioffi, N. MRS2015 Spring Meeting, San Francisco, CA (USA), 21-25/04/2015. Poster.
259. Pistidda, C.; Hardian, R.; Bergemann, N.; Horstmann, C.; Milanese, C.; Girella, A.; Capurso, G.; Bellosta von Colbe, J.M., Chaudhary, A.L.; Metz, O.; Gupta, N.; Taube, K.; Klassen, T.; Dornheim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications", Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
260. Pitzalis, F.; Cugia, F.; Salis, A.; Carboni, D.; Malfatti, L.; Innocenzi, P.; Monduzzi, M. 1st European Conference on Physical and Theoretical Chemistry, Catania (Italy), 14-18/09/2015. Poster.
261. Pogni, R. GIRSE Workshop & NIS Colloquium - EPR in Catalysis: from Model to Real Systems, Torino, 26-27/11/2015. Plenary lecture.
262. Pontiroli, D.; Magnani, G.; Gaboardi, M.; Riccò, M.; Pramudita, J.C.; Sharma, N.; Milanese, C. 2nd Parma Nanoday Workshop, Parma (Italy), 03-04/12/2015. Oral presentation.
263. Pontiroli, D.; Magnani, G.; Lenti, S.; Gaboardi, M.; Riccò, M.; Milanese, C.; Pramudita, J.C.; Sharma, N. Carbon 2015 conference, Dresda (Germany), 12-17/07/2015. Oral presentation.
264. Ridi, F. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Oral presentation.
265. Ridi, F.; Fratini, E.; Tonelli, M.; Baglioni, P.; Borsacchi, S.; Martini, F.; Calucci, L.; Geppi, M. 14th International Congress on the Chemistry of Cement, Beijing (China), 13-16/10/2015. Poster.
266. Rizzuti, A.; Mastrorilli, P.; Sportelli, M.C.; Cioffi, N.; Picca, R.A.; Agostinelli, E.; Varvaro, G.; Dassisti, M.; Caliandro, R. Amam 2015, International conference on Applied mineralogy and advanced materials, Castellaneta marina (Italy), 07-12/06/2015. Oral communication.
267. Russo Krauss, I.; Guida, V.; Gaudino, D.; Grizzuti, N.; Pasquino, R.; D'Errico, G.; Paduano, L. 1st European Conference on Physical and Theoretical Chemistry, Catania (Italy), 14-18/09/2015. Oral presentation.
268. Russo Krauss, I.; Haider, S.; Ramaswamy, S.; Parkinson, G. N. 5th International Meeting on Quadruplex Nucleic Acids: G4thering in Bordeaux, Bordeaux (France), 26-28/05/2015. Poster & flash presentation.
269. Russo Krauss, I.; Pica, A.; Spiridonova, V.A.; Tateishi-Karimata, H.; Nagatoishi, S.; Sugimoto, N.; Sica, F. 5th International Meeting on Quadruplex Nucleic Acids: G4thering in Bordeaux, Bordeaux (France), 26-28/05/2015. Poster.
270. Sacconi, S.; Tadini-Buoninsegni, F.; Moncelli M.R.; Margheri, G.; Cerboneschi, M.; Tegli, S. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
271. Salis, A. 5th NanoDrug International Scientific Meeting, Alghero, 28/06/2015-01/07/2015. Invited speaker.
272. Salis, A.; Medda, L.; Monduzzi, M. TheoBio 2015, International Theoretical Biophysics Symposium, Cagliari, 08-12/06/2015. Poster.
273. Salis, A.; Medda, M.; Monduzzi, M. 29th ECIS Conference, Bordeaux (France), 06-11/09/2015. Poster.
274. Santoru, A.; Pistidda, C.; Garroni, S.; Milanese, C.; Marini, A.; Masolo, E.; Bergemann, N.; Le, T.T.; Mulas, G.; Enzo, S.; Klassen, T., Dornheim, M. Gordon Research Conference "Hydrogen - Metal Systems: Fundamental Aspects of Hydrogen Interaction with Materials and Novel Energy Applications". Stonehill College, Easton, MA (USA), 12-17/07/2015. Poster.
275. Scarano, S.; Carretti, E.; Baglioni, P.; Dei, L.; Minunni, M. XXV Congresso della Divisione di Chimica Analitica della Società Chimica Italiana (SCI) 13-17/09/2015, Trieste. Oral presentation.
276. Scarano, S.; Mariani, S.; Ermini, M.L.; Barale, R.; Bonini, M.; Minunni, M. Biophotonics 2015, Florence (Italy), 20-22/05/2015. Oral presentation.
277. Singh, M.; Mulla, M.Y.; Manoli, K.; Magliulo, M.; Ditaranto, N.; Cioffi, N.; Palazzo, G.; Torsi, L.; Santacroce, M.V.; Di Franco, C.; Scamarcio, G. 6th IEEE International Workshop on Advances in Sensors and Interfaces, Gallipoli (Italy), 18-19/06/2015. Oral communication.
278. Smeazzetto, S.; Young, H.S.; Trieber, C.A.; Moncelli M.R.; Tadini-Buoninsegni, F. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
279. Sportelli, M.C.; Ancona, A.; Picca, R.A.; Volpe, A.; Lugarà, P.M.; Cioffi, N. Euroanalysis XVIII, the European Conference on Aalytical Chemistry, Bordeaux 06-10/09/2015. Oral communication.

280. Sportelli, M.C.; Ancona, A.; Picca, R.A.; Volpe, A.; Trapani, A.; Trapani, G.; Cioffi, N. Materials Research Society 2015 Spring Meeting, San Francisco, CA (USA), 21-25/04/2015. Oral communication.
281. Sportelli, M.C.; Picca, R.A.; Manoli, K.; Magliulo, M.; Re, M.; Pesce, E.; Tapfer, L.; Di Franco, C.; Cioffi, N.; Torsi, L. Materials Research Society 2015 Spring Meeting, San Francisco, CA (USA) 21-25/04/2015. Poster.
282. Sportelli, M.C.; Tütüncü, E.; Picca, R.A.; Valentini, M.; Valentini, A.; Kranz, C.; Mizaikoff, B.; Cioffi, N. XXV Congresso Nazionale di Chimica Analitica, Trieste 13-17/09/2015. Oral communication.
283. Strazewski, P.; Fiore, M.; D'Onofrio, A.; Emiliano, A.; Mavelli, F. Syschem 2015, Abdij Rolduc (The Netherlands), 19-22/05/2015. Oral presentation.
284. Tadini-Buoninsegni, F.; Moncelli M.R.; Peruzzi, N.; Ninham, B.W.; Dei, L.; Lo Nostro, P. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
285. Tadini-Buoninsegni, F.; Moncelli M.R.; Tegli, S. 4th International Workshop on Expression, Structure and Function of Membrane Proteins, Firenze (Italy), 28/06/2015-02/07/2015. Poster.
286. Tamasi, G.; Bonechi, C.; Rossi, C.; Cini, R.; Magnani, A. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
287. Tonelli, M.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Ridi, F.; Borsacchi, S.; Baglioni, P. 15th European Student Colloid Conference, Krakow, 08-11/06/2015. Oral presentation.
288. Toulmé, J.J.; Da Rocha, S.; Dausse, E.; Fernandez, P.; Allard, M; Kryza, D.; Janier, M.; Scarano, S.; Crispo, F.; Minunni, M.; Hassan, A.; Paurelle, O.; Azéma, L. OLIGO 2015 Oxford Antisense and therapeutic Nucleic Acids, 30/03/2015, Oxford (UK). Oral presentation.
289. Toulmé, J.J.; Dausse, E.; Fernandez, P.; Debordeaux, F.; Kryza, D.; Janier, M.; Scarano, S.; Crispo, F.; Minunni, M. Hassan, A.; Paurelle, O.; Azéma, L. 11th Annual Meeting of the Oigonucleotide Therapeutic Society, 11-14/10/2015, Lieden (The Netherlands). Oral presentation.
290. Tovar Rodríguez, J.; Fratini, E. XV Sigma-Aldrich Young Chemists Symposium, SAYCS 2015, Rimini (Italy), 27-29/10/2015. Oral presentation.
291. Tovar Rodríguez, J.; Ramírez Hernández, G.Y.; Galindo Esquivel, I.R.; Fratini, E.; De Los Reyes Heredia, J.A. XII European Congress on Catalysis, EUROPACAT 2015, Kazan (Russia), 30/08-04/09/2015. Poster.
292. Tuccitto, N.; Zappalà, G.; Vitale, S.; Licciardello, A. International SIMS Conference SIMSXX, Seattle (USA), 2015. Oral presentation.
293. Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A; Licciardello, A. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
294. Tuccitto, N.; Zappalà, G.; Vitale, S.; Giamblanco, N.; Marletta, G.; Licciardello, A. Secondary Ion Mass Spectrometry SIMS XX, Seattle (USA), 13-18/09/2015. (Poster).
295. Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. Secondary Ion Mass Spectrometry SIMS XX, Seattle (USA), 13-18/09/2015. Poster.
296. Valentini, A.; De Pascali, G.; Melisi, D.; Valentini, M.; Cioffi, N.; Casamassima, G. Amam 2015, International conference on Applied mineralogy and advanced materials, Castellaneta marina (Italy), 07-12/06/2015. Plenary lecture.
297. Valentini, A.; Fracchiolla, G.; Carbonara, G.; Rosato, A.; Cioffi, N.; Casamassima, G. Amam 2015, International conference on Applied mineralogy and advanced materials, Castellaneta marina (Italy), 07-12/06/2015. Oral communication.
298. Venditti, F.; Cuomo, F.; Ceglie, A.; Lopez, F. 15th Conference of the International Association of Colloid and Interface Scientists. Mainz (Germany), 24-29/05/2015. Poster.
299. Vitale, S.; Zappalà, G.; Tuccitto, N.; Santoni, M.P.; Campagna, S.; Licciardello, A. Secondary Ion Mass Spectrometry SIMS XX, Seattle (USA), 13-18/09/2015. Oral presentation.
300. Zappalà, G.; Vitale, S.; Tuccitto, N.; Licciardello, A. 1st European Conference on Physical and Theoretical Chemistry, Catania, 14-18/09/2015. Poster.
301. Altamura, E.; Mavelli, F. Syschem 2014, San Sebastian (Spain), 09-12/06/2014. Oral presentation.
302. Altamura, E.; Mavelli, F. Working group meeting COST Action CM1304 - Compartment Permeability, Parmenides Foundation, Munich (Germany), 20-22/11/2014. Oral presentation.
303. Baglioni, P. 1st Soft Matter School, Venice, Isola di S. Servolo, 16-20/06/2014. Invited lecture.
304. Baglioni, P. Cultural heritage and advanced technologies Symposium, Italian Institute of Culture, London, 13/11/2014. Invited lecture.
305. Baglioni, P. Director's Colloquium, University of Canberra, Leonard Huxley Lecture Theatre, Australia, 14/08/2014. Plenary lecture.
306. Baglioni, P. Royal Institute of Art, Stoccolma (Svezia), 20-21/03/2014. Invited lecture.
307. Baglioni, P. Gordon Conference: Scientific Methods in Cultural Heritage Research, Sunday River Resort in Newry, ME, USA, 27/074-01/08/2014. Invited lecture.
308. Baglioni, P. The digital future of world heritage, University of Notre Dame in Rome, 2-4/04/2014.

Invited lecture.

309. Baglioni, P. VIII Congresso Nazionale di Archeometria – Scienze e Beni Culturali: stato dell'arte e prospettive, CNR, Bologna, 5-7 febbraio 2014. Invited lecture.
310. Baglioni, P. Shaanxi Normal University, School of Material Science and Engineering, Xi'an (China), 23-29/08/2014. Invited lectures.
311. Baglioni, P. Cracow Academy of Fine Arts in Poland, Faculty of Conservation of Works of Art, Cracow (Poland), 25-28/05/2014. Invited lecture.
312. Baglioni, P. ECIS 2014, 28th International Conference of the European Colloid and Interface Society, Limassol (Cyprus), 07-12/09/2014. Invited Keynote.
313. Baratto, M.C.; Martorana, A.; Aguila, S.A.; Vazquez-Duhalt, R.; Basosi, R. Oxizymes 2014, Vienna 01-04/07/2014. Poster.
314. Basosi, R. Bogazici University Istanbul, 01/04/2014. Plenary lecture.
315. Basosi, R. EuCheMS Round Table on Energy, Environment and Food, Rome - "La Sapienza", 25/11/2014.
316. Basosi, R. London School Of Economics, 03/2014. Plenary lecture.
317. Basosi, R. Medaglia D'oro Della SCI, Università della Calabria, 07/09/2014. Invited lecture.
318. Basosi, R. Prolusione Apertura 774° A.A. Università di Siena, 16/12/2014. Invited lecture.
319. Basosi, R. SET Plan Conference, Roma, 09/12/2014. Plenary lecture.
320. Basosi, R. University Of Warsaw, 09/2014. Plenary lecture.
321. Bernini, C.; Arezzini, E.; Basosi, R.; Sinicropi, A. XXV Congresso Nazionale della SCI, Arcavacata di Rende (CS), 07-12/09/2014. Poster.
322. Bernini, C.; Zani, L.; Calamante, M.; Reginato, G.; Mordini, A.; Taddei, M.; Basosi, R.; Sinicropi, A. XXV Congresso Nazionale della SCI, Arcavacata di Rende (CS), 07-12/09/2014. Poster.
323. Berti, D. Balard Chemistry conferences: Self-Assembly of Biomolecules, La Grande Motte (France), 12-15/10/2014. Invited lecture.
324. Berti, D. Nanomedicine Symposium CEN@Politecnico: Synthesis of nanomaterials, biological applications and modelling, Politecnico di Milano (Italy), November 2014. Invited lecture.
325. Berti, D. Torino (Italia), 10/11/2014. Invited lecture.
326. Berti, D. Magnetocubosomes for Controlled Drug Delivery, Politecnico di Milano (Italia), Dicembre 2014. Invited presentation.
327. Biancalani, C.; Cerboneschi, M.; Macconi, S.; Moncelli, M.R.; Smeazzetto, S.; Biricolti, S.; Bogani, P.; Tegli, S. XX Convegno Nazionale SIPAV, Pisa (Italy), 22-24/09/2014. Poster.
328. Cerboneschi, M.; Lanzini, G.; Macconi, S.; Onor, M.; Campanella, B.; Bramanti, E.; Moncelli, M.R.; Tadini-Buoninsegni, F.; Biricolti, S.; Bogani, P.; Tegli, S. XX Convegno Nazionale SIPAV, Pisa (Italy), 22-24/09/2014. Poster.
329. Cioffi, N.; Dilonardo, E.; Di Franco, C.; Afzal, A.; Alvisi, M.; Penza, M.; Palmisano, F.; Torsi, L. COST Action TD1105 - Second International Workshop, ENEA, 25-26/03/2014, Brindisi. Invited Oral communication.
330. Cuomo, F.; Lopez, F.; Ceglie, A.; Miguel, M.G.; Lindman, B. 4th International Colloid Conference. Surface Design and Engineering. Madrid (Spain), 15-19/06/2014. Oral presentation.
331. Dassisti, M.; Mastrorilli, P.; Rizzuti, A.; Caliandro, R.; Cioffi, N. 1st WORKSHOP on the State of the art and Challenges Of Research Efforts@POLIBA, 03-05/12/2014, Politecnico di Bari (Italy). Poster.
332. Del Buffa, S.; Bonini, M.; Ridi, F.; Severi, M.; Losi, P.; Volpi, S.; Al Kayal, T.; Soldani, G.; Baglioni P. EMRS – Fall meeting, Warsaw, 15-19/09/2014. Oral presentation.
333. Del Buffa, S.; Rinaldi, E.; Carretti, E.; Bonini, M.; Ridi, F.; Baglioni, P. EMRS – Fall meeting, Warsaw, 15-19/09/2014. Poster.
334. Dilonardo, E.; Di Franco, C.; Afzal, A.; Ditaranto, N.; Alvisi, M.; Penza, M.; Palmisano, F.; Torsi, L.; Cioffi, N. ISA2014 Incontro di Spettroscopia Analitica University of Bologna, Ravenna (Italy), 05-06/06/2014. Oral communication.
335. Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. COST Action TD1105 - New Sensing Technologies for Air-Pollution Control and Environmental Sustainability - Third Scientific Meeting, organized by GEBZE and Bahcesehir University, Istanbul, 03-05/12/2014. Poster.
336. Dilonardo, E.; Penza, M.; Alvisi, M.; Di Franco, C.; Suriano, D.; Rossi, R.; Palmisano, F.; Torsi, L.; Cioffi, N. COST Action TD1105 - New Sensing Technologies for Air-Pollution Control and Environmental Sustainability - Third Scientific Meeting, organized by GEBZE and Bahcesehir University, Istanbul, 03-05/2014. Oral communication.
337. Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Cassano, G.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Poster.
338. Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Rossi, R.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. COST Action TD1105 - Second International Workshop, ENEA, 25-26/03/2014, Brindisi. Poster.

339. Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Rossi, R.; Palmisano, F.; Torsi, L.; Cioffi, N. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Oral communication.
340. Dilonardo, E.; Penza, M.; Alvisi, M.; Suriano, D.; Rossi, R.; Palmisano, F.; Torsi, L.; Cioffi, N. Secondo Convegno Nazionale Sensori, 19-21/02/2014, Roma (Italy). Oral communication.
341. Dilonardo, E.; Penza, M.; Cassano, G.; Alvisi, M.; Di Franco, C.; Palmisano, F.; Torsi, L.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (CS), 07-12/09/2014. Oral communication.
342. Ditaranto, N.; Picca, R.A.; Sportelli, M.C.; van der Werf, I.D.; Mangone, A.; Cioffi,, N.; Sabbatini, L. ISA2014 Incontro di Spettroscopia Analitica University of Bologna, Ravenna (Italy), 05-06/06/2014. Oral communication.
343. Fanti, P.; Giustarini, D.; Rossi, R.; Folli, F.; Khazim, K.; Cornell, J.; Matteucci, E.; Bansal, S. XVII International Congress on Nutrition and Metabolism in Renal Disease, Würzburg (Germany), 06-10/05/2014. Poster.
344. Ferrari, S.; Quartarone, E.; Bini, M.; Tomasi, C.; Capsoni, D.; Mustarelli, P. IMLB – The 17th International Meeting on Lithium Batteries, Como, 10-14/06/2014. Poster.
345. Ferraro, G.; Fratini, E.; Ridi, F.; Baglioni, P. XIV Sigma-Aldrich Young Chemists Symposium, SAYCS 2014, Rimini (Italy), 27-29/10/2014. Poster.
346. Garroni, S.; Santoru, A.; Pistidda, C.; Milanese, C.; Masolo, E.; Marini, A.; Dornheim, M.; Mulas, G.; Enzo, S. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Oral presentation.
347. Giorgi, R. Conference at CNCPC - Coordinación Nacional de Conservación del Patrimonio Cultural; Auditorio de la CNCPC, 21/10/2014. Oral presentation.
348. Giorgi, R. Conference at Encrym - Escuela Nacional de Restauración, Conservación y Museografía; Sala de Consejos de la ENCRyM, 22/10/2014. Oral presentation.
349. Giorgi, R. Conference at Jesuit Church in Lviv (Ukraine), 05/07/2014. Oral presentation.
350. Giorgi, R. Conference at UNAM. Instituto de Física, 20/10/2014. Oral presentation.
351. Giorgi, R. IMAT conference, Firenze, 12/11/2014. Oral presentation.
352. Giorgi, R. Keynote al XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014. Arcavacata di Rende - Università della Calabria, 07-12/09/2014. Oral presentation.
353. Giorgi, R. Keynote alla V Jornada de Conservacao-Restauracao intitolata “Conservacao e Tecnologia: caminhos da Inovacao”, Rio De Janeiro (Brasile). 22-24/09/2014. Oral presentation.
354. Giorgi, R. La Conservaciòn de la Pintura Mural en Sitios Arqueològicos - Problemàtica y Estrategias de Intervenciòn, organizzato da IPCE - School of Conservation of Archeological Wall Paintings. Najera, La Rioja (Spagna), 06-08/05/2014. Oral presentation.
355. Giorgi, R. Seminario presso la Universidad Nacional Autonoma de Mexico – UNAM. Mexico City, 18/02/2014. Oral presentation.
356. Gosalawit-Utke, R.; Meethom, S.; Pistidda, C.; Milanese, C.; Laipple, D.; Saisopha, T.; Marini, A.; Klassen, T.; Dornheim, M. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Oral presentation.
357. Grandi, S.; Achilli, C.; Guidetti, G.F.; Ciana, A.; Quartarone, E.; Capsoni, D.; Minetti, G. E-MRS: European Materials Research Society, Lille (France), 26-30/05/2014. Poster.
358. Gualdani, R.; Lentini, G.; Moncelli, M.R. 39th FEBS Congress, Paris (France), 30/08/2014-05/09/2014. Poster.
359. Gualdani, R.; Tadini-Buoninsegni, F.; Lentini, G.; Moncelli, M.R. XXII Congresso Nazionale SIBPA, Palermo (Italy), 21-24/09/2014. Oral presentation.
360. Gualdani, R.; Zanardelli, M.; di Cesare Mannelli, L.; Francesconi, O.; Ghelardini, C.; Nativi, C.; Moncelli, M.R. 39th FEBS Congress, Paris (France), 30/08/2014-05/09/2014. Poster.
361. Innocenti, M.; Cinotti, S.; Di Benedetto, F.; Lavacchi, A.; Felici, R.; Carlà, F.; Cioffi, N.; Vizza, F. 65th Annual Meeting of the International Society of Electrochemistry, Symposium 10: Electrodeposition for Energy Applications 31/08-05/09/2014 Lausanne (Switzerland). Invited oral communication.
362. Luchini, A.; Vitiello, G.; De Julian Fernandez, C.; Heenan, R.; Montesarchio, D.; D’Errico, G.; Paduano, L. IX Congresso Consorzio internuniversitario dei Sistemi a Grande Interfase (CSGI), Napoli, 01-02/07/2014. Oral presentation.
363. Luchini, A.; Vitiello, G.; De Julian Fernandez, C.; Heenan, R.; Montesarchio, D.; D’Errico, G.; Paduano, L. XXV Congresso Nazionale Società Italiana Spettroscopia Neutronica (SISN) – Italian Neutron Scattering Conference, Napoli, 03-04/07/2014. Oral presentation.
364. Magliulo, M.; Mallardi, A.; Manoli, K.; Cioffi, N.; Palazzo, G.; Torsi, L. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Invited oral communication.
365. Maranghi, S.; Parisi, M.L.; Busi, E.; Basosi, R. VIII Convegno della Rete Italiana LCA, Florence, 19-20/06/2014. Poster.

366. Mariani, S.; Ermini, M.L.; Scarano, S.; Belissima, F.; Bonini, M.; Minunni, M. COST Thematic workshop Integrated approahces for biomolecular detection: nanostructures, Biosensors and Lab on Chip devices, 28-30/04/2014, Catania (Italy). Poster.
367. Mariani, S.; Scarano, S.; Minunni, M. Giornata scientifica di Bioanalitica, Chimica Bioanalitica per La Sicurezza Ambientale ed Alimentare, Bologna, 04/07/2014. Poster.
368. Mariani, S.; Scarano, S.; Spadavecchia, J.; Minunni, M. Xxv Congresso Della Societa' Chimica Italiana, Rende 08-12/09/2014. Oral presentation.
369. Marletta, G.; Messina, G.M.L.; Giamblanco, N. N.I.C.E. 2014, 2nd International Conference on Bioinspired and Biobased Chemistry and Materials, Nice (France), 15-17/10/2014. Oral presentation.
370. Martina, M.R.; Menichetti, S.; Procacci, P.; Caminati, G. International Conference Nanotech Italy 2014, Venice, 26-28/11/2014. Oral presentation.
371. Mavelli, F. 2nd International Summit on Integrative Biology, Chicago (USA), 04-05/08/2014. Invited oral presentation.
372. Mavelli, F. IX Congresso Annuale del Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Napoli, 01-02/07/2014. Oral presentation.
373. Mavelli, F.; Altamura, E. Syschem 2014, San Sebastian (Spain), 09-12/06/2014. Oral presentation.
374. Mavelli, F.; Altamura, E. Working group meeting COST Action CM1304 - Compartment Permeability, Parmenides Foundation, Munich (Germany), 20-22/11/2014. Oral presentation.
375. Mavelli, F.; Altamura, E.; Stano P. CoSMoS Satellite Workshop of ALIFE 14, New York (USA), 29-30/07/2014. Oral presentation.
376. Messina, G.M.L.; Karakeçili, A.; Marletta, G. GRC Biointerface Science 2014, Lucca (Italy), 16-20/06/2014. Poster.
377. Messina, G.M.L.; Karakeçili, A.; Marletta, G. MRS Fall Meeting & Exhibit, Boston (USA), 29/11/-06/12/2014. Poster.
378. Meucci, V.; Minunni, M.; Vanni, M.; Sgorbini, M.; Intorre, L. Atti SISVet LXVIII. vol. LXVIII, p. 24-25, Pisa, 16-18/06/2014. Poster.
379. Milanese, C.; Aramini, M.; Gaboardi, M.; Pontiroli, D.; Girella, A.; Marzaroli, V.; Riccò, M.; Marini, A. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Poster.
380. Milanese, C.; Girella, A.; Marini, A.; Aramini, M.; Gaboardi, M. Pontiroli, D.; Riccò, M. CIMTEC – 6th Forum on New Materials, Montecatini Terme (Italy), 08-13/06/2014. Oral presentation.
381. Minunni, M. Seconda Scuola Nazionale sui Biosensori Ottici e Biofotonica, Otranto (Italy) 15-20/09/2014. Oral presentation.
382. Monduzzi, M.; Medda, L.; Salis, A. 28th ECIS Conference, Limassol (Cyprus), 07-12/09/2014 Oral presentation.
383. Murgia, S.; Caltagirone, C.; Falchi, A.M.; Meli, V.; Monduzzi, M.; Prodi, L.; Schmidt, J.; Talmon, Y. 28th ECIS Conference, Limassol (Cipro), 07-12/09/2014. Oral presentation.
384. Parisi, M.L.; Spinelli, D.; Pogni, R.; Basosi, R. VIII Congresso Nazionale dell'AIGE -Associazione Italiana Gestione Energia, Reggio Emilia (Italy), 09-10/06/2014. Oral presentation.
385. Picca, R.A.; Calvano, C.D.; Sportelli, M.C.; Fazio, B.; Priolo, F.; Irrera, A.; Cioffi, N. MRS2014 Spring Meeting, San Francisco, CA (USA), 21-25/04/2014. Poster.
386. Picca, R.A.; Sportelli, M.C.; Dilonardo, E.; Cioffi, N. IX Congresso del Consorzio per lo Sviluppo dei Sistemi a Grande Interfase – CSGI, Napoli (Italy), 01-02/07/2014. Oral communication.
387. Pogni, R. Nanoday, Siena, 25/06/2014. Oral presentation.
388. Pogni, R. Oxizymes 2014, Vienna, 01-04/07/2014. Oral presentation.
389. Pogni, R. XIX Scuola Nazionale di Chimica bioinorganica per dottorandi, Pisa, 22-24/10/2014. Plenary lecture.
390. Pogni, R.; Baratto, M.C.; Sinicropi, A.; Ruiz-Dueñas F.J.; Sáez-Jiménez, V.; Linde, D.; Martínez, A.T.; Basosi, R. XXV Congresso Nazionale della SCI, Arcavacata di Rende (Italy), 07-12/09/2014. Poster.
391. Pontiroli, D.; Gaboardi, M.; Magnani, G.; Aramini, M.; Milanese, C.; Pramudita, J.C.; Sharma, N.; Riccò, M. 2nd International Congress on Energy Efficiency and Energy Related Materials (ENEFM), Oludeniz (Turkey), 16-19/10/2014. Oral presentation.
392. Pontiroli, D.; Gaboardi, M.; Magnani, G.; Riccò, M.; Bertoni, G.; Milanese, C. 1st Parma Nanoday Workshop, Parma (Italy), 28/11/2014. Oral presentation.
393. Quinzeni, I.; Ferrari, S.; Quartarone, E.; Capsoni, D.; Mustarelli, P.; Bini, M. E-MRS: European Materials Research Society, Lille (France), 26-30/05/2014. Poster.
394. Ridi, F. Riunione Scientifica Annuale delle Unità Operative del Consorzio CSGI, Napoli, 01-02/07/2014. Oral presentation.
395. Rizzuti, A.; Mastrorilli, P.; Dassisti, M.; Sportelli, M.C.; Picca, R.A.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (CS), 07-12/09/2014. Poster.
396. Russo Krauss, I.; Parkinson, G.; Merlino, A.; Randazzo, A.; Novellino, E.; Mattia, C.A.; Mazzarella,

L.; Sica, F. Functional DNA Nanotechnology Workshop, Rome (Italy), 19-20/06/2014. Poster & flash presentation.

397. Russo Krauss, I.; Pica, A.; Merlino, A.; Mazzarella, L.; Sica, F. Functional DNA Nanotechnology Workshop, Rome (Italy), 19-20/06/2014. Poster & flash presentation.
398. Russo Krauss, I.; Pica, A.; Merlino, A.; Sica, F. XXV Congresso Annuale della Società Italiana di Spettroscopia Neutronica (SISN), Napoli (Italy), 03-04/07/2014. Poster.
399. Salis, A.; Medda, L.; Casula, M.F.; Monduzzi, M. Realizing Reformulation a Symposium on Surface and Materials Chemistry, Lund, 22-24/10/2014. Poster.
400. Salis, A.; Medda, L.; Cugia, F.; Parsons, D.F.; Ninham, B.W.; Monduzzi, M. 28th ECIS Conference, Limassol (Cyprus), 07-12/09/2014. Oral presentation.
401. Salis, A.; Medda, L.; Monduzzi, M. SiO2, Advanced Dielectrics and Related Devices, Cagliari, 15-18/06/2014. Oral presentation.
402. Santoru, A.; Garroni, S.; Pistidda, C.; Milanese, C.; Masolo, E.; Marini, A.; Dornehim, M.; Mulas, G.; Enzo, S. International Symposium on Metal – Hydrogen Systems MH 2014, Manchester (UK), 20-25/07/2014. Poster.
403. Scarano, S; Mariani, S.; Minunni, M. XXV Congresso della Società Chimica Italiana, Rende, 08-12/09/2014. Poster.
404. Scarano, S.; Mariani S.; Minunni, M. 1st IMEKO FOOD - Promoting Objective and measurable Food Quality and Safety – Rome (Italy), 13-15/10/2014. Oral presentation.
405. Scarano, S.; Mariani, S.; Minunni, M. International conference on Biophysics, section Bioispired nanotechnologies and Biosensors, RBC 2014 in Smolenice castle, 15-20/05/2014. Oral presentation.
406. Smeazzetto, S.; Cerboneschi, M.; Thiel, G.; Moncelli, M.R. Course on Biophysics of Channels and Transporters, Erice (Italy), 11-17/05/2014. Poster.
407. Smeazzetto, S.; Moncelli, M.R.; Thiel, G. 58th Biophysical Meeting, San Francisco (USA), 15-19/02/2014. Poster.
408. Sportelli, M.C.; Hoetger, D.; Picca, R.A.; Manoli, K.; Kranz, C.; Mizaikoff, B.; Torsi, L.; Cioffi, N. EMRS2014 Spring Meeting, Symposium B: Advanced functional materials for environmental monitoring and applications, Lille (France), 26-30/05/2014. Poster.
409. Sportelli, M.C.; Hötger, D.; Picca, R.A.; Manoli, K.; Kranz, Mizaikoff, B.; Torsi, L.; Cioffi, N. MRS2014 Spring Meeting, San Francisco, CA (USA), 21-25/04/2014. Oral communication.
410. Sportelli, M.C.; Nitti, M.A.; Valentini, M.; Picca, R.A.; Melisi, D.; Bonerba, E.; Sabbatini, L.; Tantillo, G.; Valentini, A.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (Italy), 07-12/09/2014. Oral communication.
411. Sportelli, M.C.; Picca, R.A.; Manoli, K.; Magliulo, M.; Torsi, L.; Cioffi, N. XXV Congresso Nazionale della Società Chimica Italiana - SCI 2014, Università della Calabria, Arcavacata di Rende (Italy), 07-12/09/2014. Keynote.
412. Sportelli, M.C.; Picca, R.A.; Manoli, K.; Torsi, L.; Cioffi, N. Società Chimica Italiana & SIGMA ALDRICH Young Chemists Symposium, 14th edition Riccione (Italy), 27-29/10/2014. Oral communication.
413. Stefan, A. Convegno: Valorizzazione dei co-prodotti come scelta strategica per la sostenibilità delle bioraffinerie da colture dedicate, Ecomondo, Rimini (Italy), 07/11/2014. Oral presentation.
414. Stefan, A.; Boiani, M.; Longanesi, L.; Hochkoeppler, A. 16th European Congress on Biotechnology, Edinburgh (UK), 13-16/07/2014. Poster.
415. Stefan, A.; Montòn-Silva, A.; Ceccarelli, A.; Hochkoeppler, A. Conference, Zing Conferences, Cambridge (UK), 31/08-04/09/2014. Poster.
416. Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Inesi, G.; Sitsel, O.; Gourdon, P.; Meloni, G.; Nissen, P. 14th International Conference 'Na,K-ATPase and related transport ATPases: Structure, mechanism, cell biology, health and disease', Lunteren (The Netherlands), 30/08-05/09/2014. Oral presentation.
417. Vitale, S.; Zappalà, G.; Leanza, D.; Napolitani, E.; Licciardello, A. SIMS Europe 2014 – IX European Workshop on Secondary Ion Mass Spectrometry, Muenster (Germania), 07-09/09/2014. Poster.
418. Vitiello, G.; D'Errico, G.; Silipo, A.; Molinaro, A.; Paduano, L. IX Congresso Consorzio internuniversitario dei Sistemi a Grande Interfase (CSGI), Napoli (Italy), 01-02/07/2014. Oral presentation.
419. Vitiello, G.; Luchini, A.; Heenan, R.K.; Silipo, A.; Molinaro, A.; D'Errico, G.; Paduano, L. XXV Congresso Nazionale Società Italiana Spettroscopia Neutronica (SISN) – Italian Neutron Scattering Conference, Napoli (Italy), 03-04/07/2014. Oral presentation.
420. Vitiello, G.; Luciani, G.; Costantini, A.; Silvestri, B.; Avossa, J.; D'Errico, G.; Pezzella, A.; Paduano, L.; Branda, F. IX Conferenza Consorzio internuniversitario dei Sistemi a Grande Interfase (CSGI), Napoli (Italy), 01-02/07/2014. Poster.
421. Zappalà, G.; Motta, V.; Vitale, S.; Torrisi, A.; Licciardello, A. SIMS Europe 2014 – IX European Workshop on Secondary Ion Mass Spectrometry, Muenster (Germania), 07-09/09/2014. Oral presentation.

Attività Editoriale

- Amedeo Marini - Editorial Board member of *Journal of Pharmaceutical Sciences* (Wiley).
- Andrea Salis - Associate Editor of *Biocatalysis* (De Gruyter).
- Claudia Crestini - Editor of the *Journal of Applied Chemistry* (Hindawi); Guest editor of *Bioresources* (NC State University); Advisory Board member of *Cellulose Chemistry and Technology Journal* (EAR).
- Claudiu T. Supuran - Editor-in-Chief of the following: *Expert Opinion on Therapeutic Patents* (Taylor & Francis), *Journal of Enzyme Inhibition and Medicinal Chemistry* (Taylor & Francis), *Current Enzyme Inhibition* (Bentham Science), *Antiinflammatory and Antiallergy Agents in Medicinal Chemistry* (Bentham Science); Senior Editor of *Infectous Diseases-Current Topics in Medicinal Chemistry* (Bentham Science); Editorial Board member of the following: *ACS Med Chem Lett* (ACS), *European Journal of Medicinal Chemistry* (Elsevier), *Bioorganic and Medicinal Chemistry Letters* (Elsevier), *Bioorganic and Medicinal Chemistry* (Elsevier), *Current Medicinal Chemistry* (Bentham Science), *Molecules* (MDPI), *Current Pharmaceutical Design* (Bentham Science), *Current Organic Chemistry* (Bentham Science), *Metal Based Drugs* (NCBI), *International Journal of Molecular Science* (John Wiley & Sons), *Turkish Journal of Biochemistry* (De Gruyter), *Marine Drugs* (MDPI), *Journal of Molecular Recognition* (Wiley), *Applied Organometallic Chemistry* (Wiley), *Anticancer Agents in Medicinal Chemistry* (Bentham Science), *Metabolites* (MDPI).
- Debora Berti - Ownership Board member of *Physical Chemistry Chemical Physics* (Royal Society of Chemistry); co-Editor in Chief of *Journal of Colloid and Interface Science* (Elsevier).
- Giovanni Marletta - Advisory Board member of the *Journal of Applied Biomaterials & Functional Materials* (Wichtig).
- Luigi Paduano - Associated Editor of *Journal of Solution Chemistry* (Springer).
- Luisa Torsi - Regional Editor for *Europe di Flexible and Printed Electronics* (IOP).
- Maria Minunni - Editorial Board member of *Sensing and Bio-Sensing Research* (Elsevier); Review Editor of *Frontiers in Chemistry*.
- Nicola Cioffi - Editorial Board member of the following: *Research & Reviews in ElectroChemistry* (Trade Science Inc.), *The Open Materials Science Journal* (Bentham Science), *Sensor Letters* (ASP), *Journal of Sensors* (Hindawi); co-Guest Editor of *Molecules* (MDPI) e *Nanomaterials* (MDPI).
- Piero Baglioni - Editorial Board member of *European Physical Journal E* (Springer); Associate Editor of *Physical Chemistry Chemical Physics* (Royal Society of Chemistry); Advisory Board member of the following: *Journal of Colloid Interface Science* (Elsevier), *Langmuir* (ACS).
- Roberto Piazza - Senior Editor of *Journal of Physics Condensed Matter per Liquids*, *Soft Matter*, *Biological Physics* (Iop Science).
- Sergio Murgia - Editorial Board member of *BioMed Research International* (Hindawi).

Organized/Chaired

- The Research Unit of CSGI-Catania, on behalf of the EuChemS division of Physical Chemistry and Physical Chemistry Division of the Società Chimica Italiana, has organized the 1st European Conference on Physical, Theoretical, and Computational Chemistry and XLII Annual Meeting of the Physical Chemistry Division of SCI, Catania (Italy), September 14-18, 2015. The Conference hosted more than 170 attendees from 15 countries, featuring 12 international Invited Speakers, more than 70 Oral presentations and 112 Poster presentations.
- Structure and Dynamics of Supercooled Water and Other Glassy Materials, Palermo, 09-11/10/2015.

Guests

- Yosef Scolnik (IYAR-Israel Institute for Advanced Research), 29/11/2016: “Deviation from identity of macroscopic properties of enantiomers via water chiral preference. Is water chiral?”.
- Maria Vallet-Regì (Departamento de Quimica Inorganica y Bioinorganica, Universidad Complutense de Madrid), 10/11/2016: “Biomaterials Design”; 16/11/2016: “Smart Nanosystems”.
- Gavin Walker, Energy Technologies Research Institute, University of Nottingham. “Multicomponent Hydride Systems for Hydrogen Storage Applications”. 15/11/2016.

- Mohammed Harir, Ph.D. Student (fellowship from the Ministery of Higher Education of Algeria), 01/10/2015–09/10/2016 “Molecular characterization of extracts produced by strains of Actinobacteria isolated from Algerian Sahara soil”.
- Flor Guadalupe Sánchez Alejandro, Ph.D student (Doctorante del Programa en Ciencias de la Vida Biotecnología Marina) from CICESE/CNyN, UNAM, Mexico, 1/05/2016-31/07/2016 “EPR spectra on three derivatives of versatile peroxidase with aromatic aminoacids in order to characterize the radical intermediates formed”.
- Pierre Joseph (Centre national de la recherche scientifique – CNRS, Laboratory for Analysis and Architecture of Systems – LAAS), 01/09/2015-31/07/2016.
- Barbara Lonetti (Centre national de la recherche scientifique – CNRS, Laboratoire des Interactions Moléculaires et Réactivité Chimique et Photochimique – IMRCP-UMR 5623), 01/09/2015-31/07/2016.
- Ignacio Rene Galindo Esquivel (Departamento de Ingegnería Química, Universidad de Guanajuato), 19/09/2015-20/07/2016.
- Stephen T. Hyde (Department of Applied Mathematics, Australian National University), 05/07/2016: “Animal, Vegetable, Mineral. A continuum of form”.
- Marco Casazza, Siena 31/05/2016 “Atmospheric aerosol pollution – an old concern, some new perspectives”. Seminario.
- Elsa Callini, Laboratory of Materials for Renewable Energy, EPFL, Switzerland. “Stabilization of gas species via incorporation in porous solids”. 29/01/2016.
- Miriam Rueda Noriega, High Pressure Processes Group Dept. Chemical Engineering and Environmental Technology University of Valladolid. “Enhanced hydrogen storage material by stabilization of a hydride in microparticles of silica aerogel”. 10/12/2015.
- Huiping Xing (School of Material Science and Engineer, Shaanxi Normal University, China), 01/09/2014-30/09/2015.
- Kondo Francois Aguey-Zinsou, Materials Energy Research Laboratory in Nanoscale School of Chemical Engineering The University of New South Wales Sydney, Australia. “From size effects to functional hydrogen stores”. 14/09/2015.
- Curtis W. Frank (Stanford University, Department of Chemical Engineering), 01/01/2015-31/07/2015.
- Jolanta Polak, Researcher (Marie Curie-Sklodowska, University Lublin, Poland) 25-30/05/2015 “Novel phenazines with antimicrobial properties synthesized by fungal laccase from Cerrena unicolor”.
- Ángel Martín, High Pressure Processes Group Dept. Chemical Engineering and Environmental Technology University of Valladolid. “Development of new materials using compressed fluids”. 26/11/2014.
- Rodolfo Guillermo Valle Altamirano, Master student (Instituto de Biotecnologia, Universidad Nacional Autonoma de Mexico, Medicina Molecular y Bioprocesos, Cuernavaca), 17/05/2014–15/06/2014 “Spectroscopic Analysis of the H2O2- resistant Zo Peroxidase Alternative Ground State (GS*) and Compound III (CIII) Species”.
- Etsuo Akiba, Department of Mechanical Engineering, Faculty of Engineering, Kyushu University, Nishi-ku, Fukuoka, Japan. “Hydrogen storage and transport: State-of-art in Japan”. 13/06/2014.
- Marzia Pentimalli, Laboratorio di Chimica e Tecnologie dei Materiali, ENEA, Centro Ricerche Casaccia, Roma, “Sviluppo di un sistema di refrigerazione a idruri metallici alimentato da calore di scarto. Caratterizzazione termodinamica dei materiali e definizione del ciclo termico”. 15/05/2014.
- Kostas Hatzixanthis (Director of Research - Procarta Biosystems Ltd, Norwich, UK), 21/01/2014: “Development of nanoparticulate Nucleic-Acid based Therapeutics, Snares™, for the treatment of infectious diseases and an introduction to EU IAPP project DNA-TRAP”.

Theses (undergraduate, master and PhD)

U.O. Bari

Bachelor in Chemistry (Laurea triennale)

- Lapenna, A.: "Sviluppo di un metodo di immobilizzazione di glicoenzimi in idrogel di alginato per applicazioni ensoristiche" (2014).
- Angelini, G.: "Immobilizzazione dell'enzima Tirosinasi da Agaricus Bisporus mediante deposizione via plasma a pressione atmosferica di un film polietilenico" (2016).
- del Sole, R.: "Controlled deposition of gold nanoparticles for Laser Induced Breakdown Spectroscopy applications" (2016).

Bachelor in Materials Science (Laurea triennale)

- Talamo, S.: "Studio preliminare della immobilizzazione di enzimi mediante deposizione via plasma a pressione atmosferica di coating polimerici" (2016).

Master in Chemistry (Laurea magistrale)

- Dilucca, M.: "Studio microstrutturale di un sistema tensioattivo commercial" (2016).

Master in Materials Science and Technology (Laurea magistrale)

- Angarano, V.: "Studio sull'immobilizzazione di enzimi mediante deposizione di coating polimerico via plasma a pressione atmosferica" (2016).
- Cimmarusti, G.M.: "Cellulose gelation in confinement" (2016).

PhD in Chemical and Molecular Sciences

- Sportelli, M.C.: "Synthesis and advanced morphological-spectroscopic characterization of transition metal nanostructures and their application in analytical methods" (2016).

U.O. Bologna

Bachelor in Industrial Chemistry (Laurea triennale)

- Perrone, A.: "Sovraespressione in Escherichia coli del sub-assemblaggio $\tau - \alpha - \varepsilon - \theta$ della DNA polimerasi III" (2014).
- Perticarari, S.: "Caratteristiche biochimiche e fenotipiche della variante D201A del dominio PHP della subunità α di Escherichia coli" (2014).
- Camerani, M.: "Sovraespressione e parziale purificazione di una DNA polimerasi di Deinococcus radiodurans" (2015).
- Caramia, S.: "Caratterizzazione cinetica di β-glucosidasi di Prunus dulcis" (2015).
- Maturi, M.: "Purificazione e caratterizzazione della DNA Polimerasi α di Deinococcus radiodurans" (2015).
- Del Grosso, I.: "Sovraespressione e purificazione della subunità α della DNA polimerasi III di Escherichia coli" (2016).

- Ottone, P.: “Tecniche analitiche in campo enologico” (2016).

Master in Industrial Chemistry or Molecular and Industrial Biotechnologies (Laurea magistrale)

- Lapenta, F.: “Caratterizzazione dell’attività pirofosfatasica associata al dominio PHP della DNA polimerasi III” (2014).
- Magri, L.: “Espressione eterologa e purificazione della istone deacetilasi umana 1 (HDAC1)” (2014).
- Martina, C.E.: “Dal frammento Klenow a HoLaMa. Ingegnerizzazione di una mini DNA polimerasi di Escherichia coli” (2014).
- Rossi, N.: “Sintesi di PNA a libertà conformazionale ridotta” (2014).
- Schipani, F.: “Sovraespressione in Escherichia coli e purificazione della istone deacetilasi umana 1 (HDAC1)” (2014).
- Tetter, S.: “Supercharged ferritin as a nanotechnological tool and transfection agent” (2014).
- Fontana, M.: “Characterization of nanofluidics devices for high-throughput single molecule fluorescence detection” (2015).
- Rocca, M.: “In vitro engineering and assembly of an artificial carboxysome” (2015).
- Perrone, A.: “Sovraespressione, purificazione e caratterizzazione cinetica della polimerasi DnaE di Deinococcus radiodurans” (2016).
- Perrucci, J.: “Sovraespressione di sub-assemblaggi della DNA polimerasi III di Escherichia coli mediante la co-trasformazione dell'ospite con plasmidi compatibili” (2016).

PhD in Biotechnological and Pharmaceutical Sciences

- Montòn Silva, A.: “Structural and kinetic characterization of DNA polymerases I and III from Escherichia coli” (2015).

U.O. Cagliari

Bachelor in Chemistry (Laurea triennale)

- Fanti, S.: “Silice mesoporosa ordinata funzionalizzata con biopolimeri come possibile sistema drug delivery. Importanza del grado di funzionalizzazione sulle proprietà strutturali e tessiturali” (2015).
- Pruner, S.: “Adsorbimento di biomolecole su Materiali Mesoporosi Ordinati” (2015).

Master in Chemical Sciences (Laurea magistrale o a ciclo unico)

- Carucci, C.: “Hofmeister phenomena in Bioelectrochemistry: The supporting Electrolyte Affects the Response of Glucose Electrodes” (2014).
- Tocco, F.: “Materiali Mesoporosi Ordinati per l’Immobilizzazione di Antibiotici” (2014).
- Becconi, O.: “Studio delle interazioni specifiche tra Li+, Na+, K+ e l'albumina del siero bovino mediante dinamica molecolare” (2016).
- Collu, M.: “Fenomeni Hofmeister in biocatalisi. Effetti specifici degli anioni sulla sintesi enzimatica del biodiesel” (2016).

- Delpiano, G.R.: “Sintesi e caratterizzazione di sistemi multifunzionali costituiti da nanoparticelle di silice mesoporosa coniugate con proteine e nanoparticelle d’oro” (2016).
- Magnolia, S.: “Sistemi "stimuli-responsive" per il drug delivery: effetto del pH su nanoparticelle di silice mesoporosa funzionalizzate con acido ialuronico” (2016).
- Medda, S.: “Studio dell'interazione tra l'albumina di siero bovino e nanoparticelle di silice mesoporosa funzionalizzate con biopolimeri” (2016).
- Sedda, S.: “Effetto degli elettroliti sull’adsorbimento fisico del lisozima su materiali a base di silice mesoporosa” (2016).

PhD in Chemical Sciences and Technologies
- Meli, V.: “Theranostic applications of fuorescent liquid crystalline nanoparticles” (2016).

U.O. Campobasso

Bachelor in Agriculture, Environment, Food (Laurea triennale)
- Tata, S.: “Ecogenicità e rilascio da liposomi indotto dal pH” (2015).
- Meli, V.: “Messa a punto e caratterizzazione di microsfere di proteine di soia-zeina per il trasporto nutraceutico controllato” (2016).

Master in Agriculture, Environment, Food (Laurea magistrale)
- Tucci, R.: “Interventi di mitigazione del rischio di liquefazione su larga scala” (2016).

U.O. Catania

Bachelor in Chemistry (Laurea triennale)
- Leanza. D.: “Ancoraggio di sistemi fotoattivi su substrati di TiO2 nanostrutturati” (2014).
- Livio, P.: “Preparazione e caratterizzazione morfologica ed elettrica su scala nanometrica di ‘nastri’ macromolecolari di Poli-3-esil-tiofene (P3HT)” (2015).
- Lo Bello, L.: “Ancoraggio di molecole fotoattive su substrati flessibili” (2015).
- Moschetto, S.: “Preparazione e caratterizzazione di film sottili ibridi di nanotubi di carbonio e polimeri coniugati” (2015).
- Valenti, A.M.G.: “Ancoraggio di sistemi fotoattivi su substrati nanostrutturati di SnO2” (2015).
- Fichera, L.: “Metodologie di “patterning” di monolayer fosfolipidici ” (2016).
- Lombardo, T.: “Sintesi stepwise, su superfici di ossidi, di sistemi organici per elettronica molecolare” (2016).
- Ruffino, R.: “Metodologie di riconoscimento selettivo di monosaccaridi in matrici biologiche modello” (2016).

Master in Materials Chemistry (Laurea magistrale)
- Eredia, M.: “Caratterizzazione chimica spazialmente risolta di sistemi organici micro- e nano- strutturati mediante ToF-SIMS” (2014).

- Scollo, M.: "Preparazione e studio di film sottili di miscele di semiconduttori organici per applicazioni fotovoltaiche" (2014).
- Tummino, A.: "Nano/Meso strutturazione e caratterizzazione di superfici polimeriche" (2014).
- Condorelli J.: "Assemblaggio e caratterizzazione di film ultrasottili per l'elettronica molecolare" (2015).
- Russo, M.R.: "Preparazione e caratterizzazione di materiali per packaging innovativo in microelettronica" - Tesi in collaborazione con ST Microelectronics (Catania) (2015).
- Spampinato N.: "Caratterizzazione chimica tridimensionale di sistemi ibridi microstrutturati mediante cluster-SIMS" (2015).
- Barillaro, S.: "Materiali elettrodici per Batterie Redox a Flusso di Vanadio" - Tesi in collaborazione con ITAE/CNR (Messina) (2016).

PhD in Materials Science

- Zappalà, G.: "Assembly and characterisation of molecular films for energetics and electronics" (2014).

U.O. Firenze

Bachelor in Chemistry (Laurea triennale)

- Gelli, R.: "Mineralizzazione di idrogel macroporosi a base di imogolite e gelatina" (2014).
- Grifoni, E.: "Nanocompositi biodegradabili a base di polisaccaridi e nanoargille: preparazione, caratterizzazione e studio delle proprietà di rilascio" (2014).
- Pastacaldi, G.: "Sintesi di nanoparticelle di silice mesoporose per il consolidamento di opere d'arte" (2014).
- Rinaldi, E.: "Nanocompositi iniettabili a base di Halloysiti e Polisaccaridi" (2014).
- Santini, S.: "Studio degli effetti di pH e specie fosfato su idrogel di PAAm" (2014).
- Sordi, G.: "Studio dell'interazione di un composto del platino con Ca-ATPasi" (2014).
- Magnani, C.: "Comprensione delle proprietà antibatteriche di agenti terapeutici nanostrutturati tramite interazione con modelli di membrane Gram-negative" (2015).
- Tanteri, V.: "Preparazione e caratterizzazione di nanocompositi biodegradabili a base di poliidrossibutirrati, polossameri e Halloysiti" (2015).
- Bolognesi, A.: "Studio degli effetti dell'addizione di alloisiti funzionalizzate su cementi a base di magnesio" (2016).
- Brandi, F.: "Caratterizzazione chimico fisica di un fluido nanostrutturato per la rimozione di film polimerici" (2016).
- Cialli, O.: "Fluidi nanostrutturati per il dewetting di film polimerici da superfici di interesse per i beni culturali" (2016).
- Giannetti, C.: "Studio dell'interazione di esametafosfato con cementi a base di silicati idrati di magnesio" (2016).
- Nardin, R.: "Gel filmogeni a base di PVA per la rimozione di patine da reperti in bronzo" (2016).

- Perdichizzi, A.: "Studio delle interazioni di cementi a base di magnesio con fasi alluminatiche" (2016).
- Salvi, M.: "Nanocarriers a Base di Complessi di Ioni Rame" (2016).

Bachelor in Diagnostics and Materials for Conservation and Restoration (Laurea triennale)

- Alterini, M.: "Rimozione selettiva di ridipinture in Arte contemporanea mediante gel chimici" (2015).
- Donatelli, A.: "Reperti archeologici copti: caratterizzazione dei materiali impiegati nel restauro" (2015).
- Guerini, L.: "Deacidificazione non acquosa di manoscritti contenenti inchiostri sintetici" (2015).
- Onorato, F.: "Dispersioni non acquose di lattato di calcio per la stabilizzazione del pH di manufatti a base di collagene" (2015).
- Potenza, P.: "Sintesi e caratterizzazione di lattato di calcio per il restauro di cuoio e pergamena" (2015).
- Rizzuti, M.: "Nanoparticelle di carbonato di calcio idrofobizzato per la deacidificazione di manoscritti contemporanei" (2015).
- Stellini, F.: "I materiali dell'arte contemporanea: degradazione fotochimica di carte ed inchiostri sintetici" (2015).
- Bortolini, M.: "Preparazione e applicazione di idrogel a base di PVA/PVP per la pulitura di opere d'arte moderna e contemporanea" (2016).
- Rivella, P.: "Microemulsioni olio in acqua a base di tensioattivo non-ionico per la rimozione selettiva di ridipinture in arte contemporanea" (2016).
- Sbolci, M.C.: "Caratterizzazione e rimozione di materiale ceroso da supporti cellulosici mediante l'applicazione di sistemi nanostrutturati" (2016).
- Vettori, I.: "Il restauro di opere d'arte in plastica: la pulitura con gel" (2016).

Master in Chemical Sciences (Laurea magistrale)

- Benvenuti, E.: "Dispositivi ibridi per emettitori modulabili di luce bianca e monocromatica" (2014).
- Fogli, S.: "Nanoparticelle Inorganiche con Corone Proteiche: sintesi e caratterizzazione chimico fisica" (2014).
- Generini, V. "Interazione di nanoparticelle di oro con sistemi modello di membrana: effetto della forma e del rivestimento della superficie" (2014).
- Nicotera, G.: "Sintesi, caratterizzazione e potenzialità applicative di nanocompositi termoresponsivi a base di PNIPAAm e Idrossiapatite" (2014).
- Sarri, F.: "Dispositivi Modulabili per Applicazioni OLED e DSSC" (2014).
- Tatini, D.: "Thermo-responsive and biocompatible polymer composite for controlled release of active agents" (2014).
- Gabbani, A.: "Adsorbimento di aminoacidi su nanotubi aluminosilicatici" (2015).
- Pomposi, C.: "Messa a punto di tecniche innovative per lo studio di disperdenti per particolato carbonioso" (2015).
- Rossi, M.: "Studio della dinamica diffusionale in idrogel chimici" (2015).
- Arias, M.: "Nuove Metodologie Bioassistite per la Pulitura di Opere d'Arte" (2016).
- Cerretani, C.: "Sintesi e caratterizzazione fotofisico di clusters di metallic nobili per applicazioni LED" (2016).

- Cipriani, A.: "Water-sensible supramolecular nanofibers as active material of a new humidity sensor" (2016).
- Feroci, E.: "Studio di un mutante di Profilina I con proprietà camaleontiche" (2016).
- Gelli, R.: "Compositi funzionali per tissue engineering", Università degli studi di Firenze (2016).
- Marsili, L.: "Sviluppo di un nuovo protocollo per la preparazione di modelli di membrane asimmetriche: un metodo microfluidico" (2016).
- Mendozza, M.: "Cristalli liquidi colloidali stabilizzati con polimeri termoresponsivi" (2016).
- Milanesi, A.: "Caratterizzazione di impasti di silicati di magnesio in presenza di polimetafosfati"(2016).
- Scudero, M.: "Preparazione e caratterizzazione di nanoparticelle mesoporose di fosfato di calcio" (2016).
- Toppi, A.: "Microsfere porose di acido poli(lattico-co-glicolico) come dispositivi per il trasporto di farmaci antitumorali" (2016).

Master in Sciences and Materials for the Conservation and Restoration (Laurea magistrale)

- Camerini, R.: "Formulazioni composite a base di idrossido di calcio per il consolidamento di materiali lapidei" (2015).
- Castri, E.: "Preparazione e caratterizzazione di idrogel a base di PVA/PVP per la pulitura di superfici artistiche" (2015).
- Sisto, A.: "Dispersioni non acquose di particelle di carbonato di calcio per la deacidificazione di materiali a base di cellulosa" (2016).
- Smiriglia, E.: "Sintesi e caratterizzazione di nanoparticelle di silice mesoporose: applicazioni per la conservazione di opera pittoriche contemporanee" (2016).

PhD in Chemical Sciences

- Castroflorio, B.: "Nanosistemi per incapsulazione e delivery di biomolecole o principi attivi terapeutici macromolecolari" (ciclo XXVIII).
- Tempesti, P.: "Nanocompositi biomimetici responsivi per ingegneria tissutale ossea" (ciclo XXVIII).
- Salvatore, A.: "Nanostructured Platforms based on Magnetic Nanoparticles for the Delivery of Therapeutic Biomolecules" (ciclo XXIX).
- Tonelli, M.: "Studio delle proprietà strutturali di cementi eco-sostenibili e valutazione delle strategie per il loro miglioramento" (ciclo XXX).

U.O. Napoli

Bachelor in Chemistry or Industrial Chemistry (Laurea triennale)

- Quinterno, M.: "Sintesi e caratterizzazione di nanoparticelle ibride titania-melanina" 2014.
- Russo, V.: "Formulazione e caratterizzazione chimico-fisica di miscele acquose acido polimetacrilico-tensioattivo etossilato" 2014.
- Buciunì, A.: "Studio cinetico dell' interazione tra il peptide β-amiloide (1-42) e una membrana lipidica mediante risonanza paramagnetica elettronica" (2015).

- Bonifazzi, M.: "Caratterizzazione mediante Risonanza Paramagnetica Elettronica dell'interazione tra dominio Pre-Transmembrana di protein di fusione virali e doppi strati fosfolipidici" (2015).
- Di Gennaro, M.: "Polimerizzazione di DHICA in presenza di un templante inorganico: il ruolo della silice" (2015).
- Savignano, L.: "Diagramma di fase di una miscela acquosa di tensioattivi di interesse industriale" (2015).
- Scermino, L.: "Caratterizzazione reologica di una miscela acquosa di surfattanti" (2015).
- Striano, A.: "Effetto dell'acido 22:6(cis) docosaesanoico sulle proprietà strutturali di un doppio strato fosfolipidico" (2015).
- Acerra, A.: "Sintesi idrotermale e caratterizzazione di nanoparticelle ibride TiO2-melanina con proprietà antimicrobiche" (2016).
- Pagano, R.: "Nanovettori liposomiali per il rilascio controllato di Sunitinib malato" (2016).
- Salzano, C.: "Effetto di nanoparticelle di magnetite funzionalizzate sulla conformazione e stabilità della transferrina umana" (2016).

Master in Chemical Sciences or Sciences and Technologies of Industrial Chemistry (Laurea magistrale)

- Del Sorbo, G.: "Caratterizzazione Strutturale del Rivestimento Lipidico di Nanoparticelle Inorganiche: verso lo Sviluppo di Nuovi Agenti Teranostici" (2015).
- Imparato, C.: "Sintesi e caratterizzazione di materiali ibridi a base di biossido di titanio come catalizzatori per la degradazione di inquinanti" (2015).
- Silvestri, S.: "Sintesi e caratterizzazione di un sistema ibrido composto da Nanoparticelle di Ossido di Zinco e Nanotubi di Carbonio per applicazioni in ambito biosensoristico" (2015).
- Liguori, S.: "Sviluppo e caratterizzazione di nanoparticelle funzionalizzate con aptameri anticoagulanti per scopi diagnostici e terapeutici" (2016).
- Tammaro, O.: "Nanoparticelle ibride TiO2-Melanina: meccanismo di azione antimicrobica" (2016).

U.O. Pavia

Bachelor in Chemistry (Laurea triennale)

- Callegari, D.: "Metodologie di sintesi del metastannato di stronzio SrSnO3" (2014).
- Gioventù, M.: "Sintesi della ferrite di bismuto BiFeO3: descrizione e confronto tra le metodologie di preparazione" (2014).
- Magagna, S.: "Sintesi e proprietà termoelettriche di Ca3Co4O9" (2014).
- Palumbo, A.: "Sintesi del niobato di litio: LiNbO3: descrizione di metodologie di sintesi" (2014).
- Valsecchi, G.: "Descrizione delle metodologie di sintesi del composto Bi4Ti3O12" (2014).
- Botti, O.: "Thermogravimetric analysis: fundaments, instrumentation and application cases" (2015).

- Cannistrà, C.: "Studio dei processi di degradazione termica di polimeri termoplastici finalizzato alla messa a punto di un metodo di misura della stabilità termica" (2015).
- Corsico, S.: "Materiali per lo stoccaggio di idrogeno allo stato solido" (2015).
- Ghidoni, S.: "Metodi di sintesi dell'ossido misto di ittrio e manganese" (2015).
- Vercesi, A.: "Metodi di sintesi innovativi di Li4Ti5O12 come anodo in batterie a ioni litio" (2015).
- Baiardi, E.: "Calorimetria differenziale a scansione a flusso di calore: descrizione della apparecchiatura ed esempi applicativi" (2016).
- Bonizzoni, S.: "Smart Materials: Leghe a memoria di forma e polimeri elettroattivi" (2016).
- Casali, E.: "Celle solari ibride organiche-inorganiche a base di perovskite CH3NH3PbI3" (2016).
- Chillè, L.: "Idruri complessi per l'immagazzinamento di idrogeno allo stato solido" (2016).
- Di Martino, G: "Il manganito di lantanio: LaMnO3. Struttura e proprietà. Metodi di sintesi" (2016).
- Olgiati, F.: "Metodi di sintesi della ferrite di lantanio LaFeO3" (2016).
- Spada, D.: "Sintesi di Perovskiti a base di lantanio: LaCoO3" 2016.

Master in Chemistry (Laurea magistrale)

- Marzaroli, V.: "Metal organic frameworks e fulleriti per lo stoccaggio di idrogeno" (2015).
- Valsecchi, G. "Preparazione e caratterizzazione chimico-fisica di sistemi idrurici innovativi per lo stoccaggio di idrogeno" (2016).

Master in Pharmacy (Laurea magistrale)

- Domenighini, M.F.: "Elettrofilati polimerici per il rilascio controllato di budesonide: preparazione e caratterizzazione chimico-fisica e farmaceutica" (2015).
- Pardi, F.: "Febantel: alla ricerca di nuovi polimorfi" (2016).
- Santagostino Baldi, F.: "Chimica e clinica dell'harpagophytum procumbens in osteoartrite e low back pain" (2016).

U.O. Siena

Bachelor in Chemical Sciences (Laurea triennale)

- Alagna C.: "Immobilizzazione della lipasi da Candida rugosa su nanofibre di poliuretano: caratterizzazione ed applicazione nella biosintesi dell'etil gallato" (2014).
- Barbetti E.: "Analisi di impatto ambientale dello Shale Gas" (2014).
- Burroni M.: "Uno studio di spettroscopia di Risonanza Paramagnetica Elettronica per la caratterizzazione di materiali fotocatalitici" (2014).
- Caforio, J.: "Utilizzo della spettrometria di massa di ioni secondari (ToF-SIMS) per la caratterizzazione geografica di prodotti agroalimentari" (2016).
- Coppola, C.: "Valutazione dell'impatto ambientale del fotovoltaico innovativo di ultima generazione: le Celle a Perovskite" (2016).

- D'Ettorre, A.: "Type II Dye Sensitized Solar Cells: the design of novel and efficient Sensitizers" (2016).
- Fineschi, G.: "Metodiche quantitative per la determinazione della Tomatina nel Solanum Lycopersicum nelle differenti fasi di sviluppo vegetative" (2016).
- Miliani, E.: "Caratterizzazione di siti di rame di tipo T3 utilizzando la spettroscopia EPR" (2016).
- Njomo Ngeumbou N.F.: "Limiti e potenzialita della biomassa algale: analisi del ciclo di vita per la produzione di biofuel" (2016).
- Sacchetta F:. "Impatti ambientali di tecnologie a totale reiniezione di fluidi per lo sfruttamento della risorsa geotermica" (2016).
- Stefanucci, E.: "Origini della contaminazione da arsenico nella Toscana meridionale: nuovi studi sul bacino del fiume Pecora" (2016).

Master in Sanitary Biology (Laurea magistrale)

- Diaz, C.: "Metodo per la misura della concentrazione del glutatione su microvolumi di sangue " (2014).
- Belvisi, R.: "Dihomo-IsoPs nel neonato asfittico con metodica LC-MS/MS: studio di un nuovo marker di danno cerebrale" (2015).
- Langialonga, A.: "Indagini sui meccanismi d'azione adatto geni di Rhodiola Rosea L." (2015).

Master in Chemistry (Laurea magistrale)

- Tabani, Z.: "Caratterizzazione di alcune uve e vini della zona Chianti Classico" (2014).
- Nencini, A.: "Sviluppo di una metodica di analisi chimica per la caratterizzazione di matrici naturali ad uso alimentare: determinazione delle proprietà chimiche delle pesche e nettarine" (2014).
- Pagliaccia M.: "Caratterizzazione del ciclo catalitico di una nuova perossidasi da Raphanus Sativus resistente all'inattivazione da perossido di idrogeno" (2014).
- Garufo G.: "Sintesi di un colorante porpora catalizzata da laccasi da Trametes versicolor" (2016).
- Mahmoudian J.: "Exploitation of Biomass for production of hydrogen and chemicals through electrochemical reforming by using nanotechnology" (2016).
- Raneri G.: "Determinazione della capacità antiossidante di un estratto da Consolida Maggiore (Symphytum Officinale) ramite standardizzazione del saggio del dpph" (2016).

Master in Pharmacy or Pharmaceutical Chemistry and Technologies (Laurea magistrale)

- Buccirossi, L.: "Caratterizzazione della composizione Terpenica in porzioni lipidiche di copaifera langsdorffii ed eugenia caryophyllat" (2016).
- Pardini, A.: "Studio delle proprietà nutraceutiche della tomatina e dei suoi derivati ottenuti da prodotti vegetali" (2016).

PhD in Chemical and Pharmaceutical Sciences

- Maranghi, S.: "Energy Efficiency Optimization Study of Microgeneration and Energy Saving Systems by LCA Analysis" (2015).
- Mohammadpourasl, S.: "Design and characterization by using computational methodologies and life cycle assessment (LCA) of devices for energy production

from renewable energy sources" (2016-2018) (Pegaso Unifi-Unipi-unisi, Univ. Siena).

RESEARCH PROJECTS

1A: Hard Matter (Nanomaterials and Solid Interfaces).....87

1B: Soft Matter (Nanomaterials and Liquid Interfaces).....121

1C: Theory and Modelling.....169

2A: Art Restoration, Environmental Remediation and Textile Chemistry.....186

2B: Metals and Ceramics.....224

2C: Biology and Biotechnology.....229

1A – Spontaneous aggregation of soil organic matter and its interaction with iron oxide particles

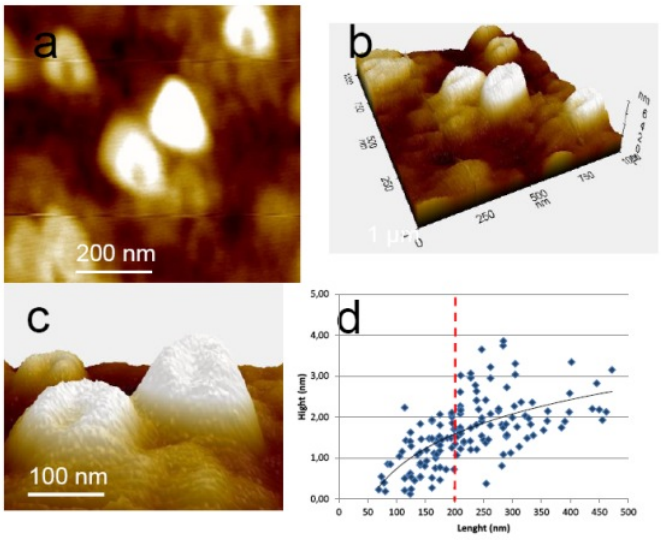
R. Angelico, G. Palumbo, C. Colombo, J. He (Centre for Eco-environmental Sciences, Chinese Academy of Sciences, Beijing, China)

Aims

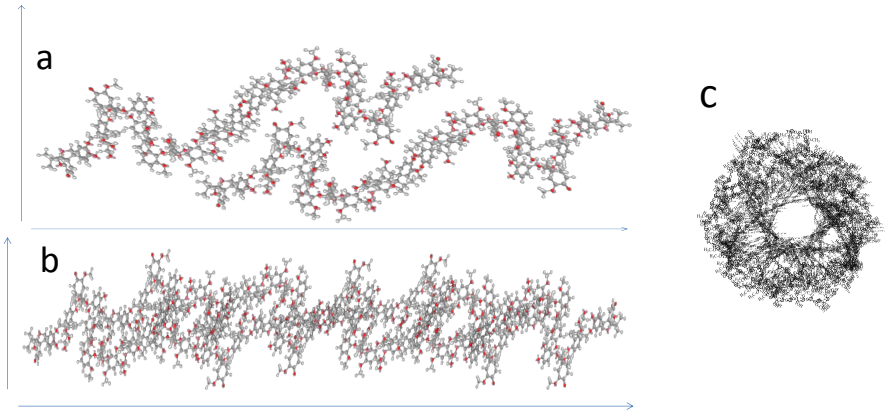
Chemical and physicochemical behaviour manifested by humic acid (HA) in natural soil and water environments is a function of its molecular structure, and dictates its organic matter mobility, interaction with clay surfaces, and aggregation in natural environments. In the present research project, Atomic Force Microscopy in contact mode (AFM-C) was used to investigate the aggregate conformation of leonardite humic acid (HA) formed at different pH values in the range 2-12. Computational molecular models of HA, based on its chemical composition as determined by NMR measurements, were also analyzed to provide a possible conformation of 3D supramolecular structure and were compared to AFM results.
Finally, we extended our investigation to the HA coprecipitation process with iron (II) oxide and studied its effect on the iron (hydr)oxide crystallinity.

Results

The structure of HA aggregates adsorbed on mica observed in AFM micrographs showed a considerable dependence on the pH of the solutions used in the preparation of the colloidal dispersions. Interestingly, HA solubilized at pH 5 showed a ring shaped supramolecular structure. (**a**) AFM-C 2D microtopography, (**b**) and **c**) 3D microtopography images of HA dispersed in water at pH 5 adsorbed and air-dried on a mica surface. (**d**) Heights of individual HA particles observed with AFM-C plotted vs. their measured lengths.



Based on molecular simulation methods, the molecular conformation of HA was performed on the Lignin–Carbohydrate Complex (LCC) model in which the parameters of the β-O-4 linkages in the oligomeric chain were optimized. The LCC model provided a possible conformation of the 3D ring structure of HA, depending on the pH employed in its preparation. These results were very helpful to understand the influence of carboxylic and phenolic group ionization on the HA molecular arrangement in terms of size, strength, and flexibility. Covalent and hydrogen bonds appeared to stabilize the oligomeric chain of the helical structure, while dipole–dipole and van der Waals interactions held the ring-like conformation. The proposed model was a significant step toward a full understanding of HA structure and function.



Molecular modelling results: (**a**) Overlapping helical structures formed by three subunits of the phenyl propanoid chain linked in a regular linear sequence, (**b**) Linear structure formed from two overlapped chains composed of six units, (**c**) 45–50 linear helix molecules looped spirally to form a ring-shaped structure. Finally, an experimental investigation performed through Transmission electron Microscopy (TEM), X-ray Diffraction (DRX) and Diffuse Reflectance Spectroscopy (DRS) was carried out to analyse the microstructure of synthetic iron coprecipitates in solid state and while their colloidal behavior as a function of pH was ascertained through Photon Correlation Spectroscopy and Laser Doppler electrophoresis.

References

Angelico, R.; Ceglie, A.; He, J.; Yu-Rong, L.; Palumbo, G.; Colombo, C. “Particle size, charge and colloidal stability of humic acids coprecipitated with Ferrihydrite”, Chemosphere 99, 239-247 (2014).

Colombo, C.; Palumbo, G.; Angelico, R.; Cho, H.G.; Francioso, O.; Ertani, A.; Nardi, S. “Spontaneous aggregation of humic acid observed with AFM at different pH”, Chemosphere 138, 821-828 (2015).

Colombo, C.; Palumbo, G.; Di Iorio, E.; Song, X.; Jiang, Z.; Liu, Q.; Angelico, R. “Influence of hydrothermal synthesis conditions on size, morphology and colloidal properties of hematite nanoparticles”, Nano-Struct. & Nano-Objects 2, 19-27 (2015).

1A – Adhesion promoters for bitumen

R. Angelico, C. Oliviero Rossi, B. Teltayev (Kazakhstan Highway Research Institute, Almaty, Kazakhstan)

Aims

All asphalt pavements consist of two main components, bitumen and mineral aggregate. The function of bitumen, which typically represents 4-7 wt % of the pavement, is to act as a binder in-between the aggregate skeleton, giving the asphalt sufficient internal cohesion. It is, therefore, of vital importance that the bitumen has a strong bond (adhesion) to the aggregate surface. In the present project, we investigate the interactions at the bitumen-aggregate interface when different types of adhesion promoters are premixed to the bitumen.

Results

From research in the road construction sector, the most common types of activators present on the market are classified according to the chemical nature of their active ingredient: amides, PolyPhosphoric Acid (PPA) esters and organosilanes. Therefore, for each of these families, the adhesive properties of the corresponding modified bitumen loaded with a fixed amount of active agent, were tested on four types of stone materials. X-Ray Powder Diffractometry (XRPD), X-Ray Fluorescence (XRF) and Environmental Scanning Electron Microscope Energy Dispersive Spectroscopy (ESEM-EDS) were carried out in order to establish the chemical and mineralogical nature and identify the agglomerate structures of the selected inert rocks. Among various screened products, the organosilane-based additive showed excellent adhesive performances, independently of the chemical composition of inorganic interfaces, as confirmed by both contact angle and boil test measurements (Figure 1).

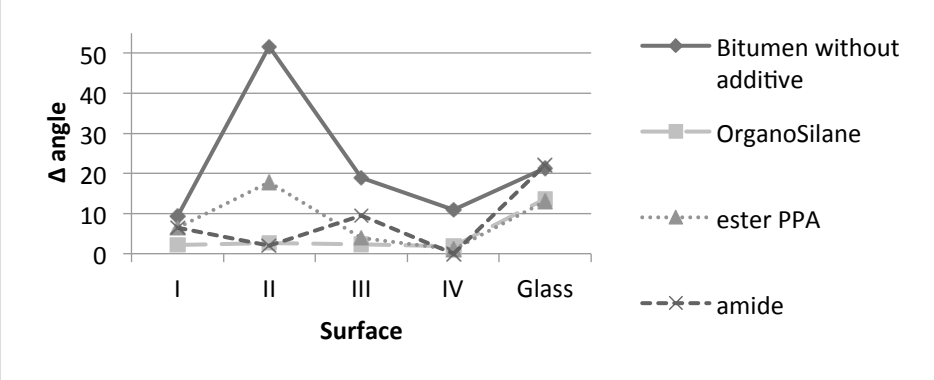
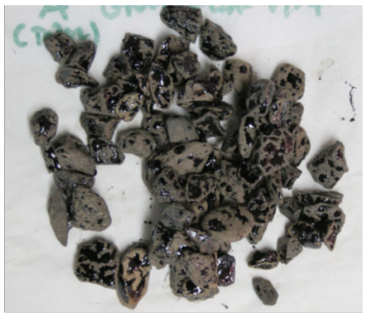


Fig. 1: Contact angles of bitumen without additives and mixed with additives, measured for various investigated aggregate surfaces: I: Quartz monzogabbro; II: White marble; III: Metamorphite; IV: Limestone.

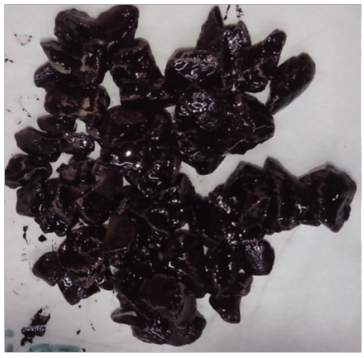
As expected, the performance of the adhesion promoters based on amide and ester of the PPA was strongly influenced by the chemical nature of the stones. This behaviour is consistent with the formation of specific chemical interactions in the adhesion process between bitumen and aggregate. On the other hand, one can argue that the

bituminous mixture based on the organosilane additive interacts with aggregates through a different mechanism driven by physical rather than chemical interactions, as confirmed by the absence of any dependence of contact angle on the type of inert stone. Therefore, the addition of 0.1 wt % organosilane to bitumen enhances remarkably its wettability onto the inert rock, independently of its chemical compositions and surface charge characteristics (either acid or basic types). Conventional boiling test results confirmed the highest coating rate recorded for the organosilane-modified bitumen, whereas samples formulated with amide and PPA ester adhesive promoters provided lower degrees of coating, as they were affected by the chemical nature of inert stones.



Pristine bitumen

Bitumen + 0.1 wt % organosilane



Bitumen + 0.1 wt % PPA ester

Bitumen + 0.1 wt % amide

References

Oliviero Rossi, C.; Spadafora, A.; Teltayev, B.; Izmailova, G.; Amerbayev, Y.; Bortolotti, V. "Polymer modified bitumen: rheological properties and structural characterization", Colloids Surf. A: Physicochem. Eng. Aspects 480, 390-397 (2015).
Oliviero Rossi, C.; Caputo, P.; Baldino, N.; Lupi, F.R.; Miriello, D.; Angelico, R. "Effects of adhesion promoters on the contact angle of bitumen-aggregate interface", International Journal of Adhesion & Adhesives 70, 297-303 (2016).

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

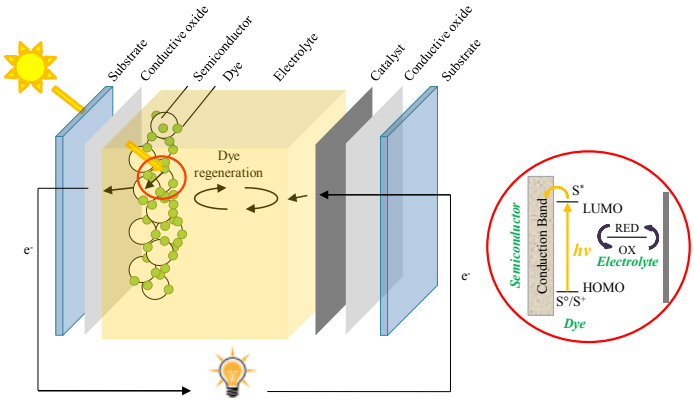
A. Sinicropi, M.L. Parisi, S. Maranghi, R. Basosi

Aims

The aim of the project is the design, computational characterization and synthesis of new organic dyes for the production of Dye Sensitized Solar Cells, along with the environmental assessment of their photovoltaic performances trough life cycle analysis.

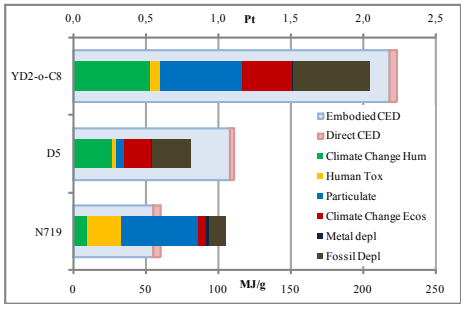
Results

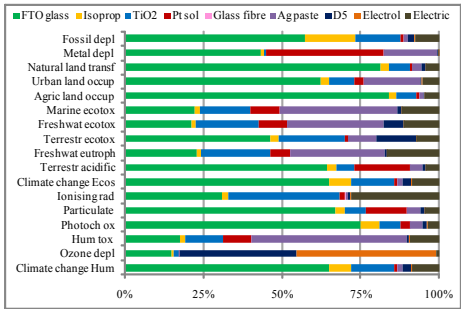
Since the pioneering work published by Grätzel and O'Reagan on the first efficiently assembled dye-sensitized solar cell (DSSC) in 1991, the research activity on photovoltaic cells based on hybrid sensitizer/nanocrystalline semiconductor systems has undergone some major developments. This present project 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.

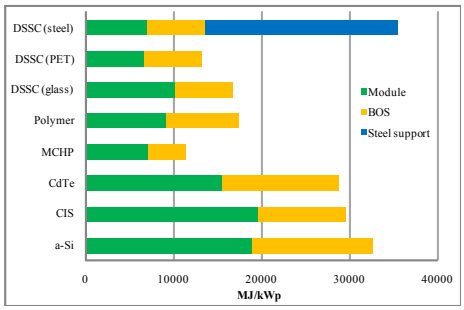


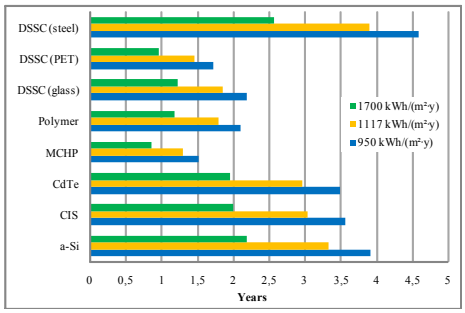
A life cycle analysis of the production process of each components of a solar cell has to be performed in order to achieve a systematic and in-depth assessment of environmental impacts and burdens (in energetic and pollution terms) deriving from all input flows, and to highlight the critical points and hot spots of the process itself. Such an evaluation represents the starting point to draw a detailed eco-profile of innovative technologies and their potential applications. Major outcomes from the project are pivotal in understanding the environmental dynamics, the benefits and

drawbacks associated with the production and employment of DSSCs in comparison with other photovoltaic crystalline silicon and other thin film technologies.









References

Dessì, A.; Calamante, M.; Mordini, A.; Peruzzini, M.; Sinicropi, A.; Basosi, R.; Fabrizi de Biani, F.; Taddei, M.; Colonna, D.; Di Carlo, A.; Reginato, G.; Zani, L. "Thiazolo [5, 4-d] thiazole-based organic sensitizers with strong visible light absorption for transparent, efficient and stable dye-sensitized solar cells", RSC Advances 5, 32657-32668 (2015).

Franchi, D.; Calamante, M.; Reginato, G.; Zani, L.; Peruzzini, M.; Taddei, M.; Fabrizi de Biani, F.; Basosi, R.; Sinicropi, A.; Colonna, D.; Di Carlo, A.; Mordini, A. "Two New Dyes with carboxypyridinium Regioisomers as Anchoring Groups for Dye-Sensitized Solar Cells", Synlett, 26, 17, 2389-2394 (2015).

Parisi, M.L.; Maranghi, S.; Basosi, R. "The evolution of the Dye Sensitized Solar Cells from Grätzel prototype to up-scaled solar applications: a life cycle assessment approach", Renewable And Sustainable Energy Review 39, 124-138 (2014).

Dessì, A.; Calamante, M.; Mordini, A.; Peruzzini, M.; Sinicropi, A.; Basosi, R.; Fabrizi de Biani, F.; Taddei, M.; Colonna, D.; Di Carlo, A.; Reginato, G.; Zani, L. "Organic dyes with intense light absorption especially suitable for application in thin-layer dye-sensitized solar cells", Chemical Communications 50, 13952-13955 (2014).

Parisi, M.L.; Maranghi, S.; Sinicropi, A.; Basosi, R. "Development of dye sensitized solar cells: a life cycle perspective for the environmental and market potential assessment of a renewable energy production technology", International Journal of Heat and Technology 31, 2, 143-146 (2013).

1A – Production and characterization of photoactive materials

M.C. Baratto, E. Fatarella (Next Technology Tecnotessile), R. Pogni

Aims

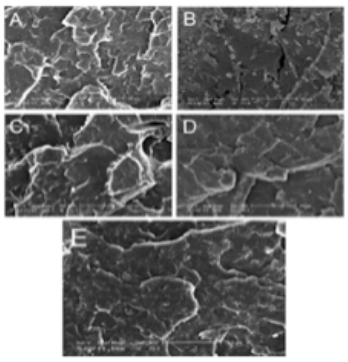
Production of a fiber with sufficient and long-lasting photoactivity and mechanical properties.

Results

Sources for indoor air pollution are cleaners, waxes, paints, pesticides, adhesives, cosmetic products, automotive products, and hobby supplies. Conventional methods to remove pollution are often ineffective, chemically and energetically intensive and suitable only for large systems. An alternative is represented by photocatalysis. TiO2, ZnO, ZrO_2, CdS, MoS_2, Fe_2O_3, and WO_3 have been used as photocatalyst and among them, titanium dioxide remained the benchmark against which alternative photocatalysts are compared. However, TiO2 nanoparticles have recently been classified by the International Agency for Research on Cancer (IARC) as an IARC Group 2B carcinogen "possibly carcinogenic to humans.". Therefore, the identification of polymeric photoactive compounds is recommended in order to reduce health problems induced by nanoparticle handling. Photocatalysts prevent the deterioration of textiles caused by insects, fungi, algae, and microorganisms. The self-cleaning property of a photoactive textile is based on the discoloration of organic stains by reactive radicals. Photocatalytic oxidation (PCO) is an emerging technology in air purification, and is also based on the decomposition of harmful substances. The use of photocatalytic textiles in antimicrobial, self-cleaning, and anti-pollution products are based on the highly reactive radicals that are generated under band-gap light irradiation.

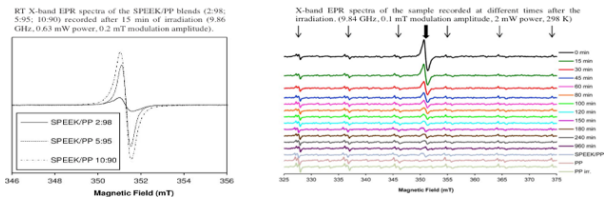
In this study, SPEEK/PP-based photoactive fibers are manufactured to provide antimicrobial, self-cleaning, and anti-pollution properties. The fibers are made in a melt spinning process, first on laboratory scale and then on a semi-industrial scale.

SEM micrograph of PP (A), SPEEK (B), SPEEK/PP 2:98 (C), SPEEK/PP 5:95 (D), and SPEEK/PP 10:90 (E)



Melt spun SPEEK/PP 5:95 filaments

The fibers are characterized regarding their mechanical properties, photochemical effectiveness, and morphology.
Based on the obtained results, their suitability in commercial textile applications is estimated. In addition to the new polymer-based textile material, the novelty of this study is the melt spinning of an unconventional polymer blend containing two totally different components and time-dependent processability. Chemical modifications of PEEK, such as sulfonation, enhance its solubility in organic solvents through electrophilic substitution reactions and promote the formation of benzophenone ketyl radicals (BPK) that could be effectively used to promote photocatalytic reactions. In fact, UV irradiation of a polar benzophenone induces an n to p* transition generating a triplet state that is highly reactive toward hydrogen atom abstraction by forming a stable radical. A hydrogen transfer reaction is involved in the initial production of the reactant radical and the generation of the final product. The selection of the appropriate hydrogen transfer agent depends on the kinetics of H-atom transfer agent and on the stabilisation of the radical induced by the chemical groups on the acceptor. Polyolefins possess a labile hydrogen atom and can therefore act as efficient chain transfer agents, whilst the sulfonated group stabilizes the radicals.



In order to evaluate the photocatalytic effectiveness of the made polymer blends, EPR spectroscopy was performed. Room temperature EPR analysis performed on a transparent casted film made from 100% SPEEK showed that after exposure to UV irradiation for 15 min free radicals are generated. The presence of PP in the SPEEK sample with increasing molar ratio significantly improves the radical formation efficiency. Stable BPK radical was detected and the characterization of the stability of the radical over several irradiation cycles was carried out. The next goal is therefore to estimate the antimicrobial, antipollution, and self-cleaning performance of the final fabrics in order to fully characterize the efficiency of the new fibers.

References

Mylläri, V.; Fatarella, E.; Ruzzante, M.; Pogni, R.; Baratto, M.C.; Skrifvars, M.; Syrjälä, S.; Järvelä, P. “Production of sulfonated polyetheretherketone/polypropylene fibers for photoactive textiles”, Journal of Applied Polymer Sceince 132, 42595, (1-8), (2015).
Fatarella, E.; Mylläri, V.; Ruzzante, M.; Pogni, R.; Baratto, M.C.; Skrifvars, M.; Syrjälä, S.; Järvelä, P. “Sulfonated polyetheretherketone/polypropylene polymer blends for the production of photoactive materials”, Journal of Applied Polymer Sceince 132, 41509, (1-8), (2015).

1A – Ordered Mesoporous Silica in Nanomedicine: Effect of Functionalization and Interactions with Proteins

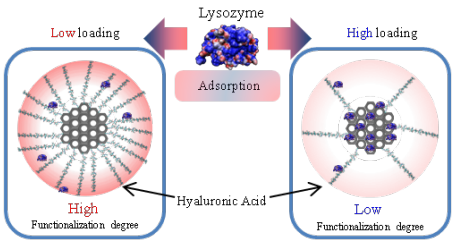
A. Salis, V. Nairi. L. Medda, F. Cugia, M. Piludu, V. Sogos, M. Monduzzi.

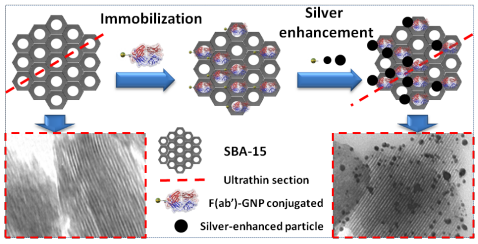
Aims

Synthesis, characterization and functionalization of ordered mesoporous silica. Adsorption and in vitro release of model drugs and proteins. Visualization of adsorbed proteins.

Results

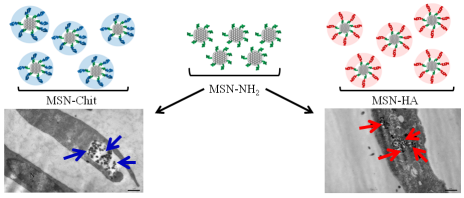
Ordered mesoporous silica (OMS) materials are receiving great attention for nanomedicine applications. OMS can be used to prepare smart depot systems for several kinds of therapeutic agents as, for example, therapeutic proteins. We focused on two types of OMS: SBA-15 and MCM-41. The former is constituted by microparticles with a pore size of about 6-7 nm. The latter is constituted by nanoparticles with a pore size of 2-3 nm. We first studied the interactions between functionalized SBA-15 mesoporous silica and lysozyme, an antimicrobial protein. In order to improve the bioadhesion properties of SBA-15 particles, they were functionalized with hyaluronic acid. SBA-15 samples having high (H-SBA) and low (L-SBA) levels of functionalization were analyzed during the three steps of the preparations: 1. introduction of the $-NH_2$ groups to obtain the SBA-NH_2 samples; 2. functionalization with hyaluronic acid to obtain the SBA-HA matrices; 3. adsorption of lysozyme. The whole of the experimental data suggests that a high level of functionalization of the silica surface allows for a negligible lysozyme adsorption mainly due to unfavorable electrostatic interactions (H-SBA-NH_2) or steric hindrance (H-SBA-HA). A low degree of functionalization of the silica surface brings about a very good performance towards lysozyme adsorption, being 71 % (L-SBA-NH_2) and 63 % (L-SBA-HA) respectively, compared to that observed for original SBA-15. A key issue is to prove that a therapeutic protein is effectively able to penetrate the pores of OMS during the adsorption step. To this purpose we immobilized an antibody fragment [F(ab′)GAMIgG] conjugated with ultrasmall gold nanoparticles (GNPs) onto amino-functionalized SBA-15 (SBA–NH_2) mesoporous silica. In order to visualize the location of the conjugates adsorbed onto SBA–NH_2 with transmission electron microscopy (TEM), due to the ultrasmall size of GNPs <1 nm, we used a silver enhancement procedure to amplify their size. In this procedure, ultrathin sections of conjugate-loaded SBA–NH_2 particles are firstly prepared. The ultrasmall GNPs located on the top side of the 70–90 nm thick slices act as microcrystallization nucleation sites for the deposition of reduced metallic silver. Consequently, the ultrasmall GNPs increase their size. This allows for the direct imaging of the





conjugates adsorbed. We clearly localized the F(ab′)GAMIgG–GNPs conjugates inside the mesopores of SBA–NH_2 through TEM.

Then we focused on mesoporous silica nanoparticles (MSNs), based on the MCM-41 mesoporous matrix. They were functionalized with amino groups, and then with hyaluronic acid (HA) or chitosan (CHIT) to fabricate bioactive conjugates. The role of the functional groups towards cytotoxicity and cellular uptake was investigated using 3T3 mouse fibroblast cells. A very high biocompatibility of MSN-NH_2, MSN-HA and MSN-CHIT was assessed through the MTS biological assay and Coulter counter evaluation. No significant differences in cytotoxicity data aroused from the presence of different functional groups in the investigated MSNs. Significant differences due to type of functionalization were instead observed both in the fluorescence microscopy experiments performed with the FITC-conjugated MSN-NH_2, MSN-HA and MSN-CHIT, and in the transmission electron microscopy experiments performed on slices of the investigated systems embedded in epoxy resins. MSN-NH_2, MSN-HA conjugates were easily internalized, being the uptake of the -HA functionalized much higher than that of the -NH_2 functionalized MSNs, whereas MSN-CHIT conjugates gave large aggregates dispersed in the medium or localized at the external surface of the cell membranes. Both fluorescence microscopy and TEM images gave clear evidence that the MSNs are distributed in the cytoplasm of the cells in the case of MSN-NH_2 and MSN-HA, whereas only few particles are internalized in the case of MSN-CHIT.



References

Salis, A.; Fanti, M.; Medda, L.; Nairi, V.; Cugia, F.; Piludu, M.; Sogos, V.; Monduzzi, M. "Mesoporous Silica Nanoparticles Functionalized with Hyaluronic Acid and Chitosan Biopolymers. Effect of Functionalization on Cell Internalization", ACS Biomaterials Science & Engineering 2, 741-751 (2016).

Salis, A.; Medda, L.; Cugia, F.; Monduzzi, M. "Effect of Electrolytes on Proteins Physisorption on Ordered Mesoporous Silica Materials", Colloids and Surfaces B: Biointerfaces 137, 77-90 (2016).

Piludu, M.; Medda, L.; Cugia, F.; Monduzzi, M.; Salis, A. "Silver-Enhancement for Trasmission Electron Microscopy Imaging of Antibody Fragment-Gold Nanoparticles Conjugates Immobilized on Ordered Mesoporous Silica", Langmuir 31, 9458-9463 (2015).

Medda, L.; Casula, M.F.; Monduzzi, M.; Salis, A. "Adsorption of Lysozyme on Hyaluronic Acid Functionalized SBA-15 Mesoporous Silica: A Possible Bioadhesive Depot System", Langmuir 30, 12996-13004 (2014).

Monduzzi, M.; Lampis, S.; Murgia, S.; Salis, A. "From Self-Assembly Fundamental Knowledge to Nanomedicine Developments", Advances in Colloid and Interface Science 205, 48-67 (2014).

1A – Carbon based nanostructures for innovative hydrogen storage systems

C. Milanese, A. Girella, P. Cofrancesco, G. Bruni, V. Berbenni, A. Marini, D. Pontiroli, M. Gaboardi*, G. Magnani*, M. Riccò* (*University of Parma, Physics Department)*

Aims

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

Results

Thanks to this project (funded by Fondazione Cariplo; number of the grant 2013-0592), started in April 2014 and ended in September 2016, we were able to demonstrate to the scientific community that alkali-cluster intercalated fullerides really constitute a novel class of materials for hydrogen storage, thanks to their proved capability to uptake reversibly high amounts of hydrogen via a complex chemisorption mechanism. We optimized the synthesis of Li, Na, and mixed Li-Na clusters intercalated fullerides, belonging to the families $Na_xLi_{12-x}C_{60}$ ($0 \leq x \leq 12$; we were the first group to explore these stoichiometries) and $Na_xLi_{6-x}C_{60}$ ($0 \leq x \leq 6$) by solid state methods, obtaining high purity and good reversibility.

The structural properties of the materials were clarified by means of in-situ neutron diffraction and the analysis of the Pair Distribution Function (PDF) obtained from high-energy synchrotron diffraction. The mechanism of hydrogenation was unveiled by Muon Spin Relaxation spectroscopy (μSR), a very powerful technique "able to see hydrogen" in the structures. Thanks to these two methods, we were able for the first time to explain the chemisorptions mechanism leading to the hydrogenation of fullerene in these structure: Li atoms help the dissociation of the hydrogen molecules on the C structures, acting as catalyst and destabilizing agent, but then capture some hydrogen in the formation of LiH. Na atoms act as a more powerful catalyst and does not hydrogenate by itself, but is not able to decrease the working temperature of the C structure. Thanks to our work, we demonstrate the importance to prepare mixed stoichiometries richer in the Li side to obtain good kinetic and thermodynamic properties. By coupled manometric - calorimetric analyses and thermogravimetric measurements, we proved that in these composites C_{60} covalently binds up to 5 wt% H_2 at moderate temperature and pressure, reaching properties similar to those of Mg hydride, the first generation material for hydrogen storage.

We also identified some strategies to further improve the absorption performance in this class of materials. For example, we succeeded to catalyze Li-fullerides with Pt and Pd nanoparticles, whose known activity towards hydrogen dissociation allows to increase the H_2 absorption up to 5.9 wt% H_2 and of about 35 % the absorption rate with respect to the pure undoped compounds.

Finally, we demonstrated that the Li decorated compounds have also very good properties for ammonia storage, a very hot topic concerning new fuels and energy vectors transportation and use.

References

Aramini, M.; Gaboardi, M.; Vlachopoulou, G.; Pontiroli, D.; Riccò, M.; Milanese, C.; Cavallari, C. "Muon spin relaxation reveals the hydrogen storage mechanism in light alkali metal fullerides", Carbon 67, 92-97 (2014).

Aramini, M.; Milanese, C.; Pontiroli, D.; Gaboardi, M.; Girella, A.; Riccò, M. "Addition of transition metals to lithium intercalated fullerides enhances hydrogen storage properties", International Journal of Hydrogen Energy 39 [5], 2124-2131 (2014).

Giglio, F.; Pontiroli, D.; Gaboardi, M.; Aramini, M.; Cavallari, G.; Brunelli, M.; Galinetto, P.; Milanese, C.; Riccò, M. "$Li_{12}C_{60}$: a lithium clusters intercalated fulleride", Chemical Physics Letters 609, 155-160 (2014).

Gaboardi, M.; Duyker, S.; Milanese, C.; Magnani, G.; Peterson, V.K.; Pontiroli, D.; Sharma, N.; Riccò, M. "In Situ Neutron Powder Diffraction of Li6C60 for Hydrogen Storage", Journal of Physical Chemistry C 119, 34, 19715-19721 (2015).

1A – Reversible hydrogen sorption for borohydrides infiltrated in silica matrices

C. Milanese, A. Girella, P. Cofrancesco, A. Marini, E. Fratini
*F. Ridi, M. Rueda Noriega**, L.M. Sanz Moral**, A. Martin***
*(** Chemical Engineering and Environmental Technology Dept., University of Valladolid, Spain)*

Aims

To realize borohydrides nanoconfinement in silica based matrices as a way to improve the reversibility and the kinetics of the H_2 sorption reactions of these complex hydrides materials; to optimize the nanoconfinement procedures; to prepare doped matrices and doped compounds to be infiltrated to further improve the hydrogen sorption kinetics.

Results

Borohydrides are very promising materials for solid state hydrogen storage thanks to their high hydrogen content (the theoretical gravimetric capacity is higher than 10 wt%, with the Department of Energy ultimate target for the whole storage tank being 6 wt %). Unfortunately, these materials suffer of poor reversibility and ciclability and work at very high temperature and hydrogen pressure (600 °C, 100 bar).
One promising way to obtain mild sorption conditions and improve the kinetics of the sorption reactions is to encapsulate the hydrogen storage systems in high porous matrices able to confine the active powders in their channels and pores, so forcing them to react in nanometric form with hydrogen gas. Few is still known on the hydrogen sorption mechanism of the powders in these conditions and the encapsulation methods are to be developed and optimized for each single borohydride, due to the different chemico-physical and solubility properties of each of them.
Concerning the borohydrides choice, we decided to start the investigation with the Mg compound $Mg(BH_4)_2$, since it is a very high-capacity hydrogen complex hydride (14.84 wt% of H_2) but its H_2 sorption reversibility remains a challenge. Its thermodynamics of dehydrogenation is calculated to be near ideal for effective hydrogen storage, but experiments reveal competing decomposition pathways with the formation of very stable intermediates limiting the lifecycle. In practice, 11 wt% H_2 reversibility was demonstrated at very high pressures and temperatures, while only 2.5wt% H_2 is exchanged at reasonable conditions. Concerning the matrices, after having demonstrate that C based materials like graphene and nanotubes react with this compound, we decided to try with silica aerogels. The group in Madrid is able to prepare these particles tuning the surface area and the pores size. Due to the properties of Mg borohydride, that melts and decomposes contextually, we cannot use the traditional melt infiltration technique. For this reason, we developed an original solid state high pressure procedure able to force the hydride to go in the silica channels in its hydrogenated form without melting and decomposition, by working at 300 °C and 110 bar of hydrogen (the borohydride melts at T higher than 350 °C at 1 bar of hydrogen pressure). The *ex-situ* BET, XRPD and IR spectroscopy help to understand the success and extent of encapsulation. Calorimetric measurements are used to describe the thermodynamic features of the

system. The hydrogen sorption performance is explored by cycling the samples in the manometric apparatus under vacuum/up to 110 bar for des/absorption at the characteristic temperatures.
In the 1:1 molar ratio borohydride:silica encapsulated system, a decrease in the dehydrogenation temperature by 60 ºC with respect to the pure hydride and a single decomposition step in the range of 220-400 ºC is observed. The kinetics of dehydrogenation at 300 ºC in the first cycle is two times faster compared to that of the bulk borohydride. 50 % of reversibility for the hydrogen sorption reaction is shown from the first to the second cycle and maintained in the 3rd one: this is the first time a so high reversibility degree is observed in Mg borohydride systems in the relatively mild working conditions proposed in our work.
We are now trying to develop a wet chemistry method for encapsulate the borohydride in the silica matrix by using a suitable solvent able to dissolve both the components without decomposition and easy to remove after the infiltration. THF gave good results concerning the encapsulation yield but demonstrated to be very hard to remove, decreasing the gravimetric capacity of the system.

References

Rueda Noriega, M.; Milanese, C.; Sanz Moral, L.M.; Girella, A.; Cofrancesco, P.; Martin, A. "Reversible Hydrogen Sorption In The Composite Made Of Magnesium Borohydride And Silica Aerogel", accepted for publication, International Journal of Hydrogen Energy, doi 10.1016/j.ijhydene.2016.07.074.

1A – Nanostructured scaffolds for tissue engineering

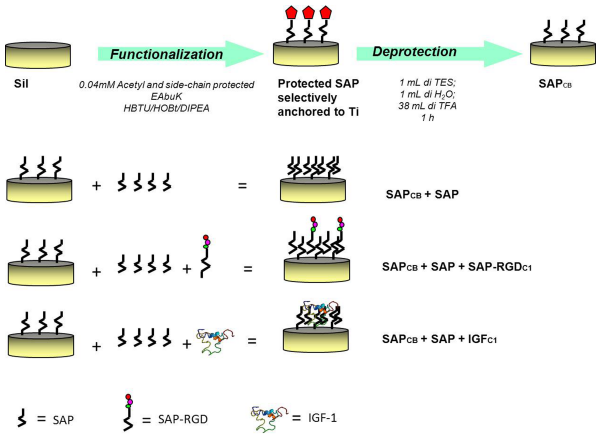
G. Messina, N. Giamblanco, A. Rapisarda, G. Marletta, A.G. Karakeçili (Chemical Engineering Department, Ankara University, Turkey), M. Gümüşderelioğlu, M.Ç. Yurtsever (Bioengineering Department, Hacettepe University, Turkey), M. Dettin (Department of Industrial Engineering, University of Padova), I. Castagliuolo, P. Brun (Department of Molecular Medicine, University of Padova)

Aims

Driving cell adhesion, spreading and proliferation by controlled nanometric biofunctionalization at solid surfaces and nanostructured hydrogels.

Recent Results

We have developed novel bioactive titanium implants, based on the anchoring of a layer of ionic-complementary self-assembling peptides (EAbuK) on Ti surfaces, which have been previously sandblasted and acid-etched. The peptide layer is anchored to the metal by covalent functionalization of titania with the self-assembling sequences (see Scheme 1).



Scheme 1: Sequence of the steps for the preparation of the different surfaces.

The peptide layer may also host a substantial amount of the Insulin-like Growth Factor-1, which can efficiently incorporated within the peptide layer. To the construct can also be added a conjugate biomimetic system obtained by chemo-selective ligation between EAbuK and a sequence of 25 residues containing 4 GRGDSP motifs per chain. XPS studies confirmed a change in the surface composition in agreement with the proposed decorations, while contact angle measurements showed a substantial change in wettability induced by the anchored peptide layer. Accordingly, the human osteoblast adhesion and proliferation assays showed an increase in adhesion for the surfaces enriched with conjugate at a concentration of 3.8 10^{-7}M and

an enhanced proliferation for samples enriched with Insulin-like Growth Factor-1 at the highest concentration tested (2.1 10^{-5}M). Further studies on the role of the different aggregation forms of various classes of ionic-complementary self-assembling peptides (EAbuK) are being investigated, both experimentally, looking at their nanoscale structure as a function of the nature of surfaces, environmental pH and electrical charges at surfaces, and in silico, by means of a mixture of Quantum Mechanical methods and Molecular Dynamic simulation.
In a parallel way, a series of methods have been developed to functionalize at nanoscale bioceramic surfaces, in order to boost efficient processes of biomineralization.

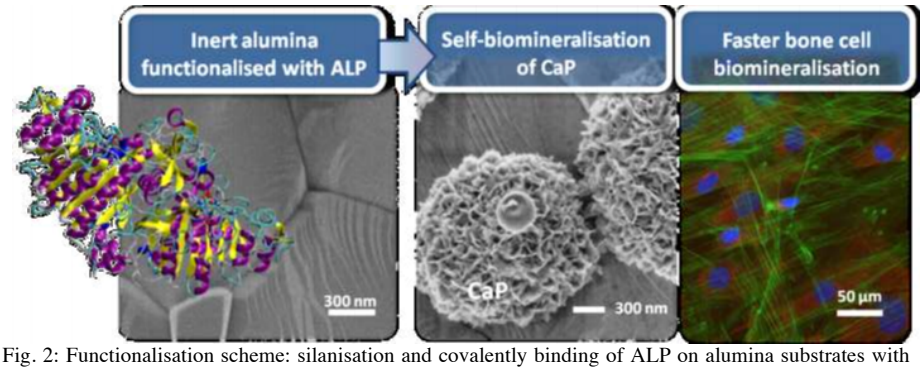


Fig. 2: Functionalisation scheme: silanisation and covalently binding of ALP on alumina substrates with N-hydroxysuccinimide (NHS) and 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC). b) Enzymatic activity of ALP immobilised in alumina discs (ASNEA) measured by pNPP assay immediately after immobilisation at three different temperatures (4 °C, 25 °C and 37 °C). Unfunctionalised alumina discs (A) were used as reference.

Thus, a bioinspired approach to induce self-mineralisation of bone-like material on alumina surfaces has been developed in collaboration with researchers of Brema University. The mineralising enzyme alkaline phosphatase (ALP) was covalently immobilised by a carbodiimide-mediated chemoligation method. The enzymatic activity of immobilised ALP and its mineralisation capability were investigated at acellular conditions as well as in the presence of human bone cells. Analytical, biochemical, immunohistochemical characterization show that ALP is efficiently immobilized, retains its activity and can trigger calcium phosphate mineralization on alumina at acellular conditions. In vitro cell tests demonstrate that ALP functionalized alumina clearly boosts and enhances bone cell mineralization (see fig.2). Our results underpin the high potential of ALP-functionalized alumina for the development of bioactive surfaces for applications such as orthopedic and dental implants, enabling potentially a fast and firm implant Osseo integration.

References

Zamuner A.; Cavo M.; Scaglione S.; Dettin M.; Messina, G.M.L.; Marletta, G. “Design of decorated self-assembling peptide hydrogels as architecture for mesenchymal stem cells”, 2D Materials 9 (2016).
Dettin, M.; Zamuner, A.; Roso, M.; Gloria, A.; Iucci, G.; Messina, GML; D'Amora, U.; Marletta, G.; Modesti, M.; Castagliuolo, I.; Brun, P. “Electrospun Scaffolds for Osteoblast Cells: Peptide-Induced Concentration-Dependent Improvements of Polycaprolactone”, PlosOne 10 (2015).

1A – Nanohybrids P3HT-based systems

N. Tuccitto, G. Sfuncia, G. Marletta

Aims

Conjugated polymeric composites with carbon nanotubes, in view of the high aspect ratio volume/surface, are expected to behave as optimal conducting materials at relatively low carbon contents. Many applications can be forecast for conjugated polymer/carbon nanotubes hybrid materials, including energy storage and energy conversion devices, sensors, etc.

Recent results

Poly(3-hexylthiophene)/carbon nanotubes composites (P3HT/NTs) are in the forefront of the research on electroactive polymers, due to their recognized role as active elements in organic photovoltaic and OFET/OLED devices. Among this class of materials, the hybrid systems based on single-walled carbon nanotubes (P3HT/SWNTs) deserve a particular interest with respect to the framework of molecular electronics, in view of the expected optimal electronic conductivity and efficiency. We have prepared high conductivity nanohybrid networks of poly(3-hexylthiophene) and single-walled carbon nanotube (P3HT/SWNTs) by spin coating deposition.

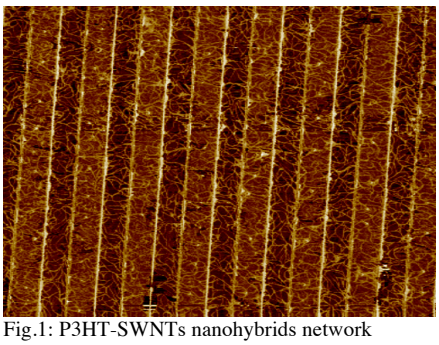


Fig.1: P3HT-SWNTs nanohybrids network deposited at 2000 RPM on IDEs.

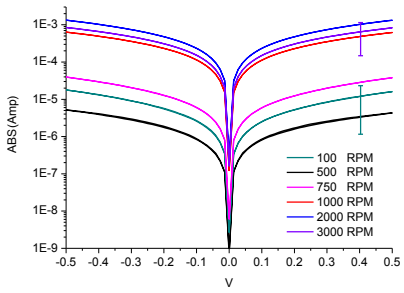


Fig. 2: I-V characteristics of nanohybrids networks deposited on IDEs at increasing spin-coating speeds (legend reports the respective RPM).

2D networks prepared at high spinning speed showed a conductivity three orders of magnitude higher than that measured for networks deposited at low spinning speed, although the individual nanotubes are not seen to form a direct connection between the electrodes.

The strong improvement of the conductivity performances is accounted for in terms of the formation of a new nanohybrid system, consisting in thin sheaths of P3HT wrapped around SWNTs, forming complex SWNT/P3HT/SWNT junctions yielding a soldering effect of the interposed P3HT sheath.

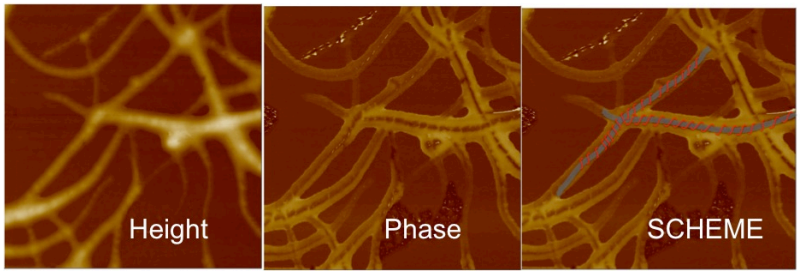


Fig. 3: The nanometric P3HT wrapping layer, therefore, acts as a conductive glue at the nanotube-nanotube junctions, allow easy tunneling of charge carriers across them.

The results open the way to molecular electronics devices exploiting the long-range conduction capability of nanotubes together with the thin P3HT sheath short range soldering effect at the hybrid nanowire junctions.

References

Sfuncia, G.; Tuccitto, N.; Marletta, G. "Preparation and Enhanced Conducting Properties of Open Networks of Poly(3-hexylthiophene) /Carbon Nanotubes Hybrids", RSC Adv. 6, 51485-51492 (2016).

Tuccitto, N.; Trusso Sfrazzetto, G.; Gangemi, C.M.A.; Ballistreri, F.P.; Toscano, R.M.; Tomaselli, G.A.; Pappalardo, A.; Marletta, G. "Memory-Driven Order-Disorder Transition of 3D-Supramolecular Architecture Based on Calix[5]arene and Porphyrin Derivatives", Chem.Comm. 52, 11681-11684 (2016).

Fraix, A.; Torrisi, V.; Marletta, G.; Sortino, S.; Mineo, P.G.; Tomaselli, G.A.; Ballistreri, F.P.; Trusso Sfrazzetto, G.; Pappalardo, A. "Supramolecular Polymer Networks Based on Calix[5]arene Chained Poly(*p*-phenyleneethynylene) and C_{60} Fulleropyrrolidine", Supramol. Chem. 28, 485-492 (2016).

Torrisi, V.; Ruffino, F.; Liscio, A.; Grimaldi, M.G.; Marletta, G. "Emerging interface dipole versus screening effect in copolymer/metal nano-layered systems", Appl. Surf. Sci. 359, 637-642 (2015).

Torrisi, V.; Squillaci, M.A.; Ruffino, F.; Crupi, I.; Grimaldi, M.G.; Marletta, G. "Schottky barrier height tuning by Hybrid organic-inorganic multilayers", MRS Proceedings, 1660, 396/1-396/6 (2014).

Ruffino, F.; Torrisi, V.; Marletta, G.; Grimaldi, M.G. "Micro-patterned nanoscale Au films on PMMA: fabrication and effect of PMMA dewetting on Au patterning", Journal of Material Science: Materials in Electronics 25, 1138-1147 (2014).

1A – Calcium phosphate-based nanostructures: synthesis in composite materials, stabilization and interaction with biologically relevant Soft Matter

R. Gelli, S. Del Buffa, P. Tempesti, F. Ridi, M. Bonini, P. Baglioni

Aims

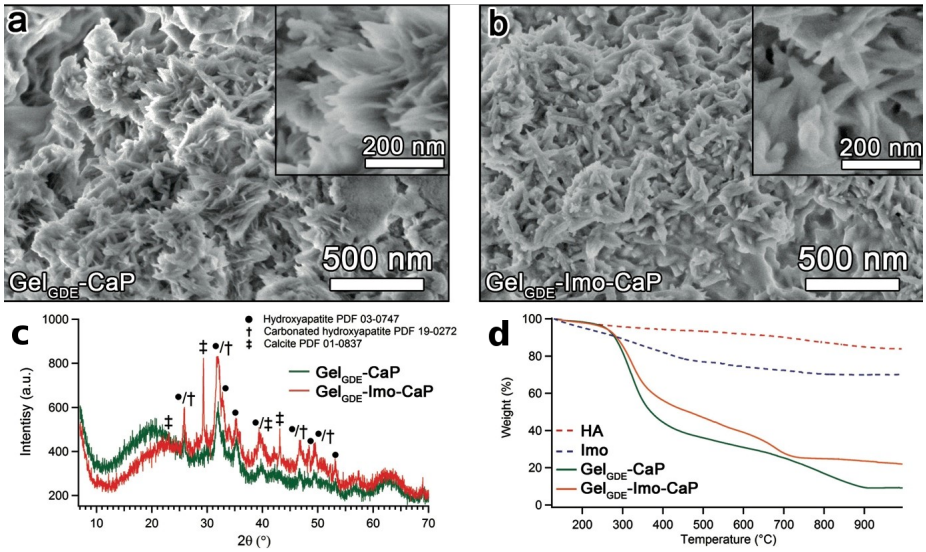
Calcium phosphate (CaP) is one of the most important biomaterials, given its essential role played in human body structure and functioning. Learning from Nature, Soft Matter can be successfully used to guide the formation of nanostructured CaPs, and the understanding of the interactions taking place between these minerals and Soft Matter itself is of special interest both in chemistry and nanomedicine. This project aims at preparing and characterizing biomimetic and nanostructured calcium-based phosphates, in order to investigate the interactions that take place between these nanostructures and biologically relevant macromolecules belonging to Soft Matter family.

Results

Inorganic nanostructured phosphates, especially calcium and magnesium-based, are essential components of the human body, since they contribute to maintain its structure and guarantee the proper functioning. CaP is the main inorganic component of human hard tissues and can be found in nanocrystalline form in bone and teeth, embedded in a soft proteic matrix. In amorphous form, CaP is present in casein micelles in human breast milk and its deposition is also involved in several pathological calcifications, such as renal calculi and atherosclerotic plaques. Mg and phosphate-based minerals are biologically relevant too, given their presence in salivary gland stones and kidneys calculi. Moreover, it has been recently found that nanoparticles of endogenous amorphous calcium phosphate formed from co-precipitation with magnesium in intestine (CaMgP) act as chaperones in the transport of macromolecules, such as orally fed protein antigens and bacterial peptidoglycan, to immune cells of intestinal tissue. The relevance of CaP nanostructures in human body, that emerges from the above mentioned examples, makes it a material of paramount importance; its applications in nanomedicine include tissue engineering, materials for dental and orthopedic applications, drug delivery and DNA transfection. Beyond its numerous applications, the study of the formation and characterization of CaPs nanostructures is important *per se*, to improve our understanding of the biomineralization process and to investigate the interactions that take place between these nanostructures and biologically relevant macromolecules.

In this framework, we investigated the formation of CaP-based nanostructures in different biocompatible polymeric matrices, taking advantage of biomimetic approaches and investigating their templating action in the crystallization of CaP and in presence of inorganic fillers. We studied the formation of hydroxyapatite nanocrystals on a macroporous gelatin hydrogel crosslinked with a bis-epoxide reactant (glycerol diglycidyl ether) and embedded with inorganic clay nanotubes-imogolites. These nanotubes have a two-fold action, acting both as inorganic fillers of the polymeric matrix and as nucleation sites for the growth of hydroxyapatite

nanocrystals. We found that the presence of imogolite promotes the formation of CaP and affects the type of crystalline phase formed.



The formation of CaP was also investigated in crosslinked Gelatin/PVA hydrogels, examining the mineral phase formed by soaking the hydrogel in a simulated body fluid, *i.e.* a solution with ionic concentration close to human plasma. In addition to polymers, this project aims at investigating how biologically relevant macromolecules belonging to Soft Matter affect and tune the precipitation of CaP and if and how they stabilize a specific crystalline phase: for this purpose, we take into account proteins, such as casein, and polysaccharides.

A significant part of this research is also devoted to the stabilization of the amorphous CaP phase: co-precipitation of CaP with Mg^{2+} ions allows the formation of amorphous CaMgP nanoparticles that mimic the biogenic nanostructures that are produced in our gut. The investigation of the interactions between these nanoparticles and complex systems, such as bacteria, can give insights about their puzzling role in our organism.

References

Ridi, F.; Meazzini, I; Castroflorio, B.; Bonini, M.; Berti, D.; Baglioni, P. "Functional calcium phosphate composites in nanomedicine", Adv Colloid Interface Sci, http://dx.doi.org/10.1016/j.cis.2016.03.006 (2016).

1A – Advanced nanostructured materials for eco-sustainable cements: investigation of the structural properties and innovative strategies for their improvement

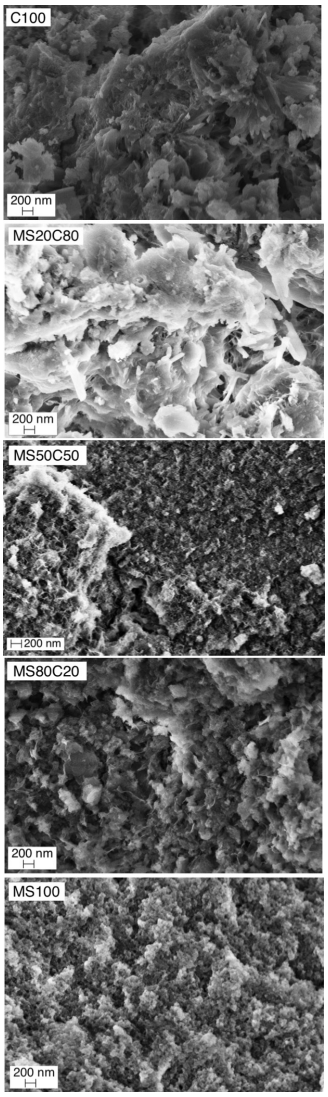
M. Tonelli, E. Fratini, F. Ridi, P. Baglioni

Aims

Structural characterization of MgO/SiO_2 cements. Simultaneous hydration of traditional Portland cement and eco-sustainable MgO-based cements. Multi-technique investigation on the kinetic of the process and the hydration products.

Results

We studied mixtures prepared by simultaneous hydration of Portland cement (C) and MgO/SiO_2 (MS) in different weight proportion, providing a physico-chemical characterization of the complex processes that occur and a detailed structural characterization of the formed amorphous binder phases. These formulations are promising in view of two compelling environmental issues: reducing the large CO_2 emissions associated to Portland production and the encapsulation of nuclear waste. The combination of TG/DTA, XRD, FT-IR and SEM analyses elucidated the effects of composition on the formation of the silicate binder phases magnesium and calcium silicate hydrate (M-S-H and C-S-H), which, in agreement with previous works, resulted to be substantially phase separated, as evident from the SEM images on the right.

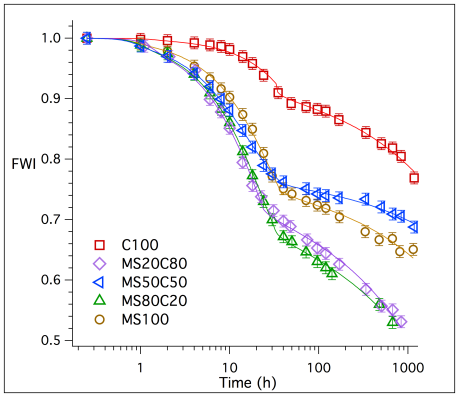


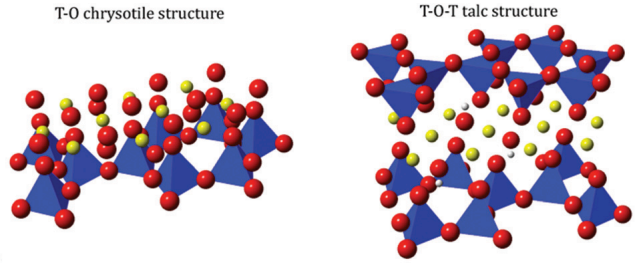
The hydration kinetic of the samples was followed over one month by reporting the free water index (FWI) as a function of time. A combination of the Boundary Nucleation and Growth Model (BNGM) with the three-dimensional diffusional model was used to describe the curves, as shown in the figure below.

Results demonstrate that the hydration of the magnesium- and of the calcium-based components affect each other: low amounts Portland cement in MgO/SiO_2 mixtures accelerate and enhance M-S-H precipitation, while low amounts of MgO/SiO_2 in Portland cement mixtures accelerate and enhance C-S-H precipitation. It could be possible to control the formation of calcium and magnesium silicate hydrate gels and the pH of the final material, which is

fundamental in order to predict its behaviour in geological repositories for radioactive waste disposal, by mixing proper amounts of MgO/SiO_2 and Portland powders.

We further performed a comprehensive structural characterization of MgO/SiO_2 cements using a multi-technique approach, including a detailed solid-state NMR investigation and, in particular, for the first time, quantitative ^{29}Si solid-state NMR data (performed in the framework of the collaboration with F. Martini, L. Calucci, S. Borsacchi and M. Geppi from the University of Pisa and ICCOM CNR of Pisa). Upon mixing highly reactive MgO and SiO_2 with water at room temperature, the binder gel phase M–S–H precipitates within the first 24 hours of hydration, and its amount increases over the entire monitored period of 1 month. The reaction proceeds through the hydration of MgO to give $Mg(OH)_2$, which then reacts with silica. Analysis of the data reveals that this reaction results in the formation of an amorphous phase that is constituted by an intimate mixture of subnanometer-sized "chrysotile-like" (*left figure*) and "talc-like" (*right figure*) sub-nanometric domains, which are approximately in a 1:1 molar ratio after long-time hydration (in the figure blue tetrahedra represent Si species; red, yellow and white spheres represent O, Mg and H atoms, respectively). This assessment of the M–S–H structure paves the way for tailoring the macroscopic properties of eco-sustainable cements by means of a bottom-up approach.





References

Tonelli, M.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Ridi, F.; Borsacchi, S.; Baglioni, P. "Structural characterization of magnesium silicate hydrate: towards the design of eco-sustainable cements", Dalton Trans. 45, 3294-3304 (2016).

Martini, F; Tonelli, M; Calucci, L; Geppi, M; Ridi, F; Borsacchi, S. "MgO/SiO_2 and Portland cement formulations: mutual effects on hydration processes and products", Cement & Concrete Composites, submitted.

Tonelli, M.; Martini, F.; Calucci, L.; Fratini, E.; Geppi, M.; Ridi, F.; Borsacchi, S.; Baglioni, P. "Traditional Portland cement and innovative MgO-based cement: a promising combination?", Physics and Chemistry of the Earth, under review.

1A – A green integrated microwave-assisted synthesis of hexagonally ordered silica sieves using a geothermal waste as silicon source

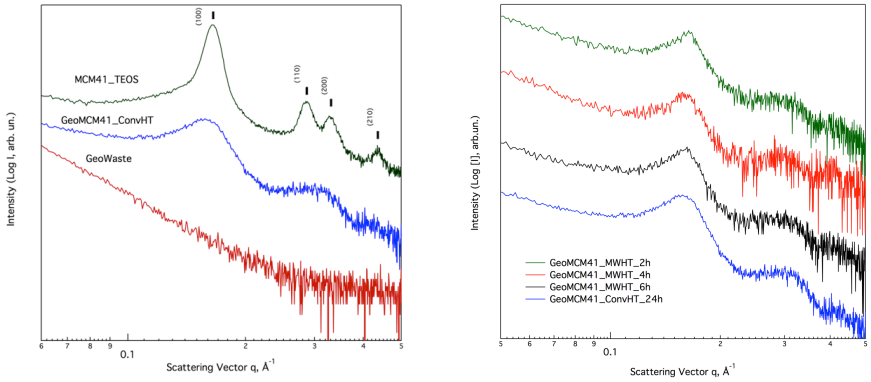
J. Tovar Rodriguez, E. Fratini, P. Baglioni

Aims

Development of an innovative eco-friendly synthesis of mesoporous silicates using a silicon waste as silicon source. Microwave irradiation (MW) for thermal activation and hydrothermal synthesis. Design of green integrated synthesis approach.

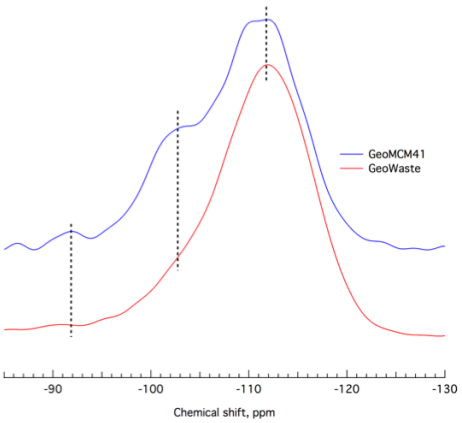
Results

A sample of inorganic geothermal waste was used as Silicon precursor for the preparation of mesoporous silicates. The green synthesis of the materials was performed by hydrothermal treatment, using a microwave-assisted Teflon-lined stainless steel high-pressure reactor. MW irradiation was applied in-situ by means of an innovative microwave coaxial antenna, which allows direct microwave application within the reaction system[1]. The following figures show the Small Angle X-Ray Scattering patterns for all prepared sieves under conventional (*left*) and MW (*right*) heating:



For comparative purposes, hexagonal MCM-41 was also prepared using tetraethoxysilane as conventional silicon source. Calcined MCM-41 features four main scattering peaks in the scattering vector interval from 0.05 to 0.5Å^{-1}, that can be assigned to the diffraction peaks of the (100), (110), (200) and (210) planes, associated to the hexagonal structure *p6mm* group[2]. The as-received geothermal waste features no ordering in the explored q vector range whereas the prepared mesoporous sieves exhibit a main scattering peak centered at around the same q vector value for MCM-41. Other two less resolved scattering peaks are observed and can be interpreted as the convolution of the (110) and (200) peaks, and the Bragg reflection of the (210) plane respectively. The intensity of the latter seems to increase as the total hydrothermal treatment time increases. Interestingly, after only two hours of MW hydrothermal synthesis it is possible to yield a material with a fair degree of ordering. Another interesting feature is the formation of surface silanol groups in the material.

The ^{29}Si NMR spectra are shown on the left diagram for the starting raw material and the hexagonal silicate. The geothermal waste has a sole spectral signal with a maximum at -112ppm (using TMS as standard) indicative of Q^4 siloxane species. For the mesoporous sieve, two other signals are observed at around -102 and -92 ppm associated to the resonances of Q^3 and Q^2 nuclei, corresponding to isolated and geminal silanol groups (Si(OH) and $Si(OH)_2$ surface groups). Considered as weak catalytic Bronsted sites, the reactivity of the silanol moiety is particularly important for surface functionalization or grafting of these silicates.



The textural properties for all prepared materials were evaluated by means of Nitrogen adsorption and desorption isotherms. Table 1 summarizes the lattice cell parameters, BET surface area and pore volume for all calcined solids. The geothermal waste by itself has a low surface area of $45m^2/g$. MCM-41 prepared under conventional heating conditions achieves a BET area of $655m^2/g$ after 24h of hydrothermal treatment while MW prepared samples exhibit areas ranging from 500 up to $700m^2/g$ as the total HT time increases from 2h to 6h. For comparative purposes, MCM-41 prepared using the alkoxide shows a BET area of $923m^2/g$. Pore volume also increases with the hydrothermal treatment time, ranging from 0.55 to $0.70cm^3/g$ for microwave prepared materials. The d_{100} and a_0 lattice cell parameters were estimated using the main Bragg diffraction peak from the SAXS curve and its value depends on the surfactant used as structure directing agent, the degree of hydrolysis of the silicon source that was used and the hydrothermal treatment time.

Table 1. Textural properties and lattice cell parameters for the prepared mesoporous sieves

Sample	HT time, h	BET Area, m^2/g	Pore vol. ml/g	d_{100}, Å	a_0, Å
GeoWaste	0	45	0.22	0	0
GeoMCM_MW2h	2	504	0.55	38.7	44.6
GeoMCM_MW4h	4	546	0.69	43.3	50.1
GeoMCM_MW6h	6	707	0.70	43.7	50.5
GeoMCM_ConvHT24h	24	655	0.62	45.5	52.5
MCM-41_TEOS	24	923	0.80	44.8	51.7

References

González-Rivera, J.; Galindo-Esquivel, I.R.; Onor, M.; Bramanti, E.; Longo, I.; Ferrari, C. "Heterogeneous Catalytic Reaction of Microcrystalline Cellulose in Hydrothermal Microwave-Assisted Decomposition: Effect of Modified Zeolite Beta", Green Chem. 16 (3), 1417-1425 (2014).

Kresge, C.T.; Roth, W.J. "The Discovery of Mesoporous Molecular Sieves from the Twenty Year Perspective". Chem. Soc. Rev. 42 (9), 3663 (2013).

1A – Microwave assisted synthesis of hexagonally ordered mesoporous silica modified by isomorphic incorporation of Yttrium

J. Tovar Rodriguez, E. Fratini, P. Baglioni

Aims

Modification of MCM-41 by isomorphic incorporation of Yttrium in the hexagonal framework. Characterisation of the textural properties of the mesoporous sieves.

Results

Yttrium-modified hexagonally ordered mesoporous silica sieves were prepared under hydrothermal conditions in a microwave-assisted synthesis approach. Hexadecyl trimethyl ammonium bromide was used as structure directing agent and tetraethoxysilane as silicon source. A series of synthesis gels were prepared with the following molar ratios: $Si(OC_2H_5)$: xYN_3O_9*$6H_2O$: 0.30 CTABr : 185 H_2O : 21.5 NH_3, Where x is the Y/Si nominal molar ratio for the desired final material and it was selected as 0.02, 0.04, 0.06 and 0.08, in order to preserve the hexagonal ordering of the pure siliceous MCM-41 parent material. Figure 1 shows the FTIR spectra *(left)* and the Small Angle X-Ray Scattering curves *(right)* for all prepared materials:

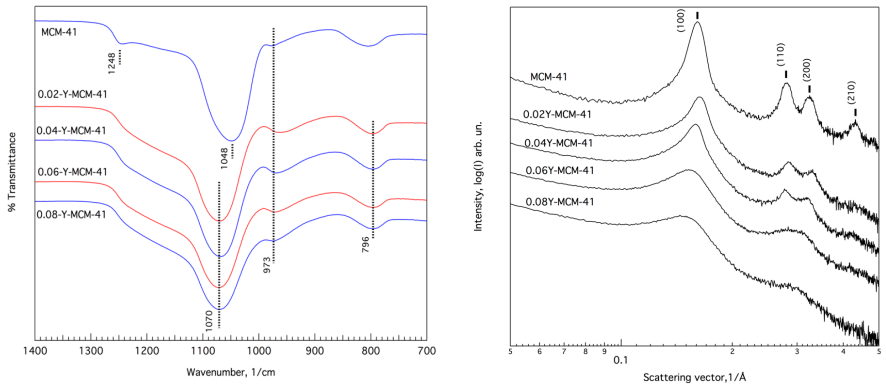


Fig. 1: FTIR spectra (left) and SAXS curves (right for Yttrium modified mesoporous silicates).

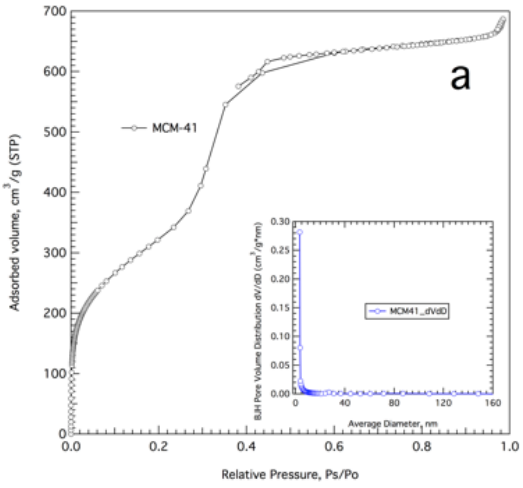
Unmodified MCM-41 features a main transmission band centered at around 1048cm^{-1} that can be associated to the internal Si-O-Si stretching vibrations[1] of the silicon tetrahedrons within the hexagonal structure. As a consequence of Yttrium incorporation, the possible formation of Si-O-Y bond may result in a band intensity reduction and its shift to a wavenumber value of 1070cm^{-1}, suggesting a successful Yttrium substitution. No significant changes are observed for the intensity of the bands located at around and 973 and 796cm^{-1} which are associated to the asymmetrical (ν_{as}(Si-O-Si)) and symmetrical (ν_{symm}(Si-O-Si)) stretching modes.
Concerning the structural features, bare MCM-41 exhibits four well-resolved scattering peaks centered around the *q* vector values of 0.16, 0.28, 0.32 and 0.43 $Å^{-1}$, which can be assigned to the Bragg diffraction peaks for the (100), (110), (200) and (210) planes associated to the hexagonal structure[2], *p6mm* group. As the amount of

Yttrium increases, the degree of hexagonal ordering of the material decreases. Considering the covalent atomic radii (1.11 Å for Si and 1.90 Å for Y)[3] the lower degree of hexagonal ordering of the materials may be explained by an effective isomorphic substitution of larger Y atoms in the hexagonal framework. Since TEOS addition is given in a dropwise step, Y^{3+} species may interact with the partially hydrolyzed silane forming Si-O-Y covalent bonds before polymerizing around the micellar arrangements of the template. Table 1 summarizes the lattice cell parameters and textural properties for all xY-MCM-41 materials.

Table 1. Lattice cell parameters and textural properties of calcined x-Y-MCM-41 materials

Sample name	d_{100} (nm)	a_0 (nm)	S_{BET} Area, m^2/g	Total pore volume ml/g	Monolayer volume, ml/g	Pore Diameter, nm
MCM41	4.46	5.15	1181	1.05	271	3.54
0.02YMCM41	4.47	5.16	693	0.77	159	4.44
0.04YMCM41	4.59	5.30	757	0.90	174	4.78
0.06YMCM41	4.78	5.52	663	1.06	152	6.39
0.08YMCM41	5.08	5.87	563	0.81	130	5.74

The textural properties were evaluated by means of nitrogen physisorption. An example of a typical isotherm is show on diagram *a)*. All samples exhibit a type IV isotherm according to the IUPAC classification. As the amount of substituted Yttrium increases in the silica network, the pore enlarges up to 60% to a final value of 5.74nm in size. The total surface area in consequence, decreases with the pore broadening. The parent material MCM-41 features a BET area of $1180 m^2/g$ and its value decreases swiftly to $563 m^2/g$ for 0.08-Y-MCM-41.



References

Holmes, S.M.; Zholobenko, V.L.; Thursfield, A.; Plaisted, R.J.; Cundy, C.S.; Dwyer, J. "In Situ FTIR Study of the Formation of MCM-41", J. Chem. Soc. Faraday Trans. 94 (14), 2025-2032 (1998).

Kresge, C.T.; Roth, W.J. "The Discovery of Mesoporous Molecular Sieves from the Twenty Year Perspective", Chem. Soc. Rev. 42 (9), 3663 (2013).

Cordero, B.; Gómez, V.; Platero-Prats, A.E.; Revés, M.; Echeverría, J.; Cremades, E.; Barragán, F.; Alvarez, S. "Covalent Radii Revisited", Dalt. Trans. 21, 2832-2838 (2008).

1A – Tuning the pore size, surface area and hydrophobicity of template-based mesoporous silica SBA-15

J. Tovar Rodriguez, E. Fratini, Y. Liu
(NCNR, Gaithersburg, MD), P. Baglioni

Aims

Tuning the pore size, pore volume and surface area of mesoporous hexagonally ordered silica SBA-15. Surface grafting for enhanced hydrophobicity.

Results

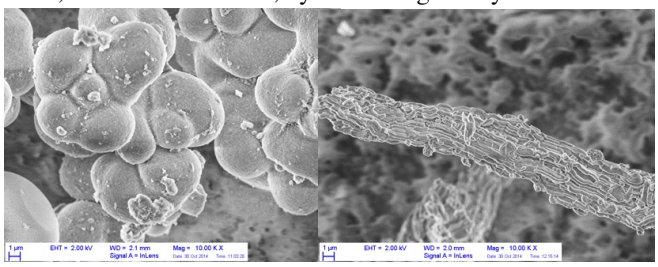
Mesoporous silica SBA-15 was synthesized by hydrothermal treatment using a non-ionic surfactant Pluronic P123 ($EO_{20}PO_{70}EO_{20}$) as structure directing agent and tetraethoxysilane as silicon source. In order to tailor the dimensions of the pore size, 1,3,5-trymethylbenzene (TMB) was used as swelling agent with the following TMB/P123 w/w ratios: 0.08, 0.16, 0.33 and 1.0. After the formation of the synthesis gel, the hydrothermal synthesis was carried out in the temperature interval from 80º to 120ºC and autogenous pressure. Textural properties were obtained by nitrogen adsorption/desorption isotherms and are shown below:

Table 1. Lattice cell parameters and textural properties for large pore silicas

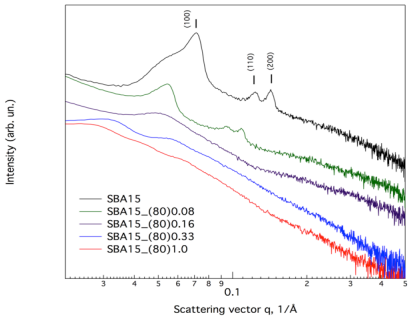
Material	TMB/P123 w/w ratio	BET Surface Area, m^2/gr	Pore size‡, nm	d_{100}, nm	a_0, nm	Pore Volume, ml/g
SBA-15	0	781	4.76	10.3	11.89	0.82
SBA-15-80§	1	716	5.61, 9.77	27.7	31.99	1.71
SBA-15-110§	1	516	14.34, 17.2	30.9	35.68	2.42
SBA-15-120§	1	464	14.35, 19.85	30.9	35.68	2.49
SBA-15-80§	0.33	560	4.30, 3.91	24.32	39.63	0.92
SBA-15-80§	0.16	631	5.3, 6.3, 3.9	15.19	17.54	0.86
SBA-15-80§	0.08	600	6.34, 3.91	13.63	15.74	0.79

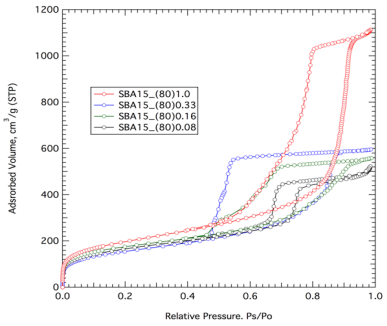
§ Indicates the Temperature for the Hydrothermal treatment; ‡ Estimated with the desorption branch of the isotherm, using the BJH method. Two given values indicate a bimodal pore size distribution.

Pure siliceous SBA-15 presents a narrow pore size distribution with an average diameter of 4.76nm. The pore size can be tuned by addition of TMB during the micellar formation, in a step previous to TEOS hydrolysis and polymerization. All mesoporous sieves exhibit a broader and bimodal size distribution, ranging from 5 to 20nm, in size. In addition, by increasing the hydrothermal temperature and pressure it is possible to yield a material with a different morphology (micrographs obtained at 10kX magnification, bar length 1μm). SBA-15 presents an elongated club-like particle size

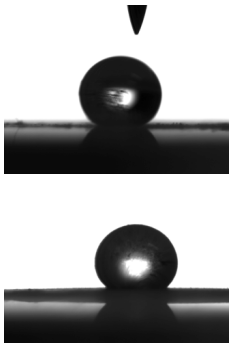


whereas higher temperature and pressure result in smaller round-like particles.
Nitrogen adsorption and desorption isotherms are shown in the next figure (*right*). According to the classification made by IUPAC[1], all prepared materials exhibit a type IV isotherm, characteristic of mesoporous materials ranging from 2 to 50nm in size. Three well-defined regions can be identified: a) Monolayer formation at low relative pressure values (P_s/P_0); b) A slope change can be attributed to the capillary condensation and the P_s/P_0 value depends on the pore size, and c) The region encompassing values until 1.0 which can be attributed to the multilayer adsorption on the external surface area of the material. All materials feature an H1-type hysteresis loop, which is indicative of capillary pores with tubular symmetry. The Small Angle X-ray scattering curves (*left*) can provide information concerning the hexagonal arrangement of the prepared solids.





SBA-15 shows three well defined diffraction peaks in the low q interval, that can be assigned to the reflections of the (100), (110) and (200) planes, associated to the hexagonal structure, *p6mm* space group[2]. As the amount of swelling agent increases, the intensity of the diffraction peaks is reduced and is shifted to lower scattering vector values, suggesting materials with a lower degree of ordering. The lattice cell parameters shown in table 1 were estimated using this value. Nonetheless, all silicas exhibit high surface areas well above the values reported for amorphous silicates. Concerning the surface grafting of SBA-15, several reports can be found in the literature on the functionalization of SBA-15[3] for specific chromatographic and adsorption purposes. Instead of the conventionally used alkyl silanes, here we present the formation of covalently attached monolayers of chlorodimethylphenylsilane, resulting in materials with contact angles over 130º, characteristic of very hydrophobic surfaces.



References

Thommes, M.; Kaneko, K.; Neimark, A.V.; Olivier, J.P.; Rodriguez-Reinoso, F.; Rouquerol, J.; Sing, K.S.W. "Physisorption of Gases, with Special Reference to the Evaluation of Surface Area and Pore Size Distribution" (IUPAC Technical Report), Pure Appl. Chem. 87 (9-10), 1051-1069 (2015).
Kresge, C.T.; Roth, W.J. "The Discovery of Mesoporous Molecular Sieves from the Twenty Year Perspective", Chem. Soc. Rev. 42 (9), 3663 (2013).
Bernardoni, F.; Fadeev, A.Y. "Adsorption and Wetting Characterization of Hydrophobic SBA-15 Silicas", J. Colloid Interface Sci 356 (2), 690-698 (2011).

1A – Nanostrategies for early diagnosis and treatment of FKBP12-related neurodegenerative amyloidosis

M.R. Martina, G. Caminati

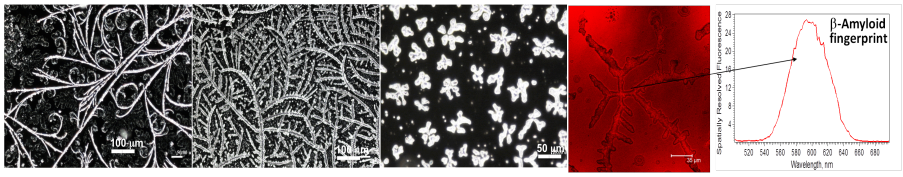
Aims

Effective inhibitors of biomarkers for neurodegenerative pathologies were investigated with the twofold aim of developing a specific sensor nanotechnology able to detect traces of biomarker in the early phases of neurodegenerative disorders and formulate biocompatible nanovectors for the delivery of the biomarker-inhibiting drug in the therapeutic stage.

Results

The FKBP protein family is at the crossroad of several important metabolic pathways due to its central role in immunosuppression and cell proliferation as specific peptidyl-prolyl-isomerase (PPI) enzyme. Members of this family, and notably FK506 binding protein (FKBP12), are involved in Multiple Sclerosis, Amyotrophic Lateral Sclerosis and cancer [1]. Recent findings also evidenced that FKBP12 is over-expressed in early stages of neurodegenerative diseases such as Parkinson's and Alzheimer's and suggest a direct role of FKBP12 in the proliferation of amyloid fibrils [2].

Phase contrast microscopy images acquired for α-SYN, α-SYN/FKBP12 samples kept under magnetic stirring at 37°C for 30 days (Figure 1), clearly show that the aggregation of α-SYN is stimulated by FKBP12 binding.



(a) (b) (c) (d)

Fig. 1: Phase contrast microscopy images of a-SYN (a), a-SYN/FKBP12 (b), and a-SYN /FKBP12/ElteN378 (c). CLSM images and spatially-resolved emission spectrum for CR.

The amyloid fingerprint of such structures, evidenced by the specific emission of Congo Red at 597 nm, was confirmed by means of Confocal Laser Scanning Microscopy combined with spatially resolved fluorescence.

A new class of nanomolar inhibitor for FKBP12 was recently designed and synthesized on the basis of theoretical modeling of the minimal structural requirements for the pharmacophore binding to the FKBP pocket: ElteX compounds [3,4].

The strong binding of ElteN378 to the protein was found to dramatically affect the amplification of fibrils proliferation as shown in fig.1 d for the system α-SYN/FKBP12/ElteN378. Addition of ElteN378 to α-SYN/FKBP12 system results in the disappearance of the extended network of fibrillar aggregates replaced by smaller and amorphous structures. Confocal Laser Scanning Microscopy combined with spatially resolved emission proved that such amorphous structures do not contain β-amyloid motifs.

References

[1] Cao, W.; Konsolaky, M. J. Biosci. 36 (3), 493-498 (2011).
[2] Gerard, M.; Deleersnijder, A.; Demeulemeester, J.; Debyser, Z.; Baekelandt, V. Mol. Neurobiology 44, 13-27 (2011).
[3] Bizzarri, M.; Tenori, E.; Martina, M.R.; Marsili, S.; Caminati, G.; Menichetti, S.; Procacci, P. J. Phys. Chem. Lett. 2 (22), 2834-2839 (2011).
[4] Martina, M.R.; Tenori, E.; Bizzarri, M.; Menichetti, S.; Caminati, G.; Procacci, P. J. of Med. Chem. 56, 1041-1051 (2013).

1A – Surface engineering of nanostructured oxide systems for solar energy conversion

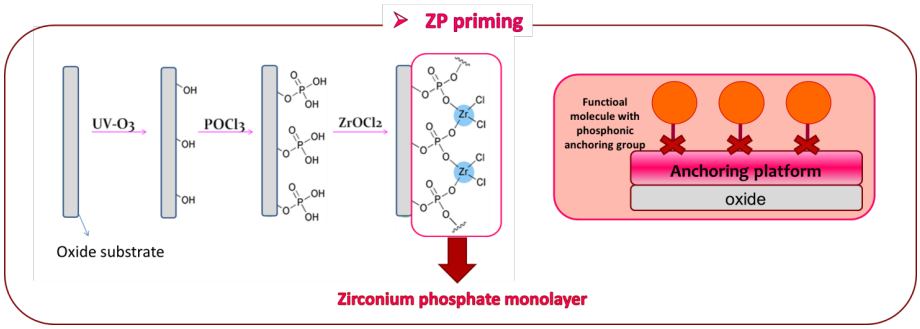
S. Vitale, G. Zappalà, N. Tuccitto, A. Torrisi, F. Ronconi, M.P. Santoni, S. Campagna, A. Licciardello

Aims

The work is aimed to develop methodologies for anchoring of functional molecules on transparent (semi)conducting oxide surfaces, for perspective applications in solar energy conversion devices. The anchoring must be robust, in order to ensure a long lifetime of the device and, at the same time, it must permit the molecule-to-oxide charge injection.

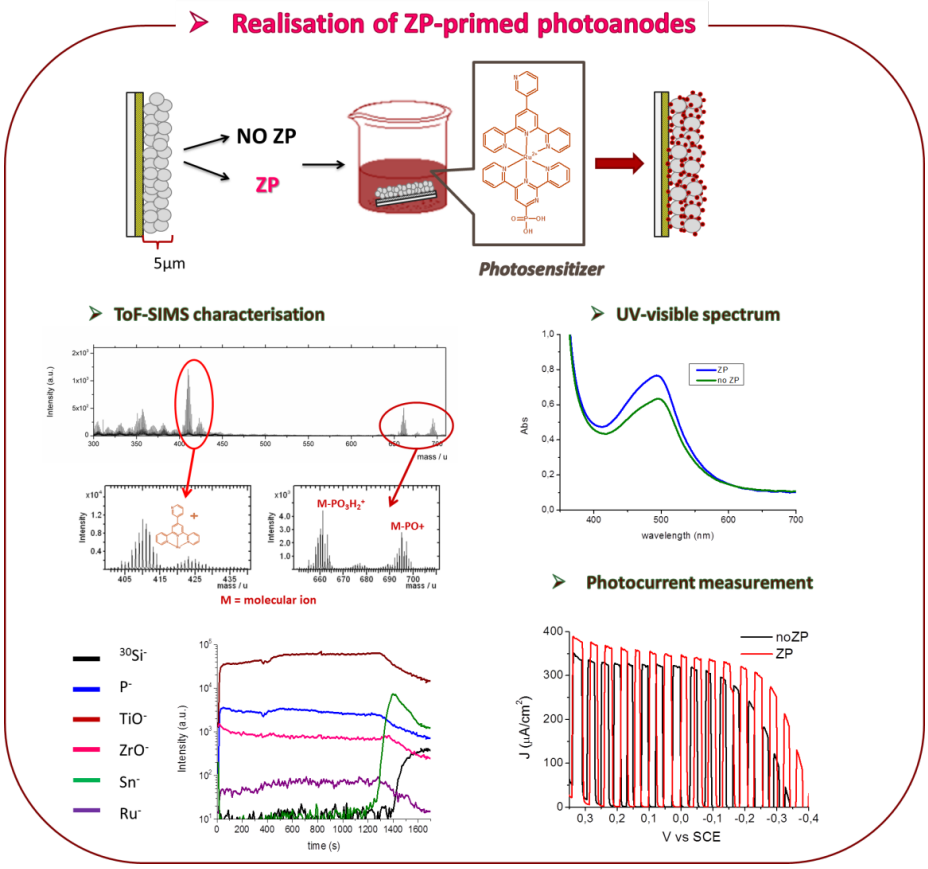
Results

The strategy, sketched in the scheme, involves the preliminary stepwise surface modification [1] based on the chemistry of zirconium phosphates/phosphonates (ZP-priming), consisting in the deposition on a zirconium-phosphate layer directly at the hydroxylated oxide surface, that allows the subsequent anchoring of a phosphonate-functionalised molecule.



The strategy was successfully applied to nanostructured, micrometres-thick TiO_2 and SnO_2 substrates. The efficacy of the method in providing a uniform priming along the entire nanostructured layer was studied and assessed by ToF-SIMS depth profiling measurements.[2] ZP-TiO_2 and ZP-SnO_2 films were subsequently used as substrates for the preparation of photoactive electrodes with perspective application in dye-sensitised cells for solar energy conversion. The ZP treatment provides a suitable anchoring platform for the sensitisation with photoactive dye RuP (a ruthenium tepryridyl-triazin complex bearing a phosphonic group). ToF-SIMS depth profiles demonstrate (as shown the uniformity Ru signal across the nanostructured film) that the sensitisation involves the whole thickness of the oxides layers, while UV-Vis spectroscopy data show the presence of a greater amount of adsorbed layer molecules compared with the conventional impregnation methods. Moreover, the anchoring obtained through the ZP methodology appears to be bore stable in accelerated lifetime tests. Finally, photoelectrochemical measurements (namely JV characteristics upon irradiation) demonstrate that the presence of the zirconium-phosphate-phosphonate layer at the interface between oxide and dye molecule does not negatively affect the

dye-to-oxide charge injection. These data show the photoelectrochemical properties are maintained and no detrimental effect occurs, and in some cases the electrode performances seem to be even improved from the ZP-treatment.



References

[1] Spampinato, V. et al., "Functionalization of Oxide Surfaces by Terpyridine Phosphonate Ligands: Surface Reactions and Anchoring Geometry," (in English), Langmuir, Article vol. 26, no. 11, pp. 8400-8406, Jun 2010.

[2] Vitale, S; Zappala, G.; Tuccitto, N.; Torrisi, A.; Napolitani, E.; Licciardello, A. "SIMS characterization of surface-modified nanostructured titania electrodes for solar energy conversion devices," (in English), Journal of Vacuum Science & Technology B, Article vol. 34, no. 3, p. 5, May-Jun 2016, Art. no. 03h110.

1A – Electrical investigation of molecular wires

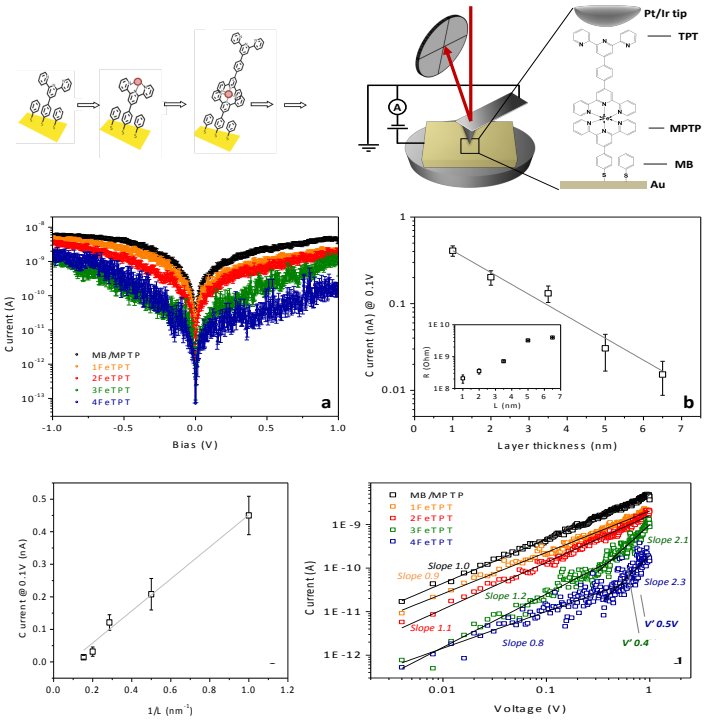
G. Zappalà, S. Vitale, N. Tuccitto, C. Musumeci, P. Samorì, A. Torrisi, A. Licciardello

Aims

Understanding the charge transfer and charge transport mechanisms is of central interest in chemistry, physics and biology, because of their crucial role in numerous processes involving molecular, supramolecular and biological systems. Here we have used a coordination chemistry strategy to fabricate Fe(II)-bis(terpyridine) conductive molecular assemblies by means of layer-by-layer growth on gold substrate, with the aim to get insights into the charge transport mechanisms of these ordered nanostructures.

Results

Supramolecular chemistry can be very useful in obtaining a wide range of system with different properties. In this particular context, polymetallic (supramolecular) complexes can be used as models for the study of electron transport mechanism in a molecular junction. Assemblies of molecular wires masked on Fe-bis(terpyridine) complexes have been grown on gold surfaces via a self-assembling stepwise method involving direct coordination reactions [1-2] at the sample surface, in order to study their electrical behaviour using the conductive AFM technique.



As easily observed, current decreases with the increasing number of layers. In particular, the dependency of the current at a fixed bias value as a function of the thickness of the multilayer shows a linear decrease. The same behavior is observed by plotting the resistance values: a linear increase is observed with increasing thickness, that is typical of ohmic conductors.

Moreover, by using the equations $I = I_0 e^{-\beta L}$ and $R = R_0 e^{\beta L}$ respectively for the current values at a fixed voltage and for low bias resistances, it is possible to determine a β value, that in our case is estimated to be β = 0.058 ±0.006 Å-1. This value provides unambiguous evidence for the existence of a hopping charge transport mechanism.[3]

The log-log plot of the I-V characteristics (d) provides a mean for understanding if is a change in transport regime as a function of the voltage is occurring. In the case of shorter wires, less than 3.5 nm long, the electrical data indicate an ohmic conduction mechanism. On the contrary, longer wires (> 4 nm) exhibit a transition in transport mechanism at certain voltages, to a regime in which the current is roughly following a quadratic dependence on the bias, indicative of a space charge limited current (SCLC) regime.

References

[1] Tuccitto, N.; Ferri, V.; Cavazzini, M.; Quici, S.; Zhavnerko, G.; Licciardello, A.; Rampi, M.A. Nat. Mater. 2009, 8, 41-46.

[2] Musumeci, C.; Zappalà, G.; Martsinovich, N.; Orgiu, E.; Schuster, S.; Quici, S.; Zharnikov, M.; Troisi, A.; Licciardello, A.; Samorì, P. Advanced Materials, 2014, 26, 1688–1693.

[3] Choi, S.H.; Frisbie, C.D.J. Am. Chem. Soc. 2010, 132, 16191.

1B – Rheology and Rheo-NMR-Imaging of lecithin-based viscoelastic solutions.

R. Angelico, L. Gentile, G.A. Ranieri, C. Oliviero Rossi
(Dept. Chem. and Chem. Technol., University of Calabria, CS)

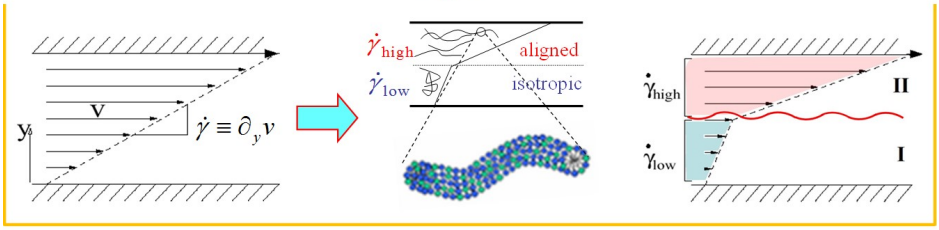
Aims

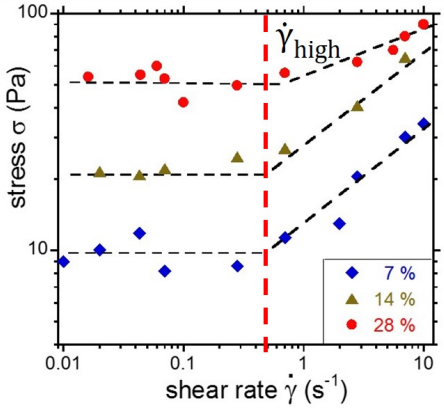
Despite the great deal of results available on the complex shear flow of aqueous wormlike micellar (WM) systems, which require the presence of cosurfactants or counter-ions, less attention has been given to the rheological response of oil continuous WM systems, which offer the advantage to neglect the electrostatic interaction played by salt concentration. To fill this gap, NMR micro-imaging and NMR velocimetry techniques, in combination with bulk rheology, have been used to understand the flow behaviour of reverse nonionic wormlike micelles stabilized by phospholipids (lecithin) in the organic solvent cyclohexane (lecithin organogel) where the amount of dispersed water corresponded to ten water molecules *per* lecithin molecule.

Results

Experimental flow curves at various lecithin volume fractions ϕ = 7, 14 and 28 wt %, were characterized by the presence of stress plateaus up to an upper shear rate limit $\dot{\gamma}_{high}$, which signed the end of the coexistence of the isotropic-nematic shear-banding regime (see Figure 1).

Figure 1





For applied shear rates $\dot{\gamma}$ within the stress plateau, ^{1}H-NMR-density weighted images of 1 mm thick 2D slices of the sample within the cell gap acquired with the Gradient Echo Fast Imaging (GEFI) pulse sequence, revealed a new phase nucleating inhomogeneously at the inner rotating cylinder (Figure 2). In steady state conditions, the shear induced (nematic) phase developed periodic fluctuations in space whose Fourier Transform analysis indicated that the perturbed flow consisted of a vortex-type pattern with wavelength $2\pi/k$, k being 3 mm^{-1} and 4 mm^{-1}, respectively, for $\dot{\gamma}$ = 0.028 s^{-1} and $\dot{\gamma}$ = 0.07 s^{-1}.
Elastic instabilities, generally observed in polymer solutions, may be responsible for the nucleation of Taylor-like vortices, developing along the neutral axis with a characteristic length-space frequency (Figure 2).
In addition, slippage phenomena have been found in flow regimes consistent with a full shear-induced nematic state.

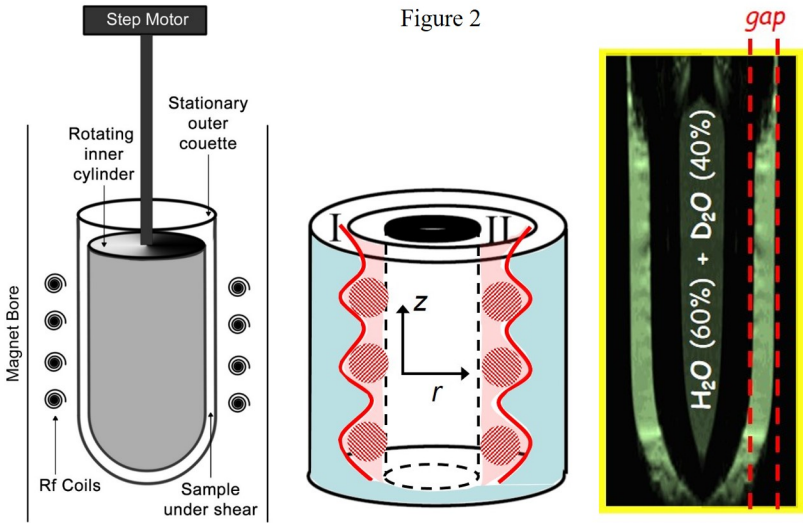


Figure 2

References

Angelico, R.; Gentile, L.; Ranieri, G.A.; Oliviero Rossi, C. "Flow Induced Structures observed in a Viscoelastic Reverse Wormlike Micellar System by Magnetic Resonance Imaging and NMR Velocimetry", RSC Advances 6, 33339-33347 (2016).
Angelico, R.; Amin, S.; Monduzzi, M.; Murgia, S.; Olsson, U.; Palazzo, G. "Impact of branching on the wormlike micelles viscoelasticity", Soft Matter, 8, 10941-10949 (2012).
Angelico, R.; Oliviero Rossi, C.; Ambrosone, L.; Palazzo, G.; Mortensen, K.; Olsson, U. "Ordering fluctuation in a shear-banding wormlike micellar system", PCCP, 12, 8856-8862, (2010).
Angelico, R.; Olsson, U.; Börjesson, J.; Ceglie, A.; Palazzo, G. "Slow dynamics of wormlike micelles", Soft Matter, 6, 1769-1777 (2010).

1B – Phyto-Liposomes as biocompatible carriers for natural drugs

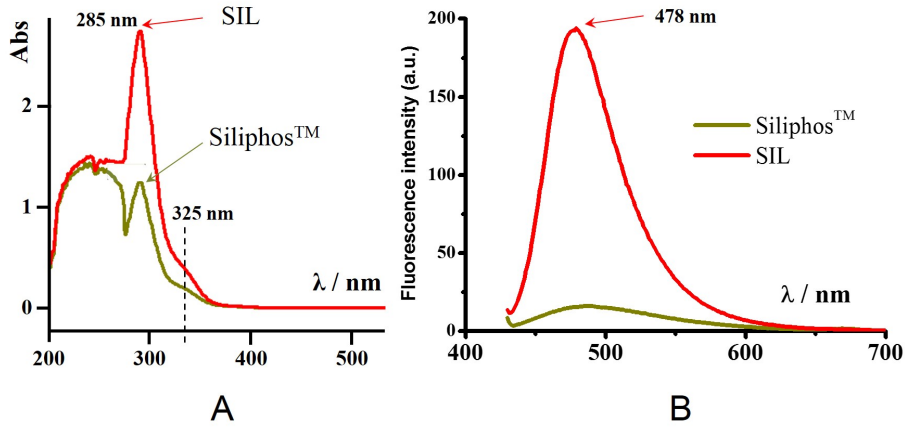
R. Angelico, A. Ceglie, P. Sacco, M. Ripoli, A. Mangia
(Liver Unit, I.R.C.C.S. Casa Sollievo della Sofferenza Hospital, S. Giovanni Rotondo, FG, Italy)

Aims

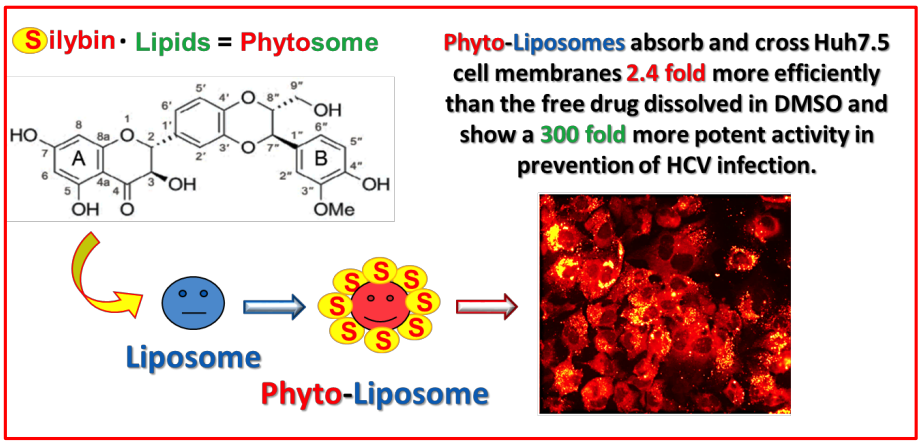
Silybin, the main component of silymarin, is a polyphenolic bioactive natural product extracted by the milk thistle plant *Silybum marianum*. Silybin possesses many health-promoting activities, such as antioxidation, anticancer and hepatoprotective. However, the benefits are curtailed by its extremely poor water solubility, which limits its bioavailability and therapeutic efficiency. Currently, the efficacy of natural extracts may be improved through their incorporation into liposomes, thanks to their versatility to control the delivery of the loaded drug to the target. Here, we developed a formulation based on the incapsulation into liposomes of a silybin-phospholipid complex, commercially available with the trade name Siliphos™, to yield a new type of supramolecular aggregates, also called *Phyto-Liposomes*. The hepatoprotective activity of new formulation was finally tested on human hepatoma cell systems supporting HCV replication and infection.

Results

First, we set up a simple preparation protocol through the reverse-phase evaporation method and investigated the physico-chemical properties of the obtained liposomial suspensions. A careful investigation of host-guest interactions was carried out by performing UV–vis (A) and spectrofluorimetry (B) experiments in non-polar solvents (1:1 mixture of DMSO and benzene), to probe the influence of phospholipids on the electronic properties of silybin and its propensity to engage H-bonding with the lipid headpolar groups (SIL=silybin; Siliphos™ = 1:1 complex silybin-phospholipids).



Then, it was demonstrated the ability of phyto-liposomes to be internalized in human hepatoma Huh7.5 cells, being 2.4 fold more efficient than the plant extract silybin.
Finally, the new formulation was tested on cell systems supporting HCV replication and infection, and its spectrum of pharmacological activities was compared with that of the active principle dissolved in DMSO, revealing a three hundreds fold more potent pharmacological activity.



Moreover, it was assessed that phyto-liposomes were unable to impair the integrity of viral particles, they had no inhibitory effects on HCV replication regardless of genotype and no competition with HCV for Chlatrin-dependent endocytosis mechanism was observed.
The maximum inhibition effect was obtained when phyto-liposomes and viruses supernatant were simultaneously added to cells, whereas no effect on previously infected cells could be detected. Considering that phyto-liposomes were able to inhibit HCV infection, they could be administered soon after the liver transplant, presumably without significant side effects. This perioperative strategy could prevent circulating or extrahepatic virions remained in the recipient to re-infect the transplanted liver, event that usually occurs within few hours after liver transplant.

References

Angelico, R.; Ceglie, A.; Sacco, P.; Colafemmina, G.; Ripoli, M.; Mangia, A. "Phyto-liposomes as nanoshuttles for water-insoluble Silybin-Phospholipid complex", International Journal of Pharmaceutics 471, 173-181 (2014).
Ripoli, M.; Angelico, R.; Sacco, P.; Ceglie, A.; Mangia, A. "Phytoliposome-based silibinin delivery system as a promising strategy to prevent Hepatitis C virus infection: an in vitro study", Journal of Biomedical Nanotechnology 12, 770-780 (2016).

1B – Formulation of liposomes functionalized with specific protein and effective in targeting highly proliferative cells

C. Bonechi, G. Tamasi, A. Donati, A. Magnani, G. Leone, C. Della Giovampaola, A. Capone, F. Rosati, P. Lupetti, M. Ziche, C. Rossi

Aims

Liposomes, used for decades to improve the therapeutic index of new and established drugs, have advanced with the insertion of active targeting.

Results

Doxorubicin-loaded liposomes functionalized (Dox-FL) with the specific target protein, that in this case preferentially binds glycans with alpha-1,2-linked fucose, have been synthesized. A target protein was introduced into the lipid bilayer of DOPC/DOPE liposomes. Functionalization of liposomes with protein did not alter size, surface charge, ζ-potential or overall structure of the vesicles.
By confocal laser microscopy we analyzed the presence and localization of *the active target* and uptake processes in two cancer cell lines. We then constructed doxorubicin-loaded functionalized liposomes. Intracellular delivery of the drug was determined *in vitro* and *in vivo* by confocal and electron microscopy.

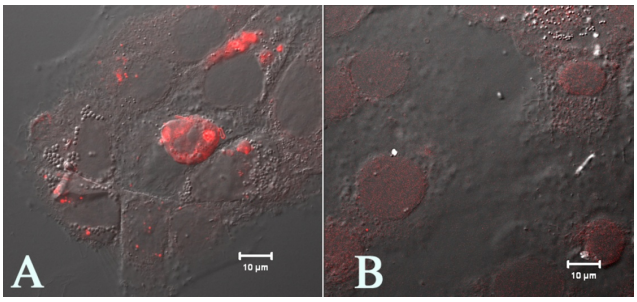


Fig. 1: Uptake for 36 hours of Dox-FL (A) and Dox-L (B) in cancer cells of the DU145 line by confocal microscope (A and B).

We confirmed the specific localization of the binding sites and the uptake mechanism in the two cell lines and determined that functionalized liposomes loaded with doxorubicin greatly increased intracellular delivery of the drug, compared to unmodified doxorubicin-loaded liposomes. The Dox-FL mechanism of entry and drug delivery was different to that of Dox-L and other liposomal preparations. Dox-FL entered the cells one by one in tiny tubules that never fuse with lysosomes. Dox-FL injected in mice with melanoma specifically delivered loaded Dox to the cytoplasm of tumor cells.

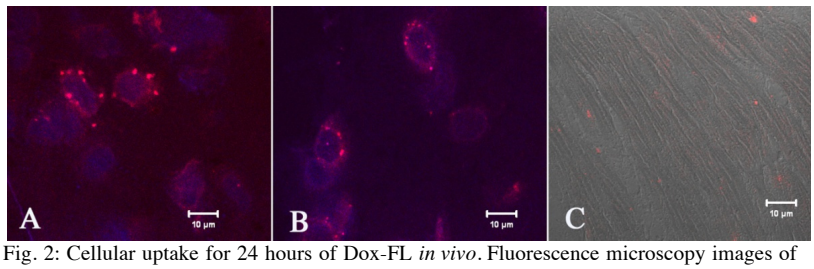


Fig. 2: Cellular uptake for 24 hours of Dox-FL *in vivo*. Fluorescence microscopy images of two sections of the melanoma tumor and one section of heart, showing the localization of Dox upon the intravenous administration of 100 µl of liposomes.

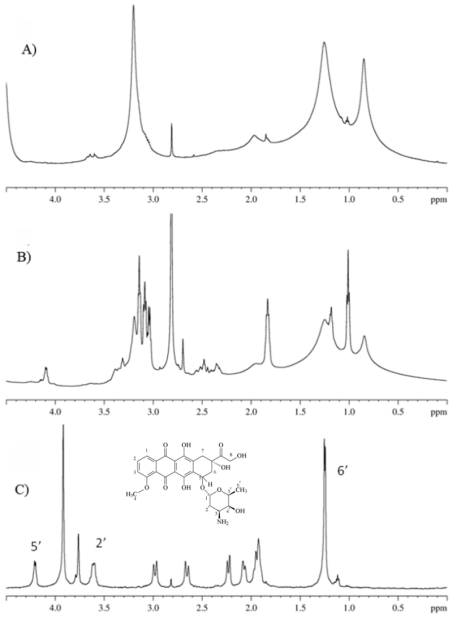


Fig. 3: 600 MHz NMR proton spectrum in D_2O (range 0-4.5 ppm) for: A) empty liposome; B) Dox-FL liposome and C) Doxorubicin (Dox)

To evaluate the interaction processes in liposome systems (Dox-FL, Figure 3B), the ^1H spectrum of doxorubicin in D_2O (figure 3C) and pure liposome (Figure 3A) were recorded. The observed signal broadening was associated with the interactions with the target protein and doxorubicin. Since it was not possible to detect preferential broadening of the polar heads or the alkyl chain signals, this effect was attributed to growth of the overall aggregates. The inclusion of specific target in a liposome formulation is a fundamental step for improving the loading and transport processes of doxorubicin. The NMR spectrum of functionalized liposomes showed that the protein does not substantially modify the structure of the liposome.

Liposome functionalization with specific target protein promises to broaden the therapeutic potential of liposomal doxorubicin treatment, decreasing non-specific toxicity.

Doxorubicin-FL functionalized liposomes promise to be useful in the development of new cancer chemotherapy protocols.

References

Bonechi, C.; Martini, S.; Ciani, L.; Lamponi, S.; Setzer, C.; Rebmann, H.; Rossi, C.; Ristori, S. "Using liposomes as carriers for polyphenolic compounds: the case of trans-resveratrol", PloS One 7, e41438. doi: 10.1371 (2012).

Aldi, S.; Capone, A.; Della Giovampaola, C.; Ermini, L.; Pianigiani, E.; Mariotti, G.; Rosati, F. "Identification of a novel, alpha2-fucosylation-dependent uptake system in highly proliferative cells", Tissue Cell. 47, 33-38 (2015).

Tahover, E.; Patil, Y.P. Gabizon, A.A. "Emerging delivery systems to reduce Doxorubicin cardiotoxicity and improve therapeutic index: focus on liposomes", Anticancer Drugs 26, 241-258 (2015).

1B – Effect of Resveratrol on Platelet Aggregation by Fibrinogen Protection: NMR, IR and SEM experiments

C. Bonechi, S. Lamponi, A. Donati, G. Tamasi, M. Consumi, G. Leone, C. Rossi, A. Magnani

Aims

The ability of resveratrol in preserving fibrinogen from denaturation and platelets from aggregation was studied using combined spectroscopic and biological analyses.

Results

Resveratrol (RSV), an antioxidant found in red wine, is able to decrease the incidence of coronary heart disease. RSV blocks platelet aggregation by the protective action characteristic of antioxidant compounds. **W**e investigated the effect of RSV in inhibiting both platelet adhesion and aggregation and fibrinogen conformational changes promoted by epinephrine, using complementary experimental techniques.

Nuclear magnetic resonance and infrared spectroscopies were used to investigate the protective effect exerted by resveratrol toward fibrinogen (FBG) in presence of epinephrine (EP) which, as well known, induces strong variations in the secondary structure of fibrinogen when reaching the stress level concentration.

The protective effect of RSV towards FBG was evident by both spin nuclear relaxation experiments, determining the thermodynamic equilibrium constants of FBG-EP interaction and infrared measurements, analyzing the EP-induced conformational changes of FBG. In particular, the spin nuclear relaxation showed that the strength of the interaction between epinephrine and fibrinogen was strongly decreased by the presence of resveratrol (Figure 1A). These data were confirmed by IR spectroscopic measurements that emphasize the protective effect of the antioxidant compound towards fibrinogen. The infrared data, in fact, showed that fibrinogen was not denatured by the interaction with epinephrine in presence of resveratrol (Figure 1B).

Resveratrol inhibits the protein interaction with the hormone and thus reduces the degree of platelet adhesion and aggregation. SEM analysis, in fact, revealed that the presence of resveratrol completely inhibited the platelet aggregation and the degree of platelet adhesion decreased by increasing the resveratrol concentration (Figure 2). Moreover, resveratrol was also able to reduce the percentage of platelet aggregation in PRP.

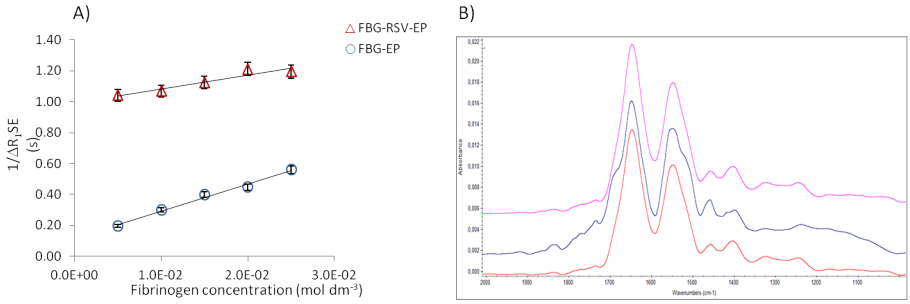


Fig. 1: A) Reciprocal of selective relaxation rate enhancements in relation to epinephrine concentration with and without RSV; B) Amide I and Amide III deconvoluted difference FTIR-ATR spectra of: native FBG (red spectrum), FBG-EP system (blu spectrum), FBG-EP-RSV system (pink spectrum) in normal saline solution

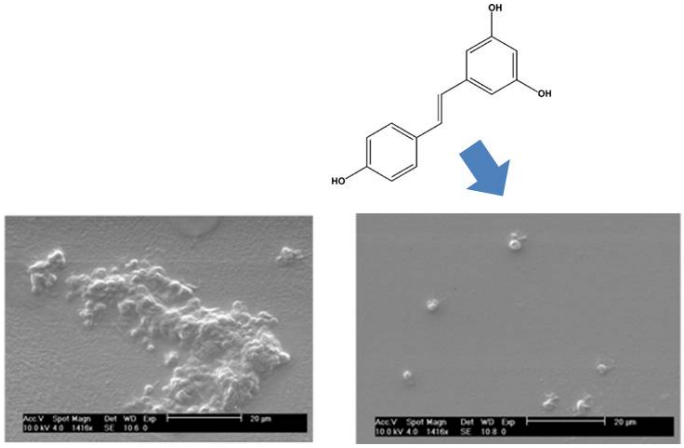


Fig. 2: Scanning Electron Microscopy images of platelets after contact with: a) EP 15 mM; b) EP 15 mM and RSV 60 mM.

The protective properties of resveratrol towards fibrinogen from the denaturant activity of epinephrine can be explained on the basis its ability to bind the catecholamine.

Our combined results pointed out that resveratrol is able to protect both fibrinogen and platelets from the denaturant and aggregating action of epinephrine at the stress level concentration.

References

Olas, B.; Wachowicz, B. "Resveratrol, a phenolic antioxidant with effects on blood platelet functions", Platelets 16, 251-260 (2005).

Bonechi, C.; Martini, S.; Rossi, C. "Interaction study of bioactive molecules with fibrinogen and human platelets determined by ^{1}H NMR relaxation experiments", Bioorganic & Medicinal Chemistry 17(4), 1630-1635 (2009).

Zordoky, B.N.M.; Robertson, I.M.; Dyck, J.R.B. "Preclinical and clinical evidence for the role of resveratrol in the treatment of cardiovascular diseases", Biochimica et Biophysica Acta 1852, 1155-1177 (2015).

1B – Effect of quercetin-loaded liposomes on induced oxidative stress in human spermatozoa

C. Rossi, C. Bonechi, E. Moretti, G. Collodel, G. Tamasi, A. Donati, A. Magnani

Aims

The study of natural compounds with antioxidant properties is appealing since it can offer the possibility of therapeutic options for male infertility and the development of new strategies of media supplementation in vitro used for semen handling. A strategy to circumvent the poor polyphenols bioavailability is to load these compounds into liposomes.

Results

We evaluated the in vitro effects of quercetin (Q) and Q-loaded liposomes on motility, viability and chromatin integrity of swim-up selected human sperm. Antioxidant power was assayed against tert-butylhydroperoxide induced lipid peroxidation (LPO) using C11-BODIPY581/591 fluorescentprobe and transmission electron microscopy. Q-loaded liposomes showed decreased toxicity for sperm motility and viability and increased DNA damage compared to quercetin. The percentage of sperm with fluorescence, marker of LPO, was decreased in samples incubated with quercetin vs Q-loaded liposomes ($P < 0.001$). The ultrastructure of acrosomes and membranes was preserved with quercetin, whereas Q-loaded liposomes did not prevent membrane injury.

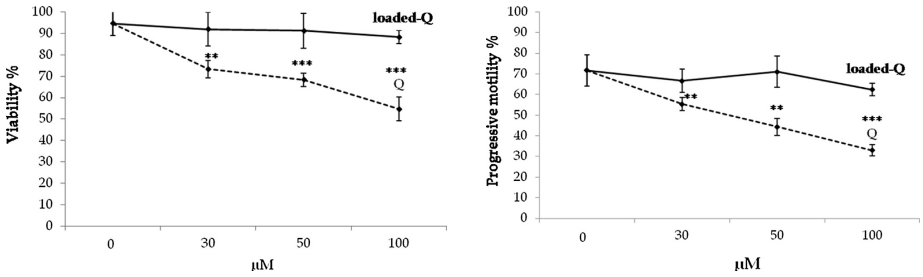


Fig. 1: Mean and SD of the percentages of viable and progressive motility sperm treated with Q-loaded liposomes and Q at different concentrations.

Respect to free Q, Q-loaded liposomes showed decreased toxicity for sperm motility and viability, increased genotoxicity, especially if used at high concentrations, and they were not active against induced LPO in human sperm. The different behavior of Q and Q-loaded liposomes could be explained by a different mechanism of action: Q may act outside the cell modulating sperm motility and counteracting LPO at plasma membrane level, the liposomes plausibly deliver Q inside the sperm cell for this reason the antioxidant effect of Q on induced LPO is decreased and the negative effect on DNA is evident.

Table 1. Size, surface charge and encapsulation efficiency of Q-free liposomes and Q-loaded liposomes.

Liposome Composition	Size (nm)	P.I.	Zeta potential (mV)	Encapsulation Efficiency (EE) %
DOPC/DOPE	105 ± 15	0.16	-11 ± 5	
DOPC/DOPE + Q (1:1)	113 ± 10	0.20	-19 ± 7	18.9 ± 5.3
DOPE/DOPA	109 ± 13	0.17	-37 ± 2	
DOPE/DOPA + Q (1:1)	125 ± 21	0.21	- 32 ± 5	14.2 ± 1.9
DOPE/DOTAP	115 ± 12	0.15	48 ± 5	
DOPE/DOTAP + Q (1:1)	124 ± 15	0.19	50 ± 9	15.6 ± 1.5

Results of the size distribution and surface charge values of Q-free liposomes and Q loaded liposomes are presented in Table 1.In all cases, there was a slight increase in liposome mean diameter when Q was incorporated. The difference in the mean diameter of Q-free liposomes and Q loaded liposomes was small indicating that Q can be well loaded in the lipid bilayers. The low polydispersity indexes (P.I.) showed that the liposomes were not altered by the interactions with Q.

References

Moretti, E.; Mazzi, L.; Terzuoli, G.; Bonechi, C.; Iacoponi, F.; Martini, S.; Rossi, C.; Collodel, G. “Effect of quercetin, rutin, naringenin and epicatechin on lipid peroxidation induced in human sperm”, Reproductive Toxicology 34, 651-657 (2012).
Bonechi, C.; Martini, S.; Ciani, L.; Lamponi, S.; Setzer, C.; Rebmann, H.; Rossi, C.; Ristori, S. “Using liposomes as carriers for polyphenolic compounds: the case of trans-resveratrol”, PloS One 7, e41438. doi: 10.1371 (2012).
Ranawat, P.; Pathak, C.M.; Khanduja, K.L. “A new perspective on the quercetin paradox in male reproductive dysfunction”, Phytother. Res. 27, 802-810 (2013).

1B – In vitro assays for the "ORAC" classification

M.C. Baratto, M.L. Parisi, M. Al Katib, R. Basosi, R. Pogni

Aims

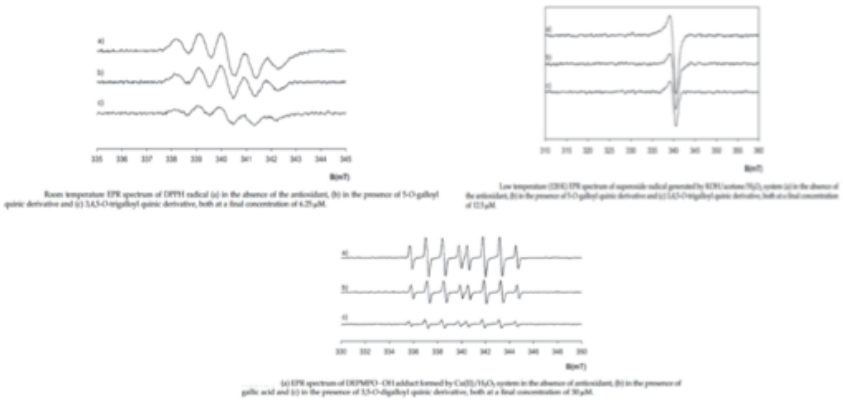
Scavenger and antioxidant activity of extracts and fractions using in vitro assays are carried out through EPR spectroscopy and spectrophotometrically.

Results

Antioxidants act against "free radicals" in order to scavenger them. The determination of antioxidant activity of single components or extracts is performed through assays (ORAC) that measure the capability of such molecules to reduce the presence of reactive radicals, mainly oxygen ones, such as ROS.

EPR (electron paramagnetic resonance) spectroscopy is a crucial technique for the analysis, determination and quantification of antioxidant activity. It is specific for the study of paramagnetic species such as radicals. As free radicals are very labile and difficult to be detected spectroscopically at room temperature, the EPR-spin trapping technique is a powerful approach in order to trap radical species and form stable adduct to be studied at room temperature. EPR spectroscopy is a non destructive technique which gives a direct analysis of the free radical quantity and an indirect measurement of the antioxidant activity. Antioxidant activity of food, extracts or single molecules is monitored and quantified through the reduction of stable radical signal present in the sample understudy.

The research carried out by the University of Siena started in 2003 with the antioxidant activity study of some galloil quinic extracts from Pistacia lentiscus leaves and some spectrophotometric and spectroscopic EPR assays were developed towards DPPH and ROS radicals.



Then the study was focused on the biochemistry of Olea europea leaves submitted to high light and salinity and the defence of leaves against oxidative damages due to water stress and salinity.

Recently antioxidant properties of polyphenolic fractions of Cistus incanus leaves and of an extract from Consalida maggiore (Symphytum Officinale) root have been tested and are still under study.

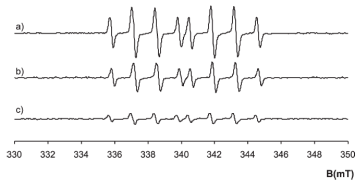


FIGURE 4 (a) EPR spectrum of DEPMPO–OH adduct formed by Cu(II)/H_2O_2 system in the absence of antioxidant, (b) in the presence of gallic acid and (c) in the presence of 3,5-O-digalloyl quinic derivative, both at a final concentration of 30 μM.

References

Baratto, M.C.; Tattini, M.; Galardi, C.; Pinelli, P.; Romani, A.; Visioli, F.; Basosi, R.; Pogni, R. "Antioxidant activity of galloyl quinic derivatives isolated from P. lentiscus leaves", Free Radical Research 37, 405-412, (2003).

Melgar, J.C.; Guidi, L.; Remorini, D.; Agati, G.; Degl'Innocenti, E.; Castelli, S.; Baratto, M.C.; Faraloni, C.; Tattini, M. "Antioxidant defences and oxidative damage in salt-treated olive plants under contrasting sunlight irradiance", Tree Physiology 29, 1187-1198, (2009).

Fini, A.; Guidi, L.; Giordano, C.; Baratto, M.C.; Ferrini, F.; Brunetti, C.; Calamai, L.; Tattini, M. "Salinity stress constrains photosynthesis in Fraxinus ornus more when growing in partial shading than in full sunlight: Consequences for the antioxidant defence system", Annals of Botany 114, 525-538, (2014).

Gori, A.; Ferrini, F.; Marzano, M.C.; Tattini, M.; Centritto, M.; Baratto, M.C.; Pogni, R.; Brunetti, C. "Characterisation and antioxidant activity of crude extract and polyphenolic rich fractions from C. Incanus leaves", International Journal of Molecular Sciences 17, 1344 (1-13) (2016).

1B – Interaction of Antimicrobial Peptides with lipid membranes

A. Bonucci (Bioénergétique et Ingénierie des Protéines, Marseille), E. Balducci (School of Biosciences and Veterinary Medicine, University of Camerino), R. Pogni

Aims

The aims of this work is to study the interaction of bioactive antimicrobial 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

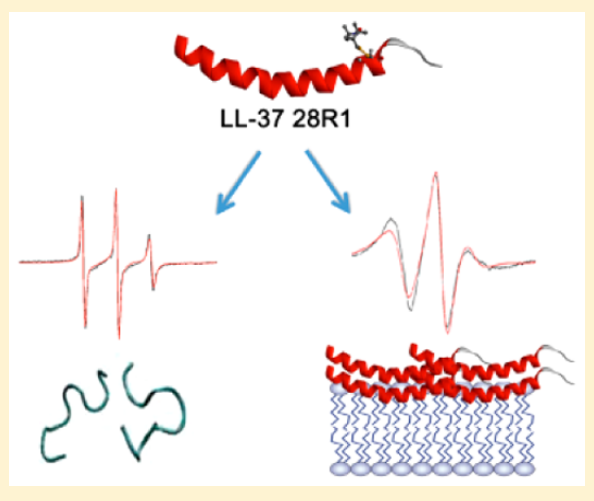
Antimicrobial peptides (AMPs) are an essential part of innate immune defence system against microbial infection. Naturally occurring AMPs are basic peptides composed of 12-50 aminoacids that are ubiquitously distributed throughout all kingdoms of life. AMPs display a broad spectrum of antimicrobial activity 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.

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 mechanism of action of human AMP LL-37 against model bacteria membranes versus host cell model membranes. In this context, antimicrobial peptide LL-37 and two variantswere studied in the presence of model membranes with different lipid compositions andcharges. The investigation was performed using an experimental strategy that combines thesite-directed spin labeling–electron paramagnetic resonance technique with circulardichroism and fluorescence emission spectroscopies. LL-37 interacts with negatively chargedmembranes forming a stable aggregate, which can likely produce toroidal pores until theamount of bound peptide exceeds a critical concentration. At the same

time, we have clearly detected an aggregate with a higher oligomeric degree for interaction of LL-37 with neutral membranes. These data confirm the absence of cell selectivity of the peptide and a more complex role in stimulating host cells.



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.

References

Bonucci, A.; Caldaroni, E.; Balducci, E.; Pogni, R. "A Spectroscopic Study of the Aggregation State of the Human Antimicrobial Peptide LL-37 in Bacterial versus Host Cell Model Membranes", Biochemistry 54, 6760-6768 (2015).

Bonucci, A.; Balducci, E.; Martinelli, M.; Pogni R. "Human neutrophil peptide 1 variants bearing arginine modified cationic side chains: effects on membrane partitioning", Biophys. Chem. 190-191, 32-40 (2014).

Bonucci, A.; Balducci, E.; Pogni, R. "HNP-1 variants bearing a reduced cationic charge: effects on membrane partitioning", Biophys. Chem. 190, 32-40 (2014).

Bonucci, A.; Balducci, E.; Pistolesi, S.; Pogni, R. "The defensin-lipid interaction: insigths of the binding state of the human antimicrobial peptide HNP-1 to model bacterial membrane", BBA-Biomem. 1828, 758-764 (2013).

Balducci, E.; Bonucci, A.; Picchianti, M.; Pogni, R.; Talluri, E. "Structural and functional consequences induced by post-translation modification in α-Defensins", Int. J. of Pep art. n. 594723 (2011).

Pistolesi, S.; Pogni, R.; Feix, J.B. "Membrane insertion and bilayer perturbation by antimicrobial peptide CM15", Biophys. J. 93, 1651-1660 (2007).

1B – EPR investigations of enzyme-ligand complex in copper containing proteins

M. Al Khatib, M.C. Baratto, R. Pogni, R. Basosi

Maher Al Khatib's PhD project is focused on the development of electron paramagnetic resonance methodologies. The central part of the work is oriented toward the implementation and application of a various range of pulsed EPR experiments to substrate of biological, biochemical and industrial interest, such as enzymes and metalloproteins. These experiments, along with the classical continuous wave (cw) EPR techniques, will provide knowledge of the structure and dynamics of the paramagnetic centers in such systems.
The pulsed experimental setup is based on a SuperQ-FT bridge which is able to generate Q band microwave pulses on the nanosecond timescale. The continuous wave experimental setup allows Q, X and S band measurements for multifrequency studies. It is important to notice that the project promotes a strong interaction between the experimental part of the work and the theoretical knowledge needed to perform it successfully. Recently, low temperature cw experiments have been performed on two new enzymes of possible industrial interest: a fungal laccase and a tyrosinase from Algerian desert soil isolates. Both these enzymes share a pair of antiferromagnetically coupled Cu(II) ions into their catalytic site ("type3" copper center, T3), even if laccases in contrast to tyrosinases, use also two other distinct mononuclear Cu(II) ions to exert their catalytic activity: the so called type1 (T1) and type2 (T2) copper centers, both EPR active (Fig. 1). In presence of exogenous ligand, the T3 antiferromagnetic coupling can be broken, making the T3 site suitable for EPR analysis.

Fig. 1: Schematic representation of the overall catalytic mechanism in laccases. Four copper ions are present. The T3 site (yellow) is the one present both in laccases and tyrosinases.

References

Pogni R.; Baratto, M.C.; Sinicropi, A.; Basosi, R. "Spectroscopic and computational characterization of laccases and their substrate radical intermediates", Cell. Mol. Life Sci. 72, 885-896, (2015).
Van Gastel, M.; Bubacco, L.; Groenen, E.J.J.; Vijgenboom, E.; Canters, G.W. "EPR study of the dinuclear active copper site of tyrosinase from Streptomyces antibioticus", FEBS Letters 474, 228-232 (2000).
Gromov, I.; Marchesini, A.; Farver, O.; Pecht, I.; Goldfarb, D. "Azide binding to the trinuclear copper center in laccase and ascorbate oxidase", Eur. J. Biochem. 266, 820-830 (1999).
Solomon, E.I.; Sundaram, U.M.; Machonkin, T.E. "Multicopper oxidases and oxygenases", Chem. Rev. 96, 2563-2605 (1996).

1B – Loading, protection and release of hydrophylic molecules entrapped in liposome based multishell nanocapsules

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

Aims

Loading and release behaviour of hydrophilic molecules as function of pH and wall thickness.

Results

Compartmentalized systems produced via the layer-by-layer (LbL) self-assembly method have been produced by alternatively depositing alginate and chitosan layers onto cores of liposomes. The possibility of encapsulating and releasing molecules from this type of nanocapsule was demonstrated by loading high (FITC-dextran 20, 40, 70 kDa) and low molecular weight (Rhodamine B) molecules into the liposome core. The release of the loaded molecules from the nanocapsule was demonstrated after liposome core dissolution.

The combination of dynamic light scattering (DLS), ζ potential, and transmission electron microscopy (TEM) techniques provides detailed information on the stability, dimensions, charge, and wall thickness of these polyelectrolyte globules. TEM microphotographs demonstrate the presence of nanocapsules with an average diameter of below 300 nm and with a polyelectrolyte wall thickness of about 20-25 nm. Even at low molecular weight, the nanocapsules appear to be appropriate for prolonged molecule compartmentalization and protection. By means of the Ritger–Peppas model, non-Fickian transport behaviour was detected for the diffusion of the entrapped molecules through the polyelectrolyte wall.

Values of the diffusion coefficient were calculated and yield useful information regarding chitosan/alginate hollow nanocapsules as drug-delivery systems. The influence of the pH and of the wall thickness on the release properties were also considered. The results indicate that vesicle templated hollow polyelectrolyte nanocapsules show great potential as novel controllable drug-delivery devices for biomedical and biotechnological applications.

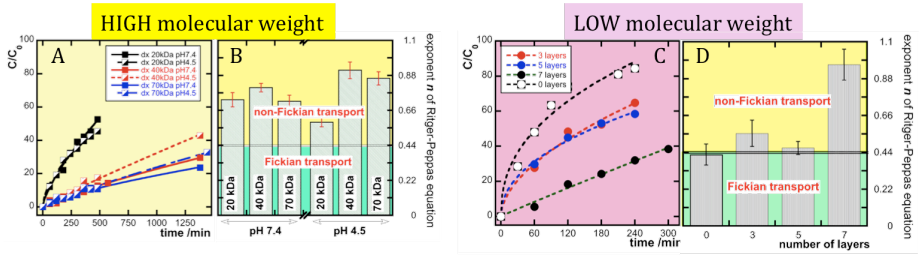


Fig.: (A) Release profiles of FITC-dextran 20, 40, 70 kDa at pH 7.2 and 4.5 from capsules made of 5 polyelectrolyte layers, (B) Release behavior of FITC-dextran extrapolated from experimental data according to the Ritger–Peppas model. (c) Release profiles of Rhodamine B from bare liposomes and from nanocapsules with three, five and seven layers at pH 7.2. (D) Release behavior of Rhodamine B extrapolated from experimental data according to the Ritger–Peppas model. The line drawn in the graphs B and D indicates the boundary between the values of n typical of Fickian (<0.43) or non Fickian diffusion (>0.43).

References

Cuomo, F.; Lopez, F.; Piludu, M.; Miguel, M.G.; Lindman, B.; Ceglie, A. "Release of small hydrophilic molecules from polyelectrolyte capsules: Effect of the wall thickness", Journal of Colloid and Interface Science 447 (1), 211-216 (2015).

Cuomo, F.; Lopez, F.; Ceglie, A. "Templated globules-Applications and perspectives", Advances in Colloid and Interface Science 205, 124-133 (2014) .

Cuomo, F.; Ceglie, A.; Piludu, M.; Miguel, M.G.; Lindman, B.; Lopez, F. "Loading and protection of hydrophilic molecules into liposome-templated polyelectrolyte nanocapsules", Langmuir 30 (27), 7993-7999 (2014).

1B – Coumarin derivative for sensing application: nucleotides identification using a micellar system

F. Cuomo, A. Ceglie, C. Caltagirone, S. Murgia, F. Lopez

Aims

Easy and controlled the use of a novel lipophilic coumarin derivative in aqueous environment for sensing application.

Results

The recognition of nucleotides is of crucial importance because they are the basic constituents of nucleic acids. The present study is focused on the selective interaction between a novel amphiphilic fluorophore containing coumarin and imidazole, CI (1-methyl-3-(12-((2-oxo-2H-chromen-7-yl)oxy)dodecyl)-1H-imidazol-3-ium bromide), and different nucleotide-monophosphates (NMPs). It was supposed that the solubilisation of the low water soluble CI in a micelle system of hexadecyltrimethylammonium chloride (CTAC) would make the coumarin moiety of CI available to the interaction with the water-soluble NMPs. Changes in CTAC critical micelle concentration suggested that CI strongly interacted with the host cationic surfactant, thus forming a positively charged interface enriched with coumarin able to interact with the anionic NMPs. Steady-state fluorescence quenching revealed that CI/CTAC system was capable of distinguish between purine- and pyrimidine-based nucleotides. A modified Stern-Volmer equation permitted the use of a quenching model that accounted for the possible interactions between the micelles and the nucleotides. The data analysis allowed calculating selective parameters that differentiated according to the type of nucleotide either at 25 or 50 °C. Our results established the utility of the novel coumarin derivative fluorophore, supported by the simple and suitable micellar systems, as a tool for DNA sensing applications.

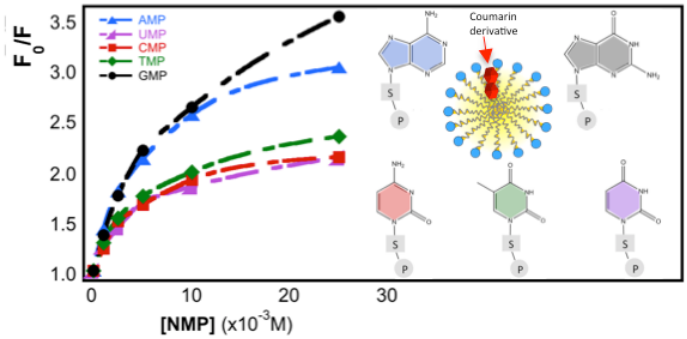


Fig. 1: Normalized fluorescence intensities at 392 nm (λexc = 325 n m) of CI solubilized in CTAC micellar solution. as function of nucleo-tide concentrations (AMP, GMP, UMP, TMP, CMP) (left). Schematic representation of the CI/CTAC system and nucleotide mono-phosphates (left).

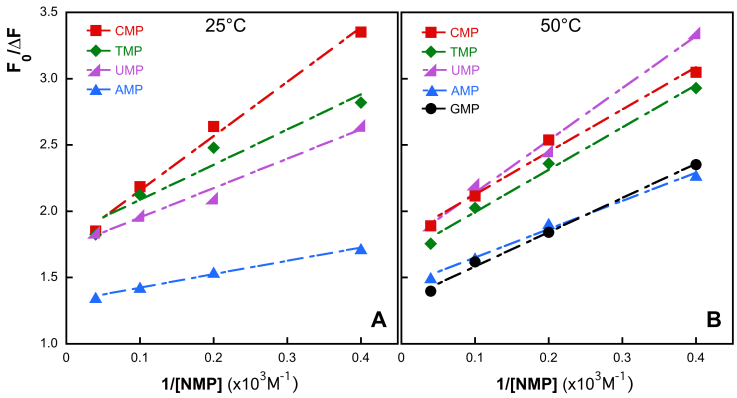


Fig. 2: Fitting of the fluorescence quenching data to the modified Stern-Volmer equation at 25 and 50°C. The intercepts of the straight lines are in agreement with the differences in terms of probe accessibility and differentiate between purine and pyrimidine based nucleotides.

References

Lopez, F.; Cuomo, F.; Ceglie, A.; Ambrosone, L.; Palazzo, G. "Quenching and dequenching of pyrene fluorescence by nucleotide monophosphates in cationic micelles", Journal of Physical Chemistry B 112 (24), 7338-7344 (2008).

Cuomo, F.; Palazzo, G.; Ceglie, A.; Lopez, F. "Quenching efficiency of pyrene fluorescence by nucleotide monophosphates in cationic micelles", Journal of Photochemistry and Photobiology A: Chemistry 202 (1), 21-27 (2008).

Bettoschi, A.; Ceglie, A.; Lopez, F.; Meli, V.; Murgia, S.; Tamburro, M.; Caltagirone, C.; Cuomo, F. "On the role of a coumarin derivative for sensing applications: Nucleotide identification using a micellar system", Journal of Colloid and Interface Science 477, 8-15 (2016).

1B – Cubosomes and hexosomes in theranostic nanomedicine

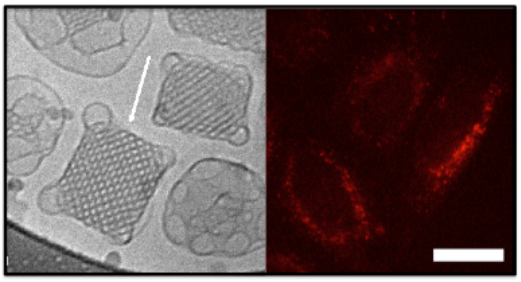
S. Murgia, C. Caltagirone, V. Lippolis, M. Monduzzi

Aims

We explored the potential of monoolein-based non-lamellar liquid crystalline nanoparticles, namely cubosomes and hexosomes, as theranostic tools.

Results

We proved that cubosomes and hexosomes allow for the encapsulation of antineoplastic poorly water-soluble drugs (quercetin, camptothecin, and docetaxel) and that the presence of such drugs within the lipid bilayer did not affect the nanostructural and morphological characteristics of the nanoparticles. Furthermore, we observed the superior cytotoxic ability of docetaxel towards HeLa cells when embedded in the cubosomes matrix with respect to its use as a free drug. Similarly, we demonstrated these nanocarriers can be simultaneously coupled with fluorescent imaging agents still preserving the original physicochemical features of pristine cubosomes and hexosomes nanoparticles. In addition, also the photophysical properties of the imaging agents, critical for the fluorescence optical imaging, are retained in the colloidal systems. Sometimes, these properties were extremely helpful for understanding the fluorophore localization in the nanoparticle (solvatochromism). In the frame of possible applications in cancer treatments, we made cubosomes and hexosomes actively targeted by decorating their surface with folic acid. Thanks to this modification the uptake of targeted cubosomes in HeLa cells considerably increases with respect to pristine cubosomes.



A detailed study of changes occurring in HeLa cells, when exposed to treatment with monoolein-based cubosomes, was conducted. Such investigation is of primary importance within the context of biomedical applications. It was observed that the uptake of cubosome formulations induced modification of the cell lipid profile, lipid droplet accumulation, mitochondrial hyperpolarization and mitochondrial ROS generation. Remarkably, these modifications did not cause significant toxicity in HeLa cells. Finally, to evaluate the potential of cubosomes as diagnostic tools in diabetes and pancreatic β-cell transplantation, a newly synthesized hydrophobic dye was entrapped with their lipid bilayer. Rat pancreatic β -cells readily took up the cubosome nanoparticles, as revealed by in vitro internalization tests, and flow-cytometric analyses confirmed the persistence of the fluorescence for up to 24 hours. All these results strongly encourage further investigation of non-lamellar lipid liquid crystalline

nanoparticles in thereanostic nanomedicine, and for pharmaceutical applications in general.

References

Murgia, S.; Falchi, A.M.; Meli, V.; Schillén, K.; Lippolis, V.; Monduzzi, M.; Rosa, A.; Schmidt, J.; Talmon, Y.; Bizzarri, R.; et al. "Cubosome Formulations Stabilized by a Dansyl-Conjugated Block Copolymer for Possible Nanomedicine Applications", Colloids Surfaces B 129, 87-94 (2015).

Caltagirone, C.; Falchi, A.M.; Lampis, S.; Lippolis, V.; Meli, V.; Monduzzi, M.; Prodi, L.; Schmidt, J.; Sgarzi, M.; Talmon, Y.; et al. "Cancer-Cell-Targeted Theranostic Cubosomes", Langmuir 30, 6228-6236 (2014).

Monduzzi, M.; Lampis, S.; Murgia, S.; Salis, A. "From Self-Assembly Fundamental Knowledge to Nanomedicine Developments", Adv. Colloid Interface Sci. 205, 48-67 (2014).

Meli, V.; Caltagirone, C.; Falchi, A. M.; Hyde, S. T.; Lippolis, V.; Monduzzi, M.; Obiols-Rabasa, M.; Rosa, A.; Schmidt, J.; Talmon, Y.; et al. "Docetaxel-Loaded Fluorescent Liquid-Crystalline Nanoparticles for Cancer Theranostics", Langmuir 31, 9566-9575 (2015).

Falchi, A.M.; Rosa, A.; Atzeri, A.; Incani, A.; Lampis, S.; Meli, V.; Caltagirone, C.; Murgia, S. "Effects of Monoolein-Based Cubosome Formulations on Lipid Droplets and Mitochondria of HeLa Cells", Toxicol. Res. 4, 1025-1036 (2015).

Caltagirone, C.; Arca, M.; Falchi, A.M.; Lippolis, V.; Meli, V.; Monduzzi, M.; Nylander, T.; Rosa, A.; Schmidt, J.; Talmon, Y.; et al. "Solvatochromic Fluorescent BODIPY Derivative as Imaging Agent in Camptothecin Loaded Hexosomes for Possible Theranostic Applications", RSC Adv. 5, 23443-23449 (2015).

Rosa, A.; Murgia, S.; Putzu, D.; Meli, V.; Falchi, A.M. "Monoolein-Based Cubosomes Affect Lipid Profile in HeLa Cells", Chem. Phys. Lipids 191, 96-105 (2015).

Miceli, V.; Meli, V.; Blanchard-Desce, M.; Bsaibess, T.; Pampalone, M.; Conaldi, P. G.; Caltagirone, C.; Obiols-Rabasa, M.; Schmidt, J.; Talmon, Y.; et al. "In Vitro Imaging of β-Cells Using Fluorescent Cubic Bicontinuous Liquid Crystalline Nanoparticles", RSC Adv. 6, 62119-62127 (2016).

1B - Poly(vinyl alcohol)-based microgels prepared through salting out: rationalising the aggregation process

M. Perfetti, G. D'Errico, L. Paduano

Aims

Rationalisation of the aggregation process of poly(vinyl alcohol) in the presence of sodium chloride, thermodynamical characterization of polymer solutions and structural properties of PVA particles obtained through salting-out.

Results

Poly(vinyl alcohol) (PVA) is a biocompatible water-soluble polymer of great interest thanks to its large-scale applications as a material for drug-delivery systems or for building sensors and membranes with selective permittivity. The cryogenic route is one of the most studied and widely employed techniques for the preparation of PVA physical hydrogels [1]: the advantages of such gels is the absence of toxic chemicals for their preparation and the consequent possibility to obtain a completely eco-friendly product [2].

In this work we propose a new route for the preparation of PVA-based microgels through the salting-out effect: after a screening of different salts belonging to the Hofmeister series, sodium chloride represented the best cosmotropic species to use in order to favour the polymer aggregation over a reasonable time-scale.

The thermodynamic properties and the kinetics of the aggregation process were deeply studied through a combined Dynamic Light Scattering (DLS), Static Light Scattering (SLS) and Small Angle Neutron Scattering (SANS) study, which allowed rationalising how such process is influenced by different parameters like salt molality, polymer concentration and time from the preparation (fig. 1).

Moreover, we were able to shed light on the structural and morphological properties of PVA particles, showing the role of the salt in the aggregation process and its effect on the supramolecular organization. In particular, we determined the molecular weight and the radius of gyration of the aggregates and we estimated the packing degree of polymer chains within the aggregates, strongly influenced by the time and the salt concentration.

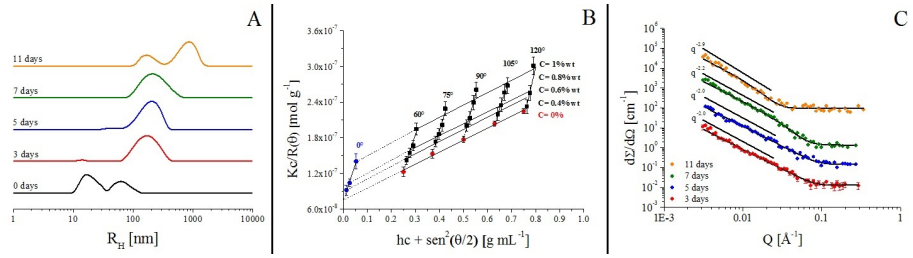


Fig. 1: PVA 1% wt, NaCl 2 mol kg-1: study of the evolution of hydrodynamic radii over time by DLS (panel A); Zimm plot obtained from SLS measurements (panel B); SANS results at different times from the preparation (panel C).

References

[1] Mangiapia, G.; Ricciardi, R.; Auriemma, F.; De Rosa, C.; Lo Celso, F.; Triolo, R.; Heenan, R.K.; Radulescu, A.; Tedeschi, A.; D'Errico, G.; Paduano, L. "Mesoscopic and microscopic investigation on poly(vinyl alcohol) hydrogels in the presence of sodium decylsulfate", J. Phys. Chem. B 111, 2166-2173 (2007).
[2] Nayak, S.; Lyon, A. "Soft nanotechnology with soft nanoparticles", Angewandte Chemie 44, 7686-7708 (2005).

1B - Neuroprotective effect of poly-unsaturated fatty acids: structure, dynamics and interaction with amyloid peptides of Omega-3 containing lipid bilayers

A. De Santis, G. D'Errico, L. Paduano

Aims

Evaluation of the Effect of Docosahexaenoic Acid on the dynamics and structures of lipid bilayers and on the interaction with peptides.

Results

Among the Omega-3 Poly Unsaturated Fatty Acids (PUFA), DocosaHexaenoic Acid (DHA) is the most important one found in cell membrane; indeed it has a pivotal role in the prevention of cardiovascular diseases and cancer and exerts a strong neuroprotective effect [1,2].

Omega-3 fatty acids were proposed to alter the physicochemical features of the membrane, once converted to phospholipids, and/or to segregate cholesterol molecules in liquid ordered domains (L_o), typically associated to the lipid rafts [3]. However, their mechanism of action is still elusive.

With the aim to understand the functional role of DHA, we investigate the influence of dipolyeneOmega3-PC (one of the possible phospholipids containing DHA) on the micro-structural properties and phase behaviour of a lipid membrane composed by 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC), Cholesterol (Chol) and Omega3-PC**.** The physico-chemical techniques employed are Electron Spin Resonance (ESR) spectroscopy with the spin-labelling approach and Neutron Reflectivity (NR).

Moving from the characterization of the lipid system, we attempt to rationalize the PUFA effect on peptide/lipid interaction, focusing on the neuroprotective effect of Omega3-PC. Through a combined ESR and Circular Dicroism (CD) study of the interaction between the Alzheimer peptide Aβ-(1–42) and a PUFA containing lipid bilayer, we show that the higher the Omega-3 lipid content the higher the membrane-peptide interaction (Figure 1) and that this interaction effectively prevent peptide aggregation. These results suggest that Aβ-(1–42) selectively interacts with DHA containing membranes and may provide hints for mechanism and therapy of Alzheimer disease [4].

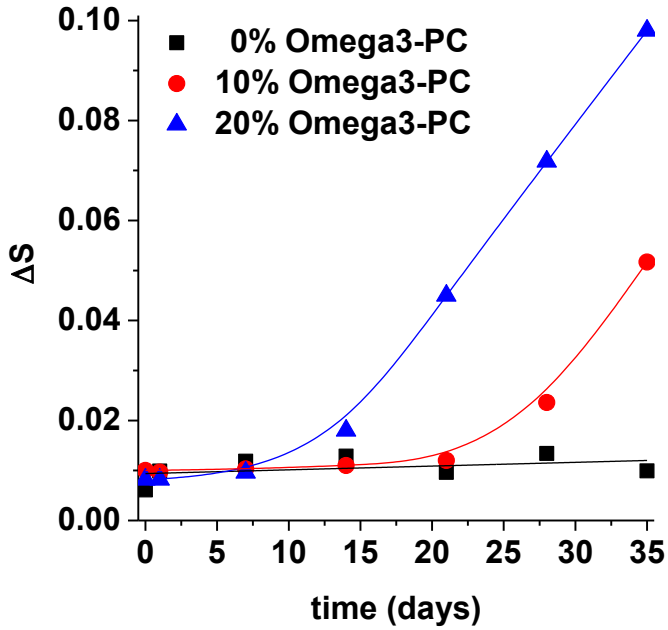


Fig. 1: Variation of the order parameter, S, in the inner apolar region of the bilayer over time, upon Aβ 1-42 peptide addition, for three lipid bilayers with increasing amount of Omega3-PC.

References

[1] Lavie, C.J.; Milani, R.V.; Mehra, M.R.; Ventura, H.O. "Omega-3 Polyunsaturated Fatty Acids and Cardiovascular Diseases", J. Am. Coll. Cardiol. 54, 585-594 (2009).

[2] Lukiw, W.J.; Cui, J.G.; Marcheselli, V.L.; Bodker, M.; Botkjaer, A.; Gotlinger, K.; Serhan, C.N.; Bazan, N.G. "A role for docosahexaenoic acid-derived neuroprotectin D1 in neural cell survival and Alzheimer disease", J. Clin. Invest. 115, 2774-2783 (2005).

[3] Georgieva, R.; Chachaty, C.; Hazarosova, R.; Tessier, C.; Nuss, P.; Momchilova, A.; Staneva, G. "Docosahexaenoic acid promotes micron scale liquid-ordered domains. A comparison study of docosahexaenoic versus oleic acid containing phosphatidylcholine in raft-like mixtures", Biochim. et Biophys. Acta. 1848, 1424-1435 (2015).

[4] Emendato, A.; Spadaccini, R.; De Santis, A.; Guerrini, R.; D'Errico, G.; Picone, D. "Preferential interaction of the Alzheimer peptide A beta-(1-42) with Omega-3-containing lipid bilayers: structure and interaction studies", FEBS Lett. 590, 582-591 (2016).

1B – Characterization of protein-NPs interaction and development of aptamer functionalized NPs

I. Russo Krauss, G. D'Errico, L. Paduano

Aims

Development of different nanoparticles as selective therapeutic and theranostic agents for biomedical applications.

Results

We investigated the interaction between superparamagnetic nanoparticles (NPs) bearing a double layer of oleic acid/oleylamine and the lysophosphatidylcholines 18LPC with different model and serum proteins, including hen egg white lysozyme, human transferrin and human serum albumin (HSA).

Effect of NPs on the small model protein lysozyme where negligible, with no effect on thermal stability of secondary and tertiary structure up to 2 days of incubation. Furthermore no clear indication of the formation of a protein corona was obtained. In the case of human transferrin, effect on the tertiary structure of the protein and formation of protein-NP aggregates where observed only upon 24 h when a 1:50 NP-protein molar ratio was investigated. Analysis on the HSA-NP system are in progress. Results collected up to now indicate a high biocompatibility of the NP system encouraging its use for biomedical applications.

At the same time we started a research line aimed at functionalize different NPs with DNA aptamer able to recognize an important biomedical target and to exert a therapeutic effect. We were able to functionalize silica NPs with a modified thrombin binding aptamer obtaining a powerful anticoagulant agent. Now we are designing hydrophobically modified aptamers to be bound on the double layer of the superparamagnetic NPs.

1B – Effect of Cardiolipin on Lipid Bilayers

A. Luchini, G. Vitiello, L. Paduano

Aims

Characterization of the effect of Cardiolipin on the structure of supported lipid bilayers in the presence of divalent ions (i.e. Ca^{2+}).

Results

The effect of CL on lipid bilayers composed by POPC and POPE in the presence and in the absence of Ca^{2+} ions has been preliminary characterized by means of Quartz-Crystal Microbalance with Dissipation monitoring (QCM-D). In these experiments the vesicle suspension were prepared in phosphate buffer (pH=7.4) with 130 mMNaCl and KCl, to which eventually 1mM $CaCl_2$ was added. The frequency shift (ΔF, evaluated from the quartz support harmonic n=3) for POPE/POPC system in the presence of 1mM $CaCl_2$ corresponds to -28 and indicates the formation of a lipid bilayer. On the other hand, in the POPE/POPC/CL system, as well in the presence of 1mM $CaCl_2$ (Figure 1, panel a), the ΔF is -35 and the different harmonics are not well superimposed (the sample does not oscillate in phase with the support). These evidences suggest that CL is responsible for a different organization of the phospholipids. The effect of 1mM $CaCl_2$ on lipid bilayer prepared with POPE, POPC and CL (40/40/20 w/w/w) was investigated by means of Neutron Reflectometry measurements (Figure 2). Even at this low concentration of $CaCl_2$ there is a detectable effect of the presence of the Ca^{2+} ions in all the explored contrasts (D_2O, H_2O and SMW). By the comparison of the experimental data it is visible a change in the shape of the curves around 0.05 and 0.16 A^{-1} that can be interpreted in a thickening of the bilayer in presence of calcium salts. All together the collected results indicate that there is an interesting effect of CL on the organization of POPE and POPC lipids both in the presence and in the absence of $CaCl_2$; this effect requires further investigation planned in the future experiments.

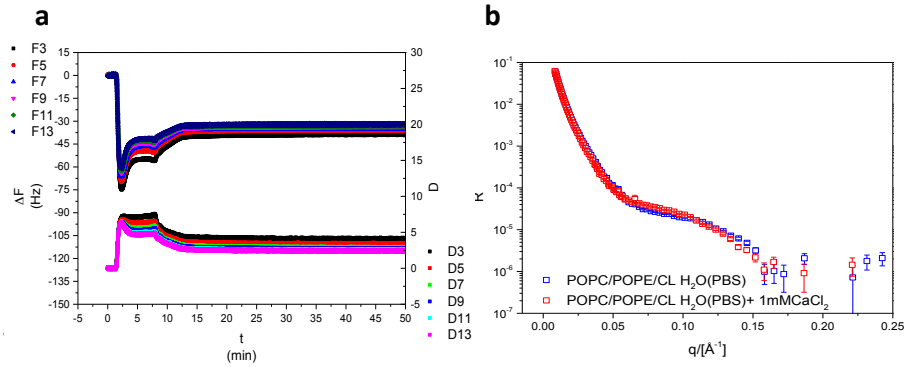


Fig. 1: QCM-D data collected for POPE/POPC/CL (40:40/20 w/w/w) in PBS + 1mM $CaCl_2$ (panel a); NR data collected during the test on FIGARO for the POPE/POPC/CL in H_2O buffer (blu curve) and POPE/POPC/CL in H_2O buffer +1mM $CaCl_2$ (red curve).

1B – Bioinspired eumelanin-based nanomaterials for antimicrobial applications

G. Vitiello, A. Pezzella, G. D'Errico, M. Varcamonti (Department of Biology, University of Naples "Federico II", Naples, Italy), G. Luciani

Aims

Design, synthesis and physico-chemical characterization of hybrid Eumelanin-TiO_2 nanomaterials with antimicrobial properties.

Results

Organo-inorganic hybrids, made by coupling inorganic phases to organic molecules, not only combine the often dissimilar characteristics of inorganic and organic components into one material, but often show unique and peculiar properties. This provides the opportunity to invent a huge set of new multifunctional materials with a wide range of applications in the fields of energy, health and electronics.

Herein, we provide a novel synthesis approach to hybrid materials whereby inorganic semiconductor materials are employed as catalysts and structure directing agents in biopolymers building up.

Following this bioinspired synthesis strategy, TiO_2 photocatalytic activity was exploited to drive 5,6-dihydroxyindole-2-carboxylic acid (DHICA) polymerization to eumelanin via complex mediated electron transfer (LMCTC) from DHICA to the TiO_2 lattice, that enables photo-activation under visible light [1-3]. This strategy led to eco-friendly melanin-TiO_2 hybrid nanostructures with unique antimicrobial activity even under visible light [2]. Mechanism underlying formation of Melanin-TiO_2 nanoparticles was outlined by integrating Photolumiscence (PL), UV-Vis, Electron Paramagnetic Resonance (EPR) and Solid-phase Nuclear Magnetic Resonance (NMR) spectroscopies [1] (Figure 1).

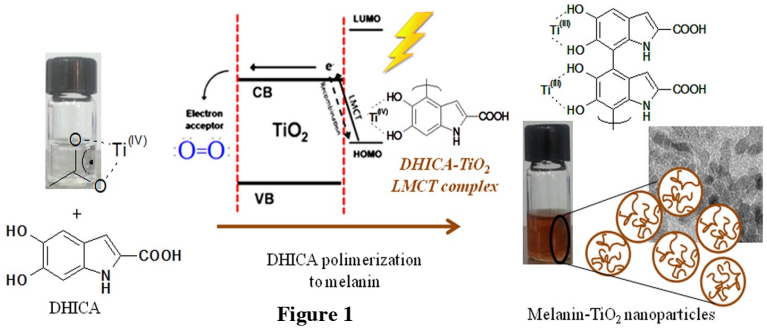


Figure 1

DHICA polymerization to eumelanin was confirmed by EPR spectrum of nanostructures, showing a single central symmetric peak at a *g*-factor value of 2.0035 ± 0.0004, which is typical of carbon-centered radicals in melanin backbone.

Furthermore, a characterization by multiple techniques allowed to link physico-chemical properties of these nanosystems to their relevant biocide efficacy. Actually, both organic and inorganic phases strongly affect each other during *in-situ* formation, as far as it concerns both morphology and microstructure. DHICA polymerization

onto TiO_2 changes final morphology of TiO_2 nanostructures, as shown by TEM micrographs (Figure 2).

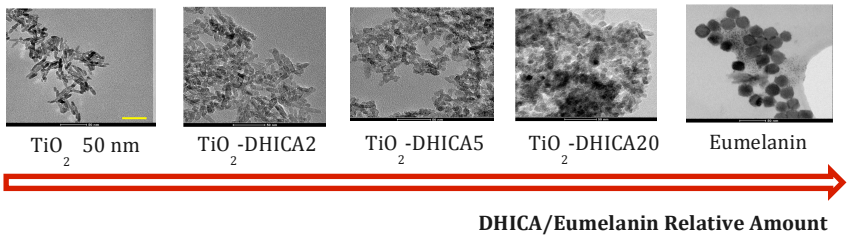


Fig. 2: TEM micrographs of bare TiO_2, TiO_2-DHICA and Eumelanin nanoparticles.

Furthermore, narrower ΔB values than bare melanin, driven from EPR spectra indicate a different spatial distribution of radical species within the hybrids, suggesting that the presence of TiO_2-sol modulates the melanin macromolecule organization, allowing an enhanced antimicrobial activity (Figure 3).

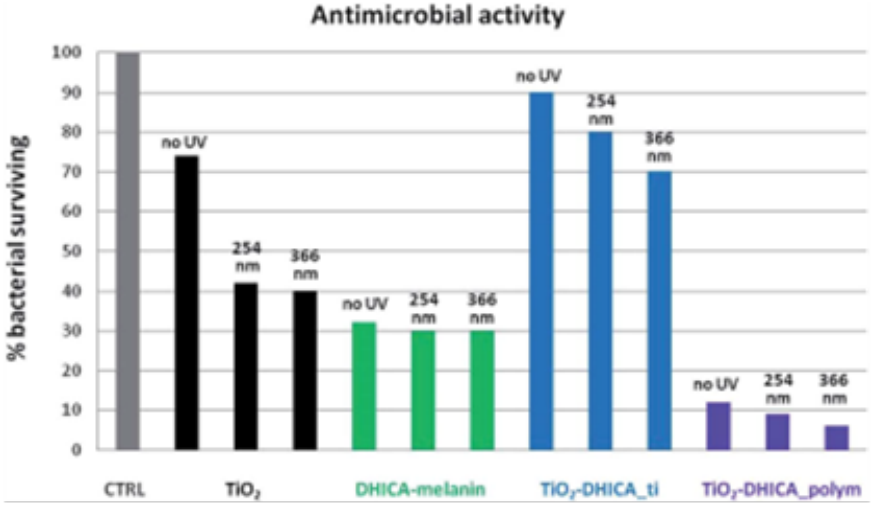


Fig. 3: Antimicrobial activity of TiO_2, DHICA-melanin and hybrid TiO_2-DHICA nanoparticles.

References

[1] Pezzella, A.; Capelli, L.; Costantini, A.; Luciani, G.; Tescione, F.; Silvestri, B.; Vitiello, G.; Branda, F. "Towards the development of a novel bioinspired functional material: Synthesis and characterization of hybrid TiO2/DHICA-melanin nanoparticles", Mater. Sci. Engin. C 33, 347-355 (2013).

[2] Vitiello, G.; Pezzella, A.; Zanfardino, A.; Varcamonti, M.; Silvestri, B.; Costantini, A.; Branda, F.; Luciani, G. "Titania as a driving agent for DHICA polymerization: a novel strategy for the design of bioinspired antimicrobial nanomaterials", J. Mater. Chem. B 3, 2808-2815 (2015).

[3] Vitiello, G.; Pezzella, A.; Calcagno, V.; Silvestri, B.; Raiola, L.; Costantini, A.; D'Errico, G.; Branda, F.; Luciani, G. "5,6-Dihydroxyindole-2-carboxylic-Acid-TiO2 Charge Transfer Complexes in the Radical Polymerization of Melanogenic Precursor(s)", J. Phys. Chem. C 120, 6262-6268 (2016).

1B – Protein trapping within nanostructured surface

G.M.L. Messina, G. Marletta

Aims

The development of a new technique enabling the fabrication of large area patterns of polymeric nanowell arrays on flat metallic surfaces, with high yield, controllable thickness, and high uniformity over large areas is described.
In particular, the proposed methodology can provide both homogenous or hybrid nanowells, providing an optimal solution to the problem of how to easily construct biosurfaces that are able to communicate with biological systems in the 'correct' way, allowing selective trapping of specific biomolecules as well as influencing their partial or complete orientation and unfolding, and finally affecting their biofunctionality.

Results

Nanostructured surfaces have generated great interest because their size, shape and local composition properties, being compatible with those of biological molecules and systems, promise in principle the manipulation of biological processes at subcellular level.
The build-up of nanostructured surfaces has been obtained by means of a large number of top-down methodologies, like photo-, electron- and ion-beam lithography, producing structures with dimensions far below 100 nm. However, these methods have the considerable drawback of involving serial and cost-consuming processes, suitable only for small area treatments.

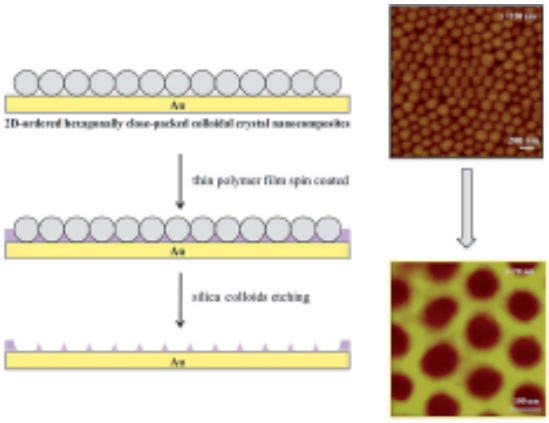


Fig. 1: Schematic representation of the procedure applied for the preparation of the nanocavity array (PMMA on Au).

Alternatively, recent research has identified the use of self-assembly processes, operating in a parallel way, as the most promising way to achieve surface nano-structuring for large areas.
These methods, globally referred to as colloidal lithography, have shown great potential to significantly improve the performance of biosurfaces.
We describe a simple and versatile method to obtain large-scale arrays of hybrid polymer/gold nanowells, able to selectively trap different types of molecules, including drugs and proteins. The appropriate choice of materials and process

conditions, such as the colloidal nanoparticle size and the post-deposition treatments (i.e., the UV-ozone), allows the volume of each nanowell to be turned and, in turn, the overall trapping capability of arrays of nanowells of given size. This implies the possibility of further developing bioactive surfaces, i.e., surfaces able to modulate the local concentration of bioactive molecules, capable of interacting with the nanometric features of cells.

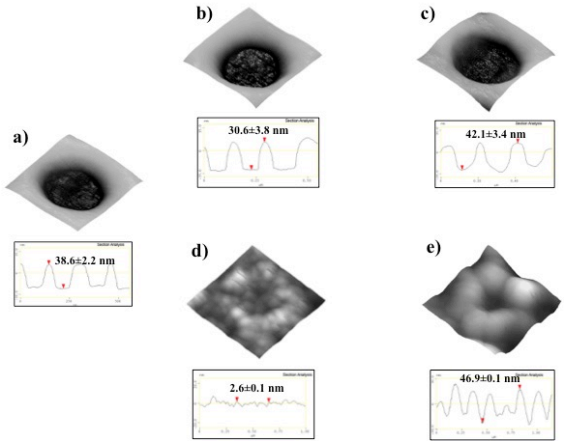


Fig. 2: AFM height images and corresponding section analysis for: (A) bare nanowell arrays, (B) nanowell arrays exposed to HSA, (C) nanowell arrays exposed to Lyz, (D) AbB HSA on HSAB containing nanowell arrays and (E) AbBLyz on nanowell exposed to Lyz.

It should be further stressed that, besides the practical interest of having bioactive surfaces, the reported results open up a wide and still little explored field of study, regarding new nanoconfinement-related properties.

Indeed, the observed counterintuitive trapping of a large protein, such as HSA, versus the untrapping of a smaller protein, like Lyz, must be considered a peculiar feature due to nanoconfinement. The proposed explanations for the phenomenon range from the nanoconfinement-induced decrease in the out-diffusion coefficient of large trapped biomolecules, to the preferential sticking of unfolded single protein molecules, to the modulation of conformational rearrangement due to the soft-hard nature of the different proteins. In fact, much more experimental and theoretical work is needed to propose a satisfactory model relating the nanoconfinement constraints to the peculiar protein behaviour. Thus, for instance, the study of the behaviour of proteins featuring similar size and overall charge could shed light on the dependence of the trapping selectivity effect on the protein softness/hardness. According to the above, we suggest that the reported results may pave the way for the construction of a new generation of bioactive surfaces, able to perform a range of actions, from filters discriminating hard–soft proteins, to more general conformationally modified biomolecules, to local providers of biosignalling molecules.

References

Messina, G.M.L.; Passiu, C.; Rossi, A.; Marletta, G. “Selective Protein Trapping within Hybrid Nanowells”, Nanoscale 8 16511-16519 (2016).

Messina, G.M.L.; De Zotti, M.; Lettieri, R.; Gatto, E.; Venanzi, M.; Formaggio, F.; Toniolo, C.; Marletta, G. “Design of lipidic platforms anchored within nanometric cavities by peptide hooks”, RSC Advances 6 46984-46993 (2016).

1B – Role of polymer molecular weight on the removal process using amphiphilic formulations

M. Raudino, G. Selvolini, P. Baglioni

Aims

Study of the interaction between a non-ionic surfactant ternary system and a thick polymer film. Effect of polymer molecular weight on the rate and the efficacy of polymer dissolution.

Results

Polymer dissolution plays a key role in a wide variety of practical applications, from industrial processes to biomedical applications and, recently, in conservation science for the removal of hydrophobic polymeric films used as consolidants. Amphiphilic formulations (micellar solutions or o/w microemulsions) are usually use as efficient cleaning media but the comprehension of the main parameters affecting the mechanism of polymer removal is still limited because of the complexity of the process.

We investigate for the first time the overall interaction process between a thick polymeric film and a water/2-butanone/non-ionic surfactant ternary system by combining different techniques, mainly confocal microscopy. Our results indicate that the cooperation between the surfactant and the organic solvent is necessary to ensure good cleaning performances to the formulation. Furthermore, this experimental approach allows to clarify different aspects of the cleaning process, such as the role of polymer molecular weight on the mechanism and the kinetics of the process.

Confocal scans acquired on polyvinyl acetates with molecular weight ranging from 75 to 855 kDa incubated with the cleaning fluid reveal that the interaction mechanism between the polymer and the liquid phase strictly depends on the molecular weight and the chain entanglement of the polymeric network: low M_w systems undergo polymer removal, while for higher M_w polymers only a partial swelling of the film occurs.

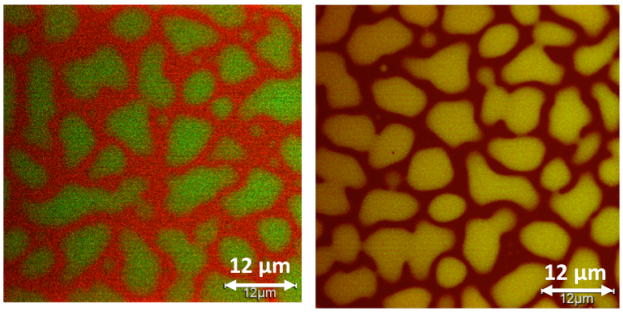


Fig. 1: Confocal horizontal scans obtained on low M_w (left) and high M_w (right) polyvinyl acetate films (red) incubated with water/non-ionic surfactant/2-butanone ternary system (green).

By analysing several confocal images of the film acquired at different incubation times with the liquid phase, we have seen that the removal efficacy strongly depends on the chain entanglement: the higher the M_w and so the entanglement of the polymeric network is, the lower is the efficacy of the cleaning medium in the detachment of the polymer from the substrate. In addition, we have observed that polymer polydispersity plays a key role in the overall removal process since it strongly affects the removal rate. In fact, polydisperse systems (in our case high M_w polymers) show a faster dissolution rate with respect to less disperse polymers probably due to an enhancement of the velocity of solvent penetration inside the polymeric network through defects.
Our results are in good agreement with the findings of literature on simple systems consisting of polymeric films in contact with good solvents and this is the first time that the influence of both M_w and polydispersity on the removal process of polymeric films is studied using complex amphiphilic formulations as cleaning media instead of neat organic solvents. Moreover, we have demonstrated that the new experimental method based on the use of confocal microscopy developed in this work can be a valuable approach to clarify the process of cleaning also in the case of complex systems.

References

Baglioni, M.; Raudino, M.; Berti, D.; Keiderling, U.; Bordes, R.; Holmberg, K.; Baglioni, P. “Nanostructured Fluids from Degradable Nonionic Surfactants for the Cleaning of Works of Art from Polymer Contaminants”, Soft Matter 10, 6798-6809 (2014).
Raudino, M.; Selvolini, G.; Montis, C.; Baglioni, M.; Bonini, M.; Berti, D.; Baglioni, P. “Polymer Films Removed from Solid Surfaces by Nanostructured Fluids: Microscopic Mechanism and Implications for the Conservation of Cultural Heritage”, ACS Appl. Mater. Interfaces 7, 6244-6253 (2015).

1B – Structure-property relation in oil soluble dispersants for lubricant media

G. Ferraro, E. Fratini, R. Rausa (Eni S.p.A. Research & Technological Innovation Department, San Donato Milanese, Italy), P. Baglioni

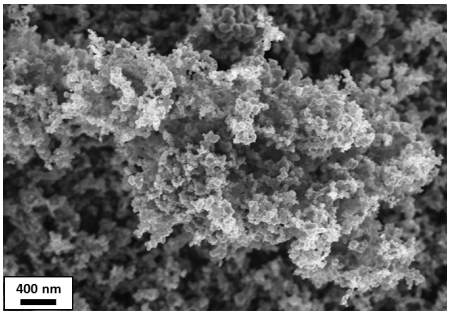
Aims

Colloidal behavior of nonionic surfactant in mineral oil. Microstructure and composition of carbonaceous deposits in lubricant media.

Results

The main objective of this work is to develop a model to connect the structural properties of dispersant additives with their efficacy against the agglomeration of carbonaceous particulates in lubricant formulations. Usually, dispersant performances are evaluated by means of expensive and time-consuming engine tests; for this reason, the research of new lab-scale methodologies to evaluate the performances of a lubricant formulation is compulsory. To accomplish this goal, we optimized different methodologies to study both the colloidal properties of the additives and their dispersant efficacy in model systems that mimic a lubricant oil. The final goal is to establish a structure-properties relation and concurrently understand the main factors affecting the dispersant ability of an additive.

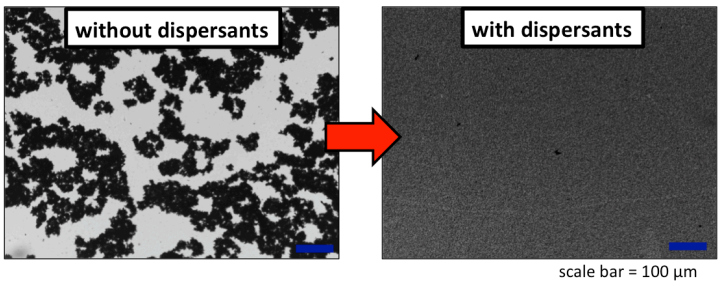
The first step of the work is the identification of a carbonaceous particulate, mainly carbon blacks, to use as a model substrate. We have separated a soot-in-oil particulate and characterized it in terms of composition (elemental analysis and infrared spectroscopy), morphology (scanning electron microscopy) and fractal dimension (small angle X-ray scattering) against commercially available carbon blacks. We found that this particulate has globular primary units with diameter ranging from 5 to 80 nm, which cluster to form aggregates.



From a compositional point of view, the particulate is mostly composed of carbon. Other elements, such as hydrogen and oxygen, are usually present in small quantities and tend to concentrate on the surface of the particle. Comparing the properties of the isolated soot with those of different commercial particulates, Vulcan XC72 was chosen as the model substrate.

The second step of the work is the study of the properties of a minimal lubricant formulation (base oil + dispersants): adsorption isotherms and optical microscopy were employed to evaluate the interaction between different dispersants and the carbonaceous substrate. In particular, we have studied a series of dispersants with different length of polar head and different number of alkyl chains. Our results indicate that, depending on the chemical nature of the amphiphile, the adsorption follows a mono-Langmuir or a di-Langmuir mechanism and the strength of the

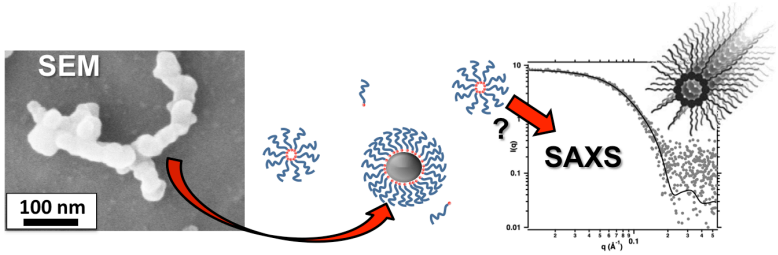
interaction increases with the surface area of the polar head. Moreover, from optical dispersion tests, the main evidences are that mono-dispersants are less efficient than bis-dispersants and their performances are strictly connected to the dimension of the polar portion. From small angle X-ray scattering measurements, we have found that all amphiphiles form inverse cylindrical micelles in oil with dimensions depending on the volume of the polar fraction of the dispersant.



The aggregation number for mono-dispersants is higher if compared to bis-dispersants: this is an evidence of the higher solubility of bis-surfactants in oil, driving their higher efficacy as compared to mono-structures.

The same kind of approach was repeated in the case of complex formulations (oil + dispersants + other additives) with the aim to understand if and how the presence of other additives influences the efficacy of the dispersants. From dispersions tests we have shown that, increasing the complexity of the formulation, the dispersant efficacy decreases significantly, especially in presence of detergents and antiwear agents. This is a clear confirmation that the interaction between the dispersants and the other additives inside the lubricant formulation causes a depletion of the active dispersant fraction in the oil.

The results of this study represent an advancement in the knowledge of lubricant chemistry and in the comprehension of the main parameters affecting the dispersant performances of different kinds of amphiphilic molecules. The simple developed lab-scale methodologies can be surely useful to rank different structures of dispersants in simple and complex lubricant oils to screen these formulations before expensive motor tests. Moreover, the correlation between the colloidal behavior of the amphiphiles and their dispersant efficacy can be used to guide the synthesis of novel oil soluble dispersants with enhanced activity against the carbonaceous particulate deposition in lubricant media.



References

Ferraro, G.; Fratini, E.; Rausa, R.; Fiaschi, P.; Baglioni, P. “Multiscale Characterization of Some Commercial Carbon Blacks and Diesel Engine Soot”, Energy Fuels 30, 9859-9866 (2016).

Ferraro, G.; Fratini, E.; Rausa, R.; Baglioni, P. “Investigation of the Diesel Soot Morphology as a function of the oil aging”. Submitted for publication.

1B – Relation between structural and diffusional properties in classical and semi-IPN hydrogels

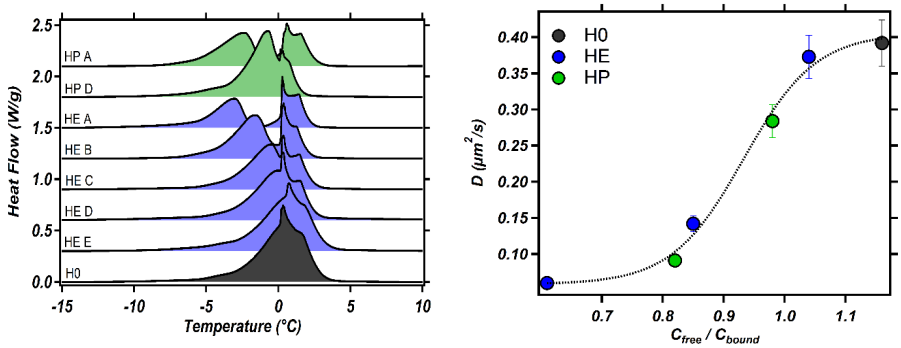
M. Rossi, G. Ferraro, E. Fratini, P. Baglioni

Aims

Synthesis and characterization of pHEMA classical and semi-interpenetrating with poly acrylic acid hydrogels. Diffusion processes of molecules and macromolecules in gels.

Results

We synthesized and characterized classic poly HEMA and semi-interpenetrating poly HEMA/PAA hydrogels having different cross-linker/monomer ratio. These differences affect the network structure and the diffusional properties of the hydrogels. Considering poly HEMA hydrogels, an increase of cross-linker percentage doesn't significantly change the nanoscale structure of the polymeric network while decreasing the free/bound water ratio (Cfree/Cbound) (left figure) and the diffusion coefficient of the molecular probe, fluorescein isothiocyanate (FITC). A sigmoidal trend of the diffusion coefficient vs Cfree/Cbound (right figure) indicates that the diffusion becomes completely activated only when the hydrogel reaches a water-percolated state.



Two series of semi-IPN poly HEMA/PAA were synthesized, one with the same ratio 8:1 between HEMA hydroxyl groups and PAA carboxylic groups and different water content (38%, 50%, 60%), the other with a water content of 38%, but different HEMA/PAA ratio (i.e. 8:1, 4:1, 2:1). SAXS analysis reveals the existence of solid-like inhomogeneity and, in the case of HEMA/PAA 8:1 series, FITC and FITC dextran 4 kDa can enter all these three hydrogels, while FITC-dextran 40 kDa can penetrate only the network with 60% H_2O. In the case of poly HEMA/PAA 4:1 and poly HEMA/PAA 2:1, it was possible to establish that FITC, FITC-dextran 4 kDa and FITC-dextran 40 kDa can diffuse into both networks. The diffusion coefficients increase with the water content and with the decrease of the amount of PAA, as the result of a lower interaction between the probes and the polymeric network.
All the results taken together provide a complete picture of the relationship between the structure, water state and diffusional properties in poly HEMA classical and semi-IPN hydrogels.

References

Wu, Y.; Joseph, S.; Aluru, N.R. "Effect of Cross-Linking on the Diffusion of Water, Ions, and Small Molecules in Hydrogels", J. Phys. Chem. B 113, 3512-3520 (2009).
Kanayaa, T.; Takahashib, N.; Nishidaa, K.; Setoc, H.; Nagaod, M.; Takebae, Y. "Dynamic and static fluctuations in polymer gels studied by neutron spin-echo", Physica B 385-386, 676-681 (2006).
Garcia, O.; Dolores Blanco, M.; Martìn, J.A., Teijòn, J.M. "5-Fluorouracil trapping in poly(2-hydroxyethyl methacrylate-co-acrylamide) hydrogels: in vitro drug delivery studies", European Polymer Journal 36, 111-122 (2000).

1B – Biomimetic membranes and interaction with nanosystems

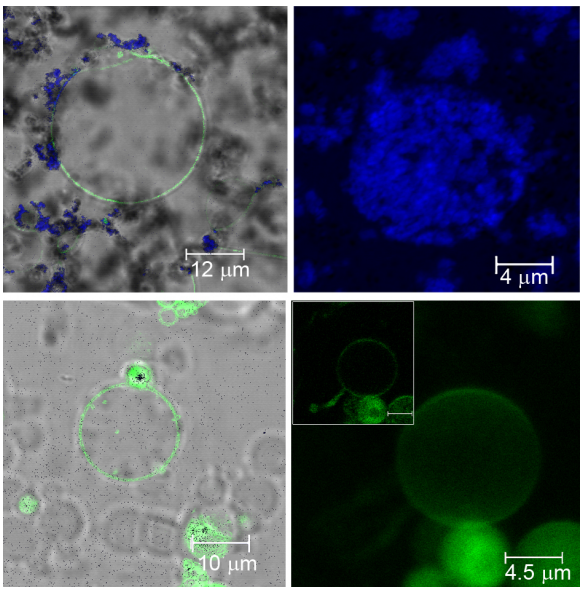
C. Montis, D. Berti, P. Bergese

Aims

Build-up reliable biomimetic membranes, capable to mimic both eukaryotic and prokaryotic cell membranes, to investigate their interaction with exogenous species, particularly nanosystems of interest for biomedical applications.

Results

Nanosystems have highly promising applications in Nanomedicine. A key issue, limiting their translation into effective application, is that the understanding of their fate in biological media and of their interaction with biological interfaces is still lacking. In this respect, artificial, biomimetic membranes have been developed. They permit working with simplified systems, and are good models to decompose the elementary events (biochemical, physical, and chemical) at stake in real biological situations.



We built-up different membrane models, of different architecture and curvature (liposomes, Giant Unilamellar Vesicles, Supported Lipid Bilayers) mimicking selected features of interest of eukaryotic and prokaryotic cells. The physicochemical characteristics of the membranes were determined in terms of morphology, structure, fluidity and permeability through Scattering methodologies (Dynamic Light Scattering, Small-angle X-ray Scattering), Steady state Fluorescence, Confocal Microscopy, Fluorescence Correlation Spectroscopy. Their interaction with exogenous species was then investigated with the same techniques, in particular: the effects of gold nanoparticles of different surface functionalization on Giant Unilamellar Vesicles; the reconstitution of membrane proteins in lipid membranes, the interaction of a nanostructured antimicrobial system with synthetic lipid membranes mimicking relevant features of prokaryotic cells.

References

Montis, C.; Maiolo, D.; Alessandri, I.; Bergese, P.; Berti, D. "Interaction of nanoparticles with lipid membranes: a multiscale perspective", Nanoscale 6 (12), 6452-6457 (2014).

Smeazzetto, S.; Tadini-Buoninsegni, F.; Thiel, G.; Berti, D.; Montis, C. "Phospholamban spontaneously reconstitutes into giant unilamellar vesicles where it generates a cation selective channel", Phys. Chem. Chem. Phys., 18, 1629-1636 (2016).

Marin-Menendez, A.; Montis, C.; Diaz-Calvo, T.; Carta, D.; Hatzixanthis, K.; Morris, C.J.; McArthur, M.; Berti, D. "Antimicrobial Nanoplexes meet Model Bacterial Membranes: the key role of Cardiolipin", Scientific Reports 7, 41242 (2017).

1B – Lipid-SPIONs mixed assemblies as smart drug delivery systems

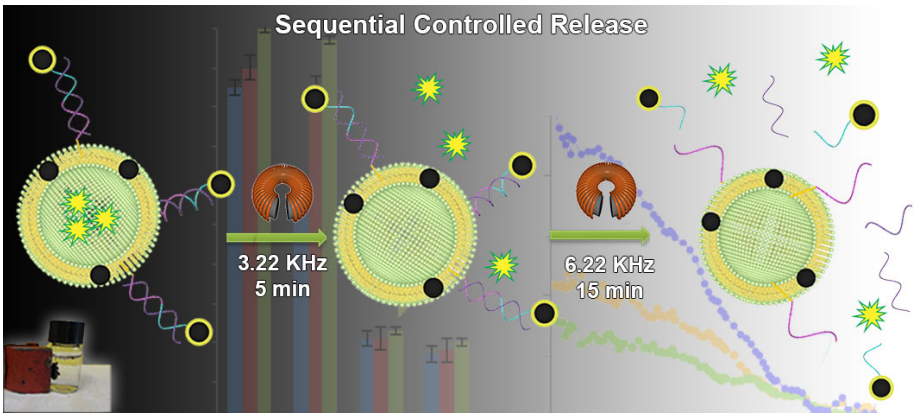
A. Salvatore, C. Montis, M. Mendozza, B. Castroflorio, D. Berti, P. Baglioni

Aims

Build-up smart drug delivery systems of lipid architectures with Superparamagnetic Iron Oxide Nanoparticles (SPIONs) embedded, responsive to different static and alternating magnetic fields in a tunable manner.

Results

The design of nanostructured drug delivery systems (DDS) that improve the efficacy of therapeutic principles by enhancing their biocompatibility, bioavailability and targeting, has been the focus of extensive research over the past years. Of particular relevance in this field is the development of multifunctional architecture that can deliver different therapeutic or diagnostic agents and release them in a controlled way.



In this context we designed, prepare and characterize DDS where hydrophilic and hydrophobic superparamagnetic iron oxide nanoparticles (SPIONs) are included in pure lipid and lipid-DNA mixed architectures to build-up multifunctional drug delivery systems, able to release their payload in a controlled way, through the application of low-frequency alternating magnetic fields of defined frequencies.

References

Montis, C.; Castroflorio, B.; Mendozza, M.; Salvatore, A.; Berti, D.; Baglioni, P. "Magnetocubosomes for the delivery and controlled release of therapeutics", JCIS 449, 317-326 (2015).

Salvatore, A.; Montis, C.; Berti, D.; Baglioni, P. "Multifunctional Magnetoliposomes for Sequential Controlled Release", ACS Nano 10, 7749-7760 (2016).

1B – Poly(ethylene glycol)-*graft*-poly(vinyl acetate) single-chain nanoparticles for the encapsulation of small molecules

A. Bartolini, P. Tempesti, C. Resta, D. Berti, P. Baglioni

Aims

Synthesis and Characterization of single chain nanoparticles (SCNPs) of poly(ethylene glycol)-*graft*-poly(vinyl acetate). Use of the so-obtained single-chain globular particles to encapsulate small hydrophobic molecules therefore promoting solubilization of flavors or drugs, which could be of interest in the food and pharmaceutical industry.

Results

This work focused on the preparation of SCNPs composed of a poly(ethylene glycol)-*graft*-poly(vinyl acetate) (PEG-g-PVAc) amphiphilic copolymer, with a very low degree of grafting. This peculiar chemical structure allows for the folding of PEG over the PVAc side chains, triggering the formation of single-chain globular objects driven by hydrophobic interactions. Both light and X-ray scattering experiments show that at 25 °C aggregation is negligible even at concentrations up to 10% w/w. When in the folded state, the hydrophobic core of these SCNPs acts as a storage compartment for small hydrophobic molecules of interest, *e.g.* flavors or drugs.

First of all, we studied the behaviour of PEG-g-PVAc aqueous solutions at different concentrations.

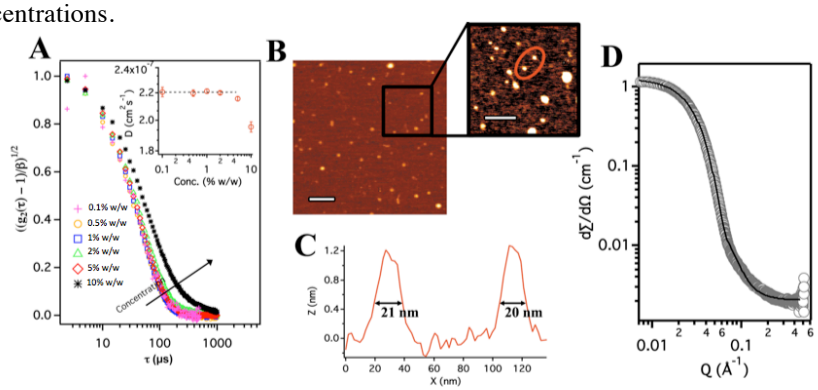


Fig. 1: (A) Autocorrelation functions of PEG-g-PVAC at various concentrations in water measured at 90°: Inset shows the diffusion coefficients obtained at different concentrations. (B) AFM image of PEG-g-PVAc SCNPs (scale bar is 200 nm, inset bar is 100 nm). (C) AFM line profile of two PEG-g-PVAc SCNPs highlighted in the inset of B (red ellipse). (D) SAXS data for sample AP1 together with the fit (black solid line).

DLS experiments (Fig. 1A) show the normalized autocorrelation functions at concentrations ranging from 0.1 to 10% w/w. The curves show the presence of one relaxation process and are superimposable up to 5% w/w. The hydrodynamic radii, obtained from the data analysis of the autocorrelation functions is invariant with concentration up to 5% w/w. This fact is indicative of the presence of PEG-g-PVAc SCNPs.[1]

AFM measurements (Figure 1B) show the presence of spherical objects with a diameter of about 20 nm (Figure 1C). Furthermore from the SAXS curve reported in Figure 2D we calculated the molecular weight of the scattering particles using the following equation:[2]

$$M_w = I(0)N_a/(\Delta\rho)^2 cv \quad (1)$$

where *I(0)* is the forward scattering intensity *i.e.*, the intensity at the lowest Q-values, $\Delta\rho^2$ is the contrast factor, N_a is Avogadro's number, c is the concentration in g mL^{-1}, and v is the polymer's specific volume in mL g^{-1} (calculated considering a 40/60% PEG/PVAc ratio). In this way a molecular weight of 10.8 kDa is obtained, which is in very good agreement with the molecular weight of a single PEG-g-PVAc molecule.

Once demonstrated the PEG-g-PVAc ability to self-fold into SCNPs, we exploited the hydrophobic nature of the core by encapsulating small molecules of interest that possess a low solubility in water. We focused on food grade molecules such as R-(+)-Limonene, p-Anisaldehyde and Terpinyl Acetate.

The fittings of the DLS autocorrelation functions of the flavor-loaded samples, shown in Figure 2A, result in an increase of the hydrodynamic radii of the particles up to 135%, indicative of an upload of molecules inside the core of the SCNPs.

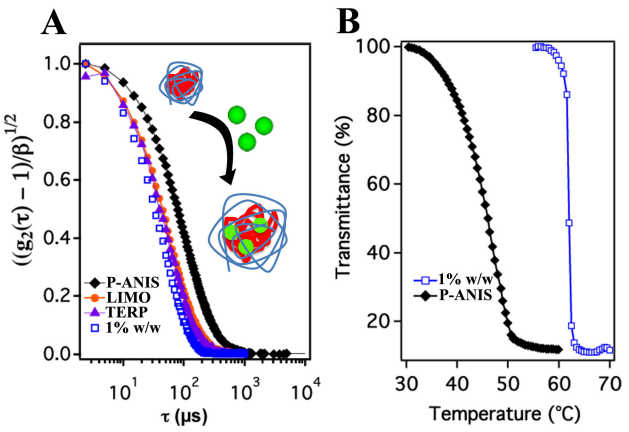


Fig. 2: (A) DLS profiles and (B) Temperature-Turbidity curves of samples containing 1% w/w of PEG-g-PVAc and different flavors.

An additional confirmation was obtained by cloud point determinations, since the incorporation of molecules in SCNPs leads to the modification of this critical temperature.[3] From the comparison between the temperature-turbidity curves of loaded and unloaded samples (Figure 2B) we observe a decrease in the cloud point of PEG-g-PVAc SCNPs, that is a straightforward evidence of a successful encapsulation.

References

Bartolini A.; Tempesti P.; Resta C.; Berti D.; Smets J.; Aouad Y.G.; Baglioni, P. "Poly(ethylene glycol)-*graft*-poly(vinyl acetate) single-chain nanoparticles for the encapsulation of small molecules", Phys. Chem. Chem. Phys. 2017, Accepted Manuscript.

Stals, P.J.M.; Gillissen, M.A.J.; Paffen, T.F.E.; de Greef, T.F.A.; Lindner, P.; Meijer, E.W.; Palmans, A.R.A.; Voets, I.K. "Folding Polymers with Pendant Hydrogen Bonding Motifs in Water: The Effect of Polymer Length and Concentration on the Shape and Size of Single-Chain Polymeric Nanoparticles", Macromolecules 47, 2947-2954 (2014).

Zemb, T.; Lindner, P. "Neutrons, X-rays and Light: Scattering Methods Applied to Soft Condensed Matter", Elsevier (2002).

1B – Delivery of nucleic acid-based therapeutics for the treatment of antibiotic-resistant pathogens

M. Mamusa, C. Montis, D. Berti; A. Ruyra, L. Sitia, M. McArthur, K. Hatzixanthis, C. W. Morris, G. Wheeler (University of East Anglia, Norwich UK); A. Gonzalez-Paredes, F. Barbero, P. Gasco (Nanovector s.r.l., Turin)

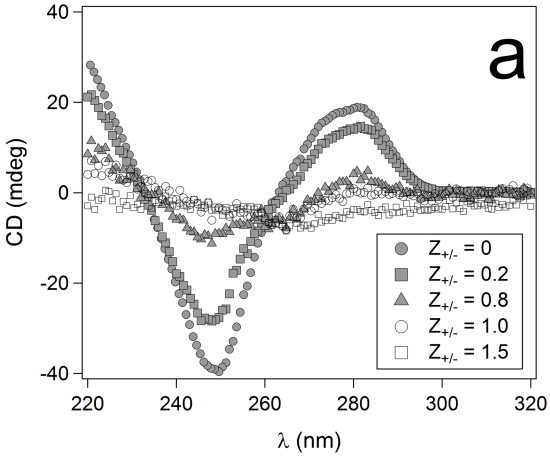
Aims

Properties of a complex between a cationic bolaamphiphile and an oligonucleotide with antibacterial action. Delivery to antibiotic-resistant bacteria by using liposomes.

Results

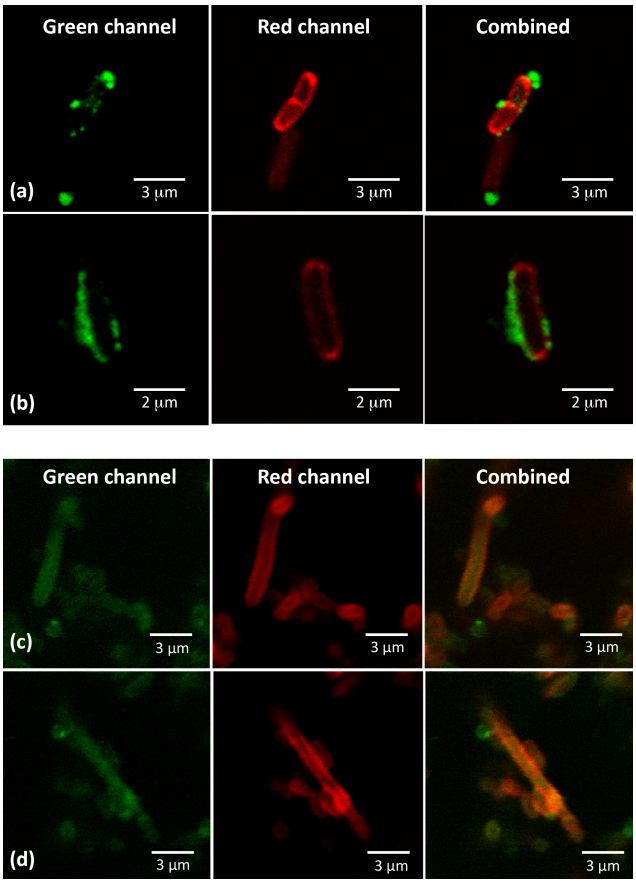
This work, funded under the 7-People Framework Marie-Curie Industry and Academia Partnerships & Pathways scheme (grant agreement nr. 612338), focused on the encapsulation and delivery of Transcription Factor Decoys (TFDs): these oligonucleotides interact with essential genetic pathways in bacteria and prevent their survival response to antimicrobial attack. TFDs have proven successful in defeating infections by antibiotic-resistant bacteria *in vivo* when coupled to a cationic bolaamphiphilic molecule, 12,12'-(dodecane-1,12-diyl)-bis(9-amino-5,6,7,8-tetrahydroacridinium) or 12-bis-THA. The latter is reminiscent of Dequalinium®, an antimicrobial molecule used in commercial topic formulations, and as such possesses intrinsic antibacterial properties.

First of all, we studied the behaviour of this bolaamphiphile in aqueous solution: thanks to DLS and cryo-TEM, we found out that 12-bis-THA (chloride salt) forms bolasomes, *i.e.* vesicles, upon strong vortexing of its dilute solutions. These structures are however kinetically unstable and can be preserved only at 4 °C for a limited time, while at room temperature they rapidly convert into one-dimensional elongated assemblies (ribbons).



Next, we demonstrated, through steady-state fluorescence spectroscopy and circular dichroism (figure on the right), that the interaction between this bolaamphiphile and the oligonucleotide leads to strong binding and condensation of the TFD, which renders it resistant to nuclease digestion. We also showed that the TFD/12-bis-THA complex is reversible by breaking it with sodium taurocholate, which competes with the TFD's polyanionic backbone for interaction with the bolaamphiphile.

However, the 12-bis-THA/TFD nanoplexes presented very scarce colloidal stability in saline solutions at physiologic ionic strength and in common buffers. We therefore designed POPC – and POPC/DOPE – based liposomes as delivery vectors to ensure colloidal stability protect the complex, and ensure its therapeutic action. DLS and Zeta- potential measurements proved that both types of liposomes were able to incorporate 12-bis-THA and possessed the appropriate size and surface charge to be used as effective DNA carriers. Both types of liposomes were loaded with a green-fluorescent TFD and challenged against a colony of *E. coli* of which the membrane had been labelled with a red-fluorescent dye for observation with confocal laser scanning microscopy. Experiments showed that POPC-only liposomes (figure on the left, panels *a* and *b*) interacted at the poles and septa of the bacteria, which are especially rich in a strongly anionic lipid, cardiolipin, suggesting a possible targeting mechanism for 12-bis-THA. However, only POPC/DOPE-based liposomes delivered the TFD into the bacterial cytoplasm, demonstrating the necessity of a fusogenic lipid to yield transfection.



References

Mamusa, M.; Resta, C.; Barbero, F.; Carta, D.; Codoni, D.; Hatzixanthis, K.; McArthur, M.; Berti, D. "Interaction between a cationic bolaamphiphile and DNA: The routetowards nanovectors for oligonucleotide antimicrobials", Coll. Surf. B 143, 139-147 (2016).

Marín-Menéndez, A.; Montis, C.; Díaz-Calvo, T.; Carta, D.; Hatzixanthis, K.; Morris, C.J.; McArthur, M.; Berti, D. "Antimicrobial Nanoplexes meet Model Bacterial Membranes: the key role of Cardiolipin", Scientific Reports 7, 41242 (2017).

Mamusa, M.; Sitia, L.; Barbero, F.; Ruyra, A.; Díaz Calvo, T.; Montis, C.; Gonzalez-Paredes, A.; Wheeler, G.N.; Morris, C.J., McArthur, M.; Berti, D. "Cationic liposomal vectors incorporating a bolaamphiphile for oligonucleotide antimicrobials", submitted to Bioph Bioch Acta (2017).

1B – Complexation of short ds RNA/DNA oligonucleotides with Gemini micelles: a time resolved SAXS and computational study

S. Falsini, E. Di Cola (ESRF, Grenoble, France),
M. In (University of Montpellier, France),
S. Borocci (University of Tuscia, Italy), S. Ristori

Aims

One major challenges in gene therapy is the development of non-viral vectors for genetic material, such as plasmids and small interfering nucleic acids. The molecular properties of complexes between carriers and nucleic acids are of fundamental importance to obtain efficient transfection. In this contribution we describe the structural evolution of oligonucleotide (siRNA or siDNA) during complexation with micelles of divalent cationic surfactants, i.e. Gemini bis (quaternary ammonium) bromide with variable spacer length (12-3-12, 12-6-12, 12-12-12).

Results

The kinetics of complexation was studied by time resolved Small Angle X Ray Scattering (SAXS) performed at the European Synchrotron Radiation Facility (Grenoble, France) and by molecular dynamics. In SAXS experiments all the systems contained a fixed amount of surfactant and different concentrations of oligonucleotide at charge ratios (+/-) 0.75 and 1.25. SAXS intensity diagrams showed that complexes appear in solution immediately after mixing (10-20 ms) and, therefore, the study of their formation requires fast experimental techniques. The obtained aggregates have internal arrangement constituted by layers of squeezed micelles alternating the nucleic acids. Moreover, we found that there are relevant differences in the structure of the nucleic acid/micelles complexes due to the nature of the nucleic acid (siRNA and siDNA). To illustrate this point figure 1 shows the comparison of SAXS profiles obtained for siRNA and siDNA complexed with 12-6-12 micelles.

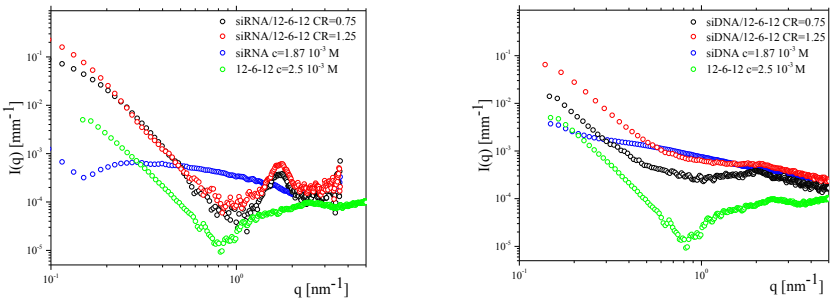


Fig. 1: SAXS diagrams of siRNA/12-6-12 and siDNA/12-6-12 (20 ms after mixing).

Molecular dynamics simulations were carried out to obtain an atomistic description of the interaction between the nucleic acid molecules and the surfactant aggregates. The systems composed by siDNA or siRNA, 27 molecules of Gemini 12-6-12 (CR = 0.75), ~15000 water molecules and ions (40 Na+ and 54 Br-) were simulated for 100 ns (after 20 ns of equilibration) at P = 1 bar and T = 298 K. The corresponding snapshots are reported in figure 2.

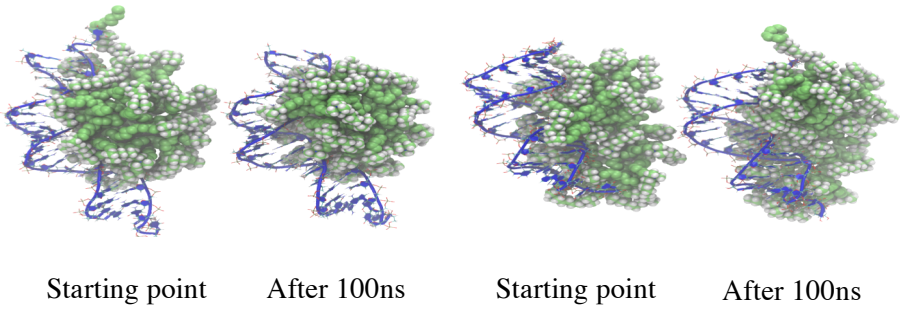


Fig. 2: Snapshots of the siRNA/12-6-12 (right) and siDNA/12-6-12 (left) complex at the starting point and after 100ns of MD simulation.

The analysis of MD trajectories put into evidence a preferential interaction of the micellar aggregates with the minor groove of the nucleic acid. The siRNA associated with the micelles conserve a more compact structure (~1.9nm) respect to the siDNA (~2.2nm). Moreover, the siDNA associated to the micellar aggregates presents a greater deformation respect to siRNA, as evidenced by the root mean square deviation, calculated respect to initial structure of siDNA and siRNA, that reaches the value of 0.80 and 0.51 nm respectively.
These results are in agreement with those obtained by SAXS and provide refined information on the structure of complexes formed by Gemini micelles and siRNA or siDNA oligonucleotides.

References

Falsini, S.; Ristori, S. “Lipoplexes from Non-Viral Cationic Vectors: DOTAP-DOPE Liposomes and Gemini Micelles” in Non-Viral Gene Delivery Vectors: Methods and Protocols. G. Candiani Ed., ISSN: 1064-3745, Springer NY 1445, 33-43 (2016).
Falsini, S.; Di Cola, E.; In, M.; Giordani, M.; Borocci, S.; Ristori, S. “Complexation of short ds RNA/DNA oligonucleotides with Gemini micelles: a time resolved SAXS and computational study”, Phys. Chem. Chem. Phys. 19, 3046-55 (2017).

1B – Nitric oxide assisted C60-SIMS for molecular depth profiling of polyelectrolyte multilayers

G. Zappalà, S. Vitale, N. Tuccitto, A. Torrisi, A. Licciardello

Aims

Molecular depth profiling of polymers is an important demand in many technological applications that has been increasingly fulfilled by the introduction and development of cluster SIMS methodologies. SIMS with polyatomic primary ions provides a successful tool for molecular depth profiling of polymer systems, relevant in many technological applications. Widespread C_{60} sources, however, cause in some polymers extensive damage with loss of molecular information along depth. We studied a method, based on the use of a radical scavenger, for inhibiting ion beam-induced reactions causing sample damage.

Results

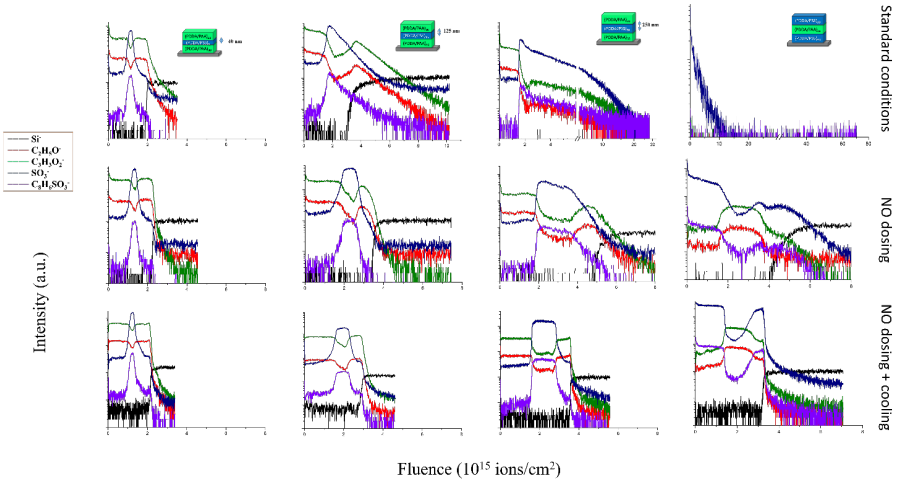
The introduction of reactive gases during SIMS analysis turned out to be an interesting aid in organic and polymer depth profiling, either for obtaining an increase of ionization efficiency [1] or for interfering with adverse ion beam-induced reaction (such as crosslinking) that in some cases prevent the accomplishment of a successful molecular depth profile. The latter approach, initially proposed by our laboratory, consists in the use of a radical scavenger, namely nitric oxide (NO), and it has been recently shown to be a valid and cheap tool, in alternative to the more effective GCIBs, for extending the use of fullerene beams in depth profiling of difficult polymers [2]. Moreover NO flooding in conjunction with fullerene primary beams allows the analysis of hybrid organic-inorganic systems [5] and, in addition, it can supply some additional indication useful for a deeper understanding of the ion-beam induced chemistry in polymers.

We present some recent results obtained on multilayers with NO-assisted C_{60}-SIMS depth profiling. In particular we prepared and examined some test samples based on layer-by-layer (LbL) deposition of polyelectrolytes, which is a versatile technique that allows to cover any kind of surfaces with well-ordered films by fine tuning of thickness and composition. In particular, we used polydiallyldimethylammonium chloride (PDDA), poly acrylic acid (PAA) and polystyrene sulfonate (PSS) as polyelectrolites and combined them in order to obtain multilayers with different sequences of the threee components.

Such layers where profiled by C_{60}-SIMS and the influence of NO and sample temperature in terms of damage accumulation, erosion yield and depth resolution was investigated.[3].

As shown in Figure, C_{60} depth profiling in standard conditions (i.e. without NO-dosing and at RT) does not allow to obtain satisfactory molecular depth profiles when relatively thick PSS-based layers are involved, due to ion-beam-induced crosslinking occurring in this system. By contrast, the introduction of NO allows to obtain in all cases good molecular depth profiles and to discriminate, on the basis of the intensity of structure-related fragments, among all the layers, with satisfactory depth resolution and sputter yield. A further improvement in the quality of the profiles can be obtained by cooling the sample down to 150 K. Actually it has been already reported that

temperature affects[4] the quality of depth profiles of polymers, and this is not surprising if we consider that chemical reactions are involved in the erosion process.



The above findings confirm the ability of nitric oxide to inhibit radical reactions leading to cross-linking and damage accumulation during C_{60} SIMS depth profiling of polymers and prompt NO-dosing method as a valuable one for the SIMS characterization of polymer multilayers with C_{60} primary beams. Although similar and even better results have been recently obtained by means of large polyatomic argon clusters (GCIB), NO-dosing has the advantage of allowing to continue to use the widespread C_{60} sources and, moreover, it is expected to be useful when profiling hybrid organic/inorganic multilayers. Indeed GCIBs are not able to profile inorganic materials at the low energies per constituent atom that are suitable for organic molecular depth depth profiling, while a fullerene beam with the aid of NO-dosing should be suitable for this purpose.

References

[1] Mouhib, T.; Delcorte, A.; Poleunis, C.; Bertrand, P. J Am Soc Mass Spectrom 2010, 21, 2005-2010.
[2] Havelund, R.; Licciardello, A.; Bailey, J.; Tuccitto, N.; Sapuppo, D.; Gilmore, I.S.; Sharp, J.S.; Lee, J.L.S.; Mouhib, T.; Delcorte, A. Anal. Chem. 2013, 85, 5064-5070.
[3] Zappalà, G.; Motta, V.; Tuccitto, N.; Vitale, S.; Torrisi, A.; Licciardello, A. Rapid Commun. Mass Spectrom. 2015, 29, 2204-2210.
[4] Moellers, R.; Tuccitto, N.; Torrisi, V.; Niehuis, E.; Licciardello, A. Applied Surface Science 2006, 252, 6509-6512.
[5] "Nitric oxide dosing in C60-SIMS depth profiling of polymer/inorganic hybrid multilayers". SIMS Europe 2012, Muenster, Germany, September 9-11, 2012.

1C – Active sites of copper-trafficking proteins: density functional structural and spectroscopy studies on copper(I) models

C. Rossi, G. Tamasi, C. Bonechi, A. Donati, A. Magnani

Aims

Several proteins are believed to be actively involved in copper trafficking and storage, and even small biomolecules such as glutathione (GSH) play an important role in binding copper *in vivo*, and sometimes copper proteins are involved in serious human diseases like Parkinson and Menkes pathologies. Structural studies at metal sites might help in understanding the molecular mechanism of such health disorders. In the present work, selected structures optimized via density functional (DFT) methods of some models of copper(I) binary and ternary complexes, with low-molecular weight ligands, on the relevant selected computed structural parameters, spectroscopic data, and energy aspects, are reported. These data can help in interpreting structural data of complex biological systems and in constructing reliable force fields for molecular mechanics computations.

Results

The work provided rationale for several structural features of selected copper protein systems involved in copper trafficking found experimentally at the solid state and in the solution phase via X-ray diffraction and NMR techniques, especially those that involve mononuclear coordination.

A series of mononuclear binary and ternary Cu(I) complexes with formato, formamide, methylphenol, and methanethiolato ligands were optimized at DFT-B3LYP/6-31G** and DFT-B3LYP/6-311++G** levels of theory. The solvent effect was taken into account via PCM method.

The investigation of estimated qualitative energy of formation of the computed models explained that the linear $Cu(I)S_2$ coordination mode was the most favorable both for thiolato (RS–) and thiol (RSH) ligands when compared to Cu(I)S, $Cu(I)S_3$ and $Cu(I)S_4$ modes. Then, the grafting on the $Cu(I)S_2$ skeleton by certain hard donor groups like alcohol/phenol(ROH) and carboxylate and amide functions are suitable for further stabilizing the overall coordination scaffolding. The treatment of solvation effects via PCM methods (solvent, water) has been also considered, showing that it did not have dramatic influence on structural parameters and on reaction energies.

The formation energies of $[Cu(HSCH_3/SCH_3)(OOCH)]^{0/-1}$ were higher than those of $[Cu(HSCH_3/SCH_3)_2]^{+/-}$ on starting from $[Cu(HSCH_3/Cu(SCH_3)]^{+/0}$ by *ca.* 10 kcal mol^{-1} (DFT-PCM-B3LYP/6-311++G** levels of theory). The structural arrangements, bond distances, and angles as well as computed spectroscopic parameters resulted in good agreement with experimental data for corresponding to synthetic complexes and with metal site regions of several copper(I)-proteins.

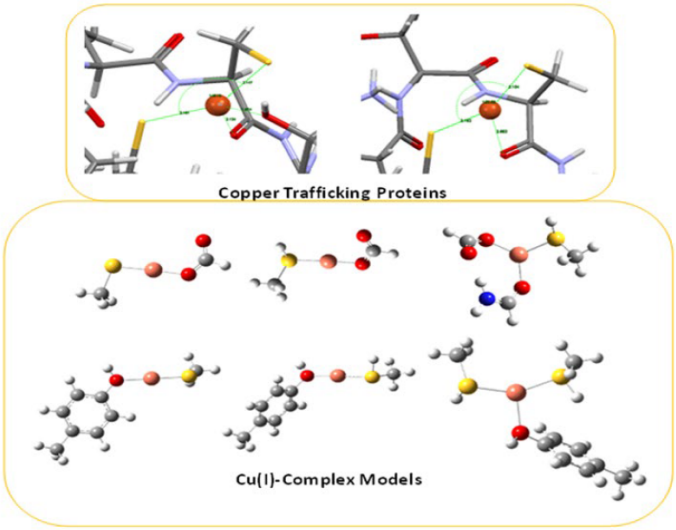


Fig. 1: Cu(I)-complex models for copper trafficking protein structures.

References

Maryon, E.B.; Molloy, S.A.; Kaplan. J.H.; "Cellular glutathione plays a key role in copper uptake mediated by human copper transporter 1", Am. J. Physiol. Cell Physiol. 304, C768-C779 (2013).

Freedman, H.J.; Ciriolo, M.R.; Peisach. J., "The role of glutathione in copper methabolism and toxicity" J. Biol. Chem. 264, 5598-5605 (1989).

Puno, M.R.; Patel, N.A.; Moller, S.G.; Robinson, C.V.; Moody, P.C.E.; Odell. M. "Structure of Cu(I)-bound DJ-1 reveals a biscysteinate metal binding site at the homodimer interface: insights into mutational inactivation of DJ-1 in Parkinsonism", J. Am. Chem. Soc. 135, 15974-15977 (2013). PDB ID: 4BTE.

Girotto, S.; Cendron, L.; Bisaglia, M.; Tessari, I.; Mammi, S.; Zanotti, G.; Bubacco, L. "DJ-1 is a copper chaperone acting on SOD1 activation", J. Biol. Chem. 289, 10887-10899 (2014).

DeSilva, T.M.; Veglia, G.; Opella S.J. " Solution structures of the reduced and Cu(I) bound forms of the first metal binding sequence of ATP7A associated with Menkes disease", Proteins 61, 1038-1049 (2005). PDB ID: 1KVJ.

Tamasi, G.; Mangani, S.; Cini R. "Copper(I)-alkyl sulfide and -cysteine tri-nuclear clusters as models for metallo proteins: a structural density functional analysis", J. Biomol. Struct. Dynam. 30, 728-751 (2012).

1C – Biopolymers and Biomacromolecules Solvent

C. Rossi, C. Bonechi, A. Foletti, G. Tamasi, A. Donati, A. Magnani

Aims

In this paper we developed a strategy, based on Nuclear Magnetic Resonance Spectroscopy, to define the dynamical contribution of the biomacromolecules to the water molecules belonging to their hydration shells.

Results

Biomacromolecules in solution modify the structure and the dynamics of the bulk water at the solute-solvent interface. The ordering effects of biomolecules, in particular proteins, are extended for several angstroms. The role of the hydration shells around a protein has yet to be completely understood. Hydrated proteins maintain more dynamic flexibility with respect to the dried system, which is an important property in protein-protein and/or protein-ligand recognition processes.

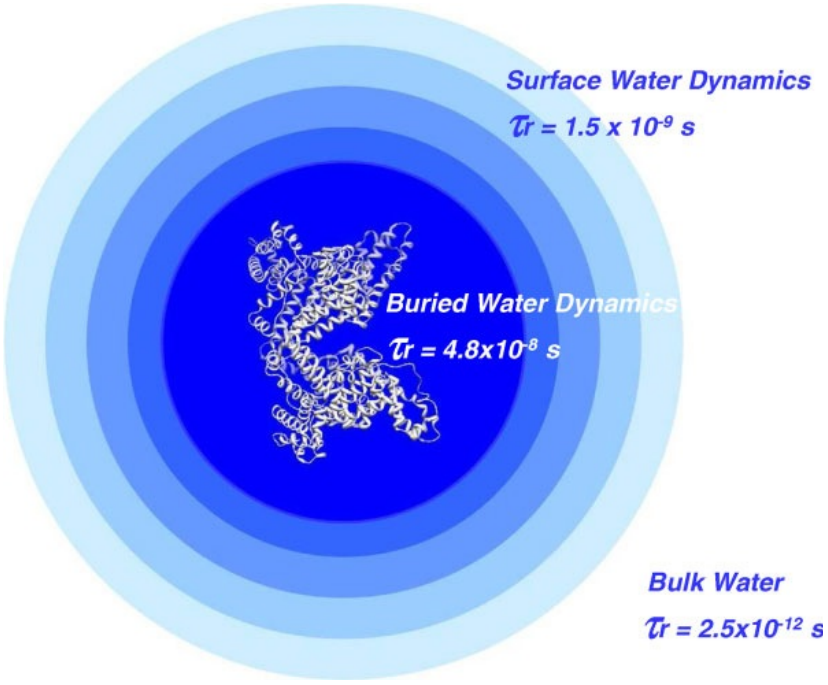


Fig. 1: Effect of the ordering effect of proteins on water. Three water environments defined by their dynamical properties can be observed: bulk, surface and buried water environments

We propose a method for analyzing the dynamical properties of the water molecules present in the hydration shells of proteins. The approach is based on analysis of the effects of protein-solvent interactions on water protons
NMR relaxation parameters. The water proton spin-lattice relaxation rate in protein solution is analyzed considering all possible dipolar contributions from coupled protons environments. The analysis of both selective and non-selective water spin-

lattice relaxation rates allowed the calculation of the average effective correlation time for the water molecules at the protein interface and the evaluation of the long range ordering effect of the protein surface.
In diluted protein solutions, the bulk water proton relaxation shared the contributions from the water molecules in the protein hydration shell. These water molecules differ from the bulk water, mainly because of their correlation times, which is are short for bulk water and longer for the protein hydration waters.

References

Martini, S.; Bonechi, C.; Rossi, C. “Interaction between vine pesticides and serum albumin studied by nuclear spin relaxation data”, J. Agr. Food Chem. 58, 10705-10709 (2010).
Martini, S.; Consumi, M.; Bonechi, C.; Rossi, C.; Magnani, A. “Fibrinogen-catecholamines interaction as observed by NMR and Fourier Transform Infrared Spectroscopy”, Biomacromolecules 8, 2689-2696 (2007).
Bhattacharjee, N.; Biswas, P. “Structure of hydration water in proteins: a comparison of molecular dynamics simulations and database analysis”, Biophys Chem. 158 (1), 73-80 (2011).

1C – In silico design of Dyes for DSSC

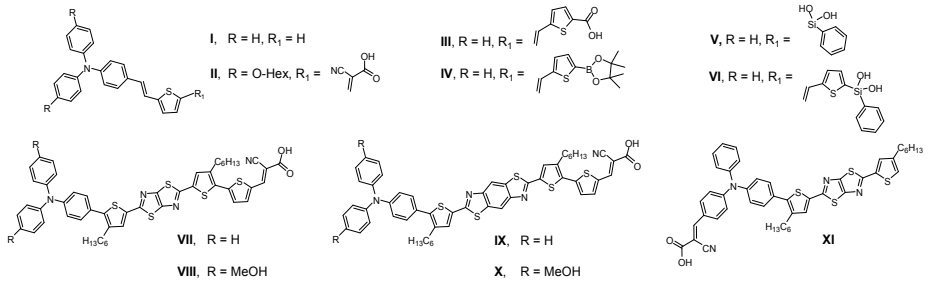
A. Sinicropi, C. Bernini, S. Mohammadpourasl, M. Taddei, R. Basosi

Aims

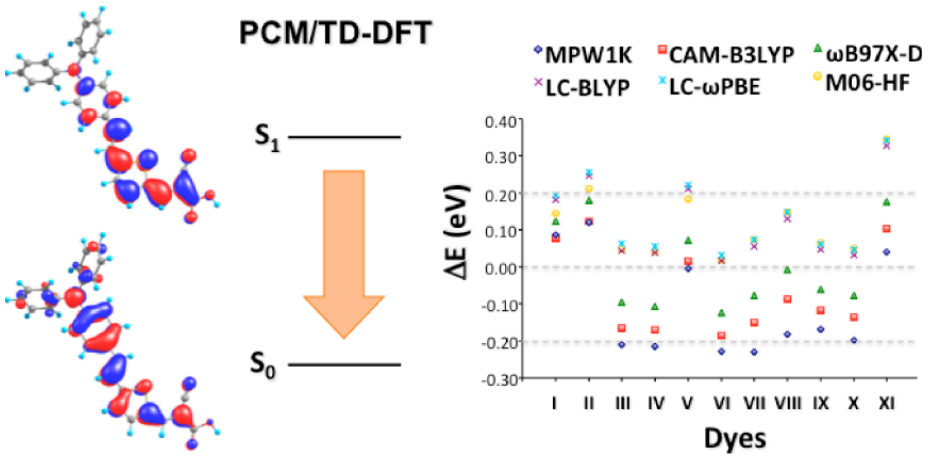
Computational chemistry methods are applied for the calculation of the electronic and molecular properties of designed compounds to be used as dyes for DSSC (Dye Sensitized Solar Cells). The main goal is to verify, even prior to the laboratory synthesis, whether: i) the semiconductor/dye/redox mediator system has a good "alignment" between the energy levels and the relevant electrochemical potentials and ii) the sensitizer has an energy gap wide enough to exploit a large portion of the solar spectrum. The computational study also allows for the characterization of the photostability of these compounds since, to be of practical interest, they must be stable in operation conditions.

Results

Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) have been used for the simulations, either in gas phase or in solution, of the absorption properties of dye molecules, mainly based on a D-π-A structure (i.e., featuring a π conjugated backbone connecting donor and acceptor/anchoring groups), providing very accurate results. Furthermore, as a first step toward the exploration of the excited state potential energy surface of the dyes and, therefore, the evaluation of the photostability, the excited state geometries and emission maxima of several organic dyes used as sensitizers in DSSCs (see molecules I–XI) have been computed and compared to the available experimental data using TD-DFT and a polarizable continuum model (PCM), both in the Linear-Response (LR) and in the State-Specific (SS) formalisms, to take into account solvent effects.



The results showed that the use of six different functionals (LC-ωPBE, LC-BLYP, CAM-B3LYP, ωB97X-D, M06-HF, MPW1K) within the PCM/TD-DFT method allowed for the accurate calculation of the low-lying singlet excited state of the D-π-A dyes obtaining emission data that compare well with the experimental values. Indeed, the mean absolute error (MAE) is, in the best cases, 0.10 eV. The inclusion of solvent effects at the optimization stage is crucial to obtain results that are consistent with experimental values (ca. 0.2 eV). The use of a SS-PCM model further reduces the discrepancy with experiments (within 0.15 eV).



To the best of our knowledge, this is (i) the first extensive TD-DFT computational study that focuses on the emitting properties of D- π -A dyes in which the role of the solvation in affecting the excited state geometries has been explored and (ii) the first computational investigation of excited state geometry and emission properties of one of the most representative organic dyes for DSSC, i.e., the D5 dye (molecule I).
The present benchmarking study opens the way to the evaluation of the photostability of D- π -A sensitizers and thus to the design of more robust organic dyes, in terms of excited state stability, through substitutions and/or insertion of different molecular units.

References

Bernini C.; Zani L.; Calamante M.; Reginato G.; Mordini A.; Taddei M.; Basosi R.; Sinicropi, A. "Excited state geometries and vertical emission energies of solvated dyes for DSSC: a PCM/TD-DFT benchmark study", Journal of Chemical Theory and Computation 10 (9), 3925-3933 (2014).
Dessì, A.; Calamante, M.; Mordini, A.; Peruzzini, M.; Sinicropi, A.; Basosi, R.; Fabrizi de Biani, F.; Taddei, M.; Colonna, D.; Di Carlo, A.; Reginato, G.; Zani, L. "Organic dyes with intense light absorption especially suitable for application in thin-layer dye-sensitized solar cells", Chemical Communications 50, 13952-13955 (2014).
Dessì A.; Calamante M.; Mordini A.; Peruzzini M.; Sinicropi A.; Basosi R.; Fabrizi de Biani F.; Taddei M.; Colonna D.; Di Carlo A.; Reginato G.; Zani L. "Thiazolo [5, 4-d] thiazole-based organic sensitizers with strong visible light absorption for transparent, efficient and stable dye-sensitized solar cells", RSC Advances 5, 32657-32668 (2015).
Franchi, D.; Calamante, M.; Reginato, G.; Zani, L.; Peruzzini, M.; Taddei, M.; Fabrizi de Biani, F.; Basosi, R.; Sinicropi, A.; Colonna, D.; Di Carlo, A.; Mordini, A. "Two New Dyes with carboxypyridinium Regioisomers as Anchoring Groups for Dye-Sensitized Solar Cells", Synlett 26, 17, 2389-2394 (2015).

1C– Computational spectroscopy of protein radicals

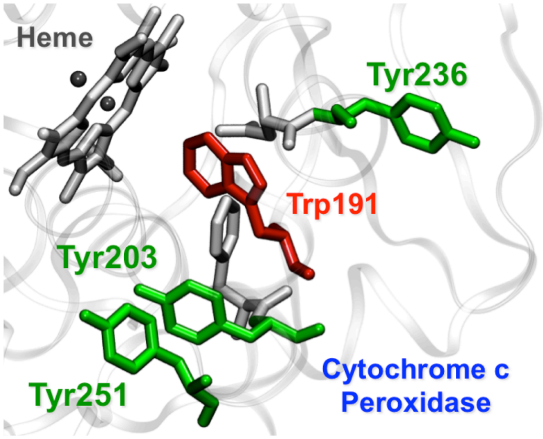
C. Bernini, R. Basosi, A. Sinicropi

Aims

State-of-the-art quantum-mechanics/molecular-mechanics (QM/MM) methods are used to characterize the electronic, vibrational, and magnetic properties of redox-active amino acids involved in long-range electron transfer pathways in proteins. 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.

Results

Hybrid QM/MM methods, 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). 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, it allows to obtain a mechanistic description of the proton-coupled electron transfer process leading to the radical formation and to provide 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.



More recently, we built models of tryptophan and tyrosine radicals within the protein matrix of the cytochrome c peroxidase (CcP) from *Saccharomyces cerevisiae*. Cytochrome c peroxidase (CcP) is a heme-containing enzyme involved in the mitochondria electron transport chain. Similar to other heme peroxidases, the ferric resting form of CcP is first oxidized by H2O2 to a two-electron oxidized intermediate (Cp-I), in which one oxidizing equivalent is stored as an oxoferryl species, while the second one as a protein radical. Cp-I is then reduced by two molecules of Cytochrome c to cycle back

to the resting enzyme. Electron paramagnetic resonance (EPR) and electronic and nuclear double resonance (ENDOR) measurements indicated that both a tryptophan and a tyrosine radical contributed to Cp-I. Despite this, no definitive answer on the assignment of the radical species to a specific tryptophan and tyrosine residue has yet been provided. Moreover, so far, the neutral or charged nature of the tryptophan radical has not been clearly indicated. The results show that the models correctly predict the magnetic, electronic and vibrational properties of the observed amino acid radicals of Cp-I and demonstrate that a tryptophan cationic radical (Trp191•+) and three tyrosine residues (Tyr203, Tyr236 and Tyr251), located along two possible ET pathways involving Trp191•+, are possible candidates to host the Cp-I radical species.

References

Bernini C.; Arezzini E.; Basosi R.; Sinicropi A. "In silico spectroscopy of tryptophan and tyrosine radicals involved in the long-range electron transfer of Cytochrome c Peroxidase", Journal of Physical Chemistry B 118, 9525-9537 (2014).

Bernini, C.; Andruniów, T.; Olivucci, M.; Pogni, R.; Basosi, R.; Sinicropi, A. "Effects of the Protein Environment on the Spectral Properties of Tryptophan Radicals in Pseudomonas aeruginosa Azurin", Journal of the American Chemical Society 135, 4822-4833 (2013).

Bernini, C.; Pogni, R.; Basosi, R.; Sinicropi, A. "The nature of tryptophan radicals involved in the long-range electron transfer of lignin peroxidase and lignin peroxidase-like systems: Insights from quantum mechanical/molecular mechanics simulations", Proteins: Structure, Function, and Bioinformatics 80, 1476-1483 (2012).

Bernini, C.; Pogni, R.; Ruiz-Dueñas, F.J.; Martínez, A.T.; Basosi, R.; Sinicropi, A. "EPR Parameters of Amino Acid Radicals in P. eryngii Versatile Peroxidase and its W164Y variant computed at the QM/MM level", Physical Chemistry Chemical Physics 13, 5078-5098 (2011).

1C– A complex system's view of the rebound effect in energy efficiency

A. Facchini (IMT School for Advanced Studies, Lucca), L. Valori, A. Scala (IMT School for Advanced Studies, Lucca), M.L. Parisi, R. Basosi

Aims

The project aims to provide a characterization of the rebound effect by means of complex systems methods (nonlinear systems dynamic and complex networks).

Results

There is evidence that energy efficiency improvements do not ultimately produce the expected results in terms of energy savings. This phenomenon is due to the so called *rebound effect*. Indeed, for households and firms an energy efficiency improvement is equivalent to a reduction of the cost of the energy service that has been improved, that is, they can obtain the same amount of useful work from the improved energy service (e.g. thermal comfort, travelled kilometers, lighting, etc.) at less cost (or alternatively, more useful work at the same cost), which would lead to a subsequent increase in the energy consumption, offsetting partially or completely the energy savings derived from the energy efficiency improvement.

Even when maintaining the same useful work at the same cost, an energy efficiency improvement produces qualitative changes in energy service in the form of improving attributes or characteristics, therefore resulting in an alternative form of rebound effect. Regarding this, there is a general agreement between energy economists about the existence of rebound effect. Disagreement however centers on the sources and especially from the size it achieves. Some authors claim that it is less than 100%, that is, the energy efficiency improvements produce a net reduction of energy consumption. Alternatively some of them argue that it is higher than 100% and therefore energy efficiency improvements lead to a "backfire", producing an increase in the final energy consumption.

Understanding this distinction involves an effort and the need of a paradigm shift when dealing with the rebound effect.

In the present project, we make the assumption that the rebound effect is the result of a set of nonlinear interaction producing an emergent behavior that can be modeled by means of the methods typical of complex systems sciences. Our starting point is the consideration that evolutionary systems, such as biological or even socio-economic systems, may evolve towards more complex structure under the pressure of an increasing flow of energy and materials, driven by the higher conversion rate of greater efficiency. Higher complexity, due to a greater energy density rate, counteracts the positive effects of energy efficiency, resulting in a increase of resource consumption.

More specifically, our aim is to apply the methods of complex networks and systems dynamics to model, explain, and quantify the rebound effect in the energy systems, with an application to urban ecosystems and transport infrastructures (also including the effect of rebound dynamics in a scenario of wide diffusion of electric mobility).

We use the above mentioned methods because:

1) **Complex networks** are a well established paradigm for modeling and describing different systems interconnected both in a physical and functional way. This characteristics makes them suitable to model the connection of urban infrastructures, that as the city evolved become more an more interconnected, as showed in figure 1.
2) **Nonlinear Systems dynamics** is the appropriate framework to describe the temporal evolution of systems with nonlinear feedbacks that, due to bifurcations and changes in their stability characteristics can be useful in modeling the rebound dynamics.

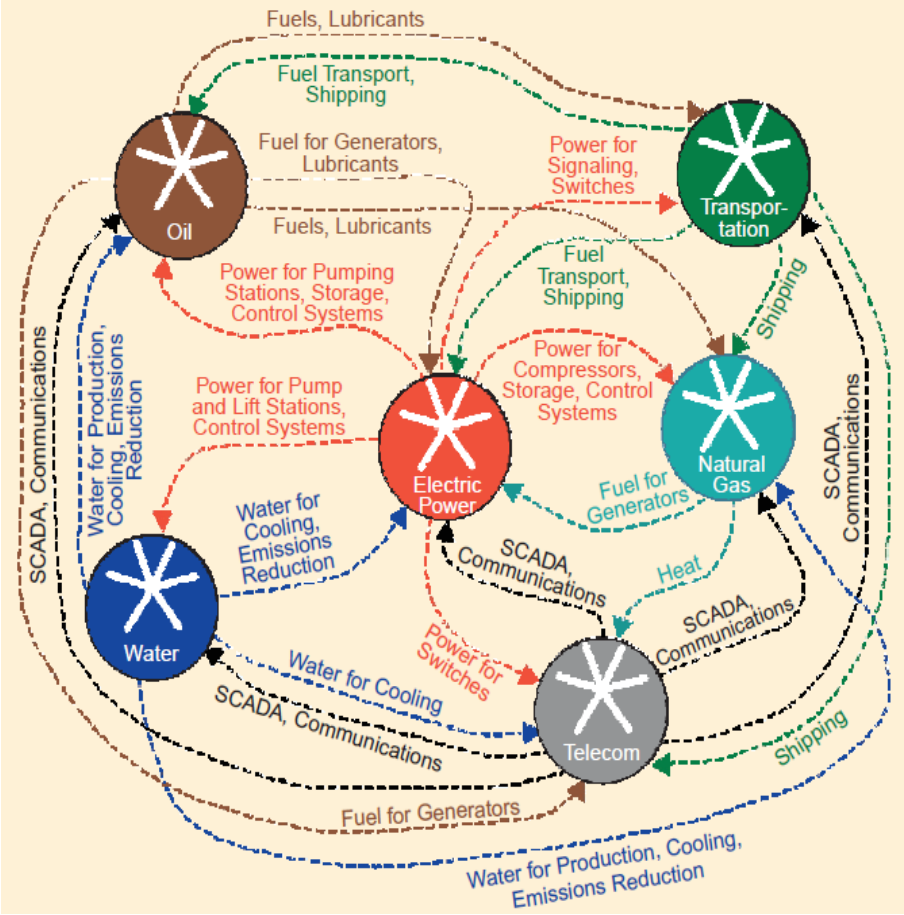


Fig. 1 Interdependence of urban infrastructures

References

Valori L.; Giannuzzi G.L.; Facchini A.; Squartini T.; Garlaschelli D.; Basosi R. "A generation-attraction model for renewable 1 energy flows in Italy: a complex network 2 approach", The European Physical Journal, Special topics, 1-15 (2016).
Ruzzenenti, F.; Basosi, R.; "The rebound effect: An evolutionary perspective", Ecological Economics 67 (4), 526-537 (2009).
Ruzzenenti, F.; Basosi, R. "Energy growth, complexity and efficiency", Energy efficiency, 27-49 (2010).
Sorrell, S.; Dimitropoulos, S. "The rebound effect: microeconomic definitions, limitations and extensions", Ecological Economics (2007).

1C - Leather production ultrasound-assisted as best available technology to reduce damages to workers health

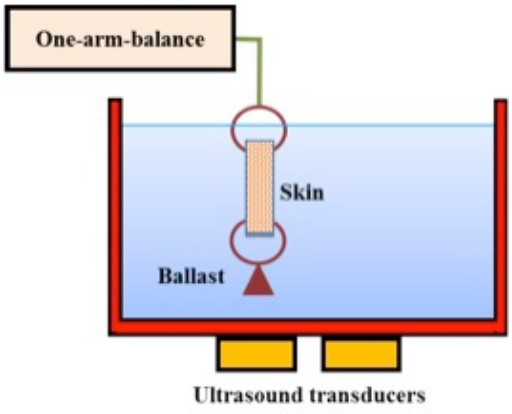
G Bufalo, F. Di Nezza, L. Cimmino, F. Cuomo, L. Ambrosone

Aims

One of the purposes of this paper is to show how applying ultrasound to tanning-alum-water greasing approach to produce mink fur with desired quality.

Results

The environmental impact of fur industry is quite relevant. Measurements carried out on mink fur show that ultrasound have a limited effect on the diffusion rate, but increase the capacity of the tanning-greasing agent only after attainment of the equilibrium. Experimental results indicate that cavitation greatly improves the greasing-tanning stage increasing the skin absorption of 25%. This implies a reduction of volatile solvents load of 50%. Since the mink fur is machined in open standing paddle, such reduction significantly increases the working place healthiness. Experimental results can be transposed to industrial scale in two possible arrangements. However, the configuration with all transducers outside of the reactor appears to be more suitable for the mink fur production. This is because with standing paddle open and fixed one is able to irradiate a well-defined area, increasing the quality of the final fur. In this way, the equipment costs are lowered, the environmental impact is reduced, the toxicity of the volatile solvents partially torn down and finally the product quality is optimized.



References

Bufalo, G.; Di Nezza, F.; Cimmino, L.; Cuomo, F.; Ambrosone L. “Leather production ultrasound-assisted as best available technology to reduce damages to workers health ” J. Clear Prod. (2016 in press).

1C – Specific Ion Effects in Protein Systems

A. Salis, L. Medda, F. Cugia, M. Monduzzi,
D.F. Parsons (Murdoch University),
B.W. Ninham (Australian National University).

Aims

Investigation of specific ion effects in protein systems. The specific effect of cations suggests that they operate through two opposite mechanisms. A new theoretical modelling is being developed.

Results

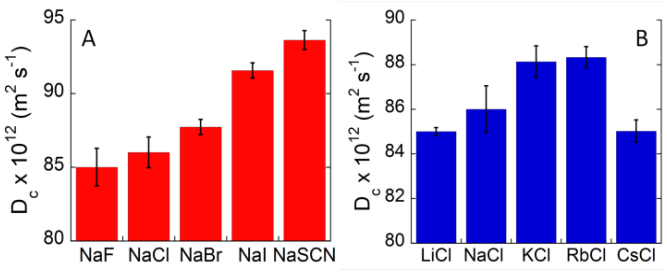
Specific ion effects are those variations in properties which are not anticipated from classical electrostatic theory of salt solutions. They were firstly observed in 1888 by Franz Hofmeister who studied the effect of salt addition on the aggregation of egg white proteins. He ordered the salts, with the same cation but different anions, according to their ability in promoting the precipitation (salting-out) or the solubility (salting-in) of a protein in aqueous solution. A conventional 'Hofmeister series' is:

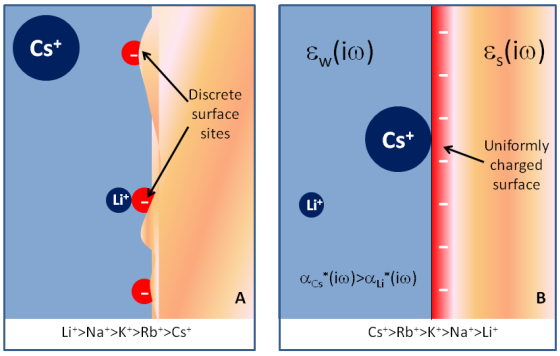
$HPO_4^{2-} > SO_4^{2-} > F^- > Cl^- > Br^- > NO_3^- > ClO_4^- > SCN^-$

The 'salting-out' anions (left side of the series) are strongly hydrated, while salting-in' anions (right side) are only weakly hydrated. A similar series for cations was also observed:

$NH_4^+ > K^+ > Na^+ > Li^+ > Mg^{2+} > Ca^{2+}$

The 'conventional' cation series has a substantial difference compared to the case of anions.[5] Indeed, salting-out cations are weakly hydrated (NH_4^+) and salting-in cations are strongly hydrated (i.e. Li^+ and Mg^{2+}). Substantially, anions and cations behave in the opposite way. The understanding of the specific cation behaviour is very interesting because many cations (i.e. Na^+, K^+, Mg^{2+}, Ca^{2+}) play a crucial role in fundamental biological systems. We investigated the specific effect of salts on the molecular motion of a concentrated solution of a model protein (bovine serum albumin, BSA) in physiological conditions. To investigate the subtle molecular protein-electrolyte interactions the 'Brownian' diffusion coefficient, D_c, obtained through dynamic light scattering (DLS) measurements is an extremely sensitive and convenient parameter. The diffusion coefficients increase according to the typical Hofmeister sequence for anions ($SCN^- > I^- > Br^- > Cl^- > F^-$), usually observed for pH > pI. The observed trend is consistent with a specific anion adsorption on BSA surface, despite its negative net charge at pH 7. The higher negative charge induced by SCN^- adsorption at BSA surface strengthens the repulsion among protein molecules and, hence, higher D_c values are measured. The effect of different cations was then studied by measuring D_c values for BSA solutions (40 mg/mL) at pH 7 in the presence of





$\Delta H_{hydr.\ anion} - \Delta H_{hydr.\ cation} \approx 0$

$$U_{disp}(x) = \frac{kT}{2x^3}\sum_{n=0}^{\infty}\frac{\alpha^*(i\omega_n)}{\varepsilon_w(i\omega_n)}\frac{[\varepsilon_w(i\omega_n)-\varepsilon_s(i\omega_n)]}{[\varepsilon_w(i\omega_n)+\varepsilon_s(i\omega_n)]}$$

different 0.1 M chloride salts. Differently from the anions case, here the D_c values do not follow a monotonic series but, rather, a "bell-shaped" trend: $Rb^+ \sim K^+ > Na^+ > Cs^+ \sim Li^+$. Cesium and lithium, two cations that are considered to be at the opposite sides of the Hofmeister series, behave very similarly giving rise to the lowest values of D_c. Rubidium and potassium, instead, increase BSA motion, while sodium is in between the two extremes. A similar "bell-shaped" series for cations is a clear sign of two different mechanisms that operate in opposite directions. In the early attempts to include dispersion forces the dispersion energy, $U_{dispersion}$, was estimated from ion static polarizabilities. Since polarizability increases going from Li^+ to Cs^+, a stronger adsorption for Cs^+ rather than Li^+ at a protein surface is expected. But if we consider Collins' "law of matching water affinities" (LMWA) the formation of ion pairs between a cation and a negatively charged kosmotropic carboxylate would follow the order $Li^+ > Na^+ > K^+ > Rb^+ > Cs^+$. That is, the two approaches would predict exactly the opposite sequences. Our experimental results clearly show that both mechanism are at work and the observed macroscopic phenomenon, i.e. Brownian motion is due to a delicate interplay of these two microscopic mechanisms. On the basis of our experimental results, we are currently working to improve specific ion effects in protein systems by the theoretical point of view. The new theoretical model considers the two different hypothesized mechanisms: i. physisorption at neutral protein surface and ii. chemisorption at charged sites. Both involve, besides the conventional electrostatic forces, also polarizability-dependent ion dispersion forces.

References

Parsons, D.F.; Salis, A. "Hofmeister effects at low salt concentration due to surface charge transfer", Current Opinion in Colloid and Interface Science 23, 41-49 (2016).

Salis, A.; Monduzzi, M. "Not only pH. Specific Buffer Effects in Biological Systems", Current Opinion in Colloid and Interface Science 23, 1-9 (2016).

Salis, A.; Medda, L.; Cugia, F.; Monduzzi, M. "Effect of Electrolytes on Proteins Physisorption on Ordered Mesoporous Silica Materials", Colloids and Surfaces B: Biointerfaces 137, 77-90 (2016).

Parsons, D.F.; Salis, A. "Impact of the Competitive Adsorption of Ions at Surface Sites on Surface Free Energies and Surface Forces", Journal of Chemical Physics 142, 134707 (2015).

Medda, L.; Monduzzi, M.; Salis, A. "The Molecular Motion of Bovine Serum Albumin Under Physiological Conditions is Ion Specific", Chemical Communications 51, 6663-6666 (2015).

Salis, A.; Ninham, B.W. "Models and Mechanisms of Hofmeister Effects in Electrolyte Solutions, Colloid and Protein Systems Revisited", Chemical Society Reviews 43, 7358-7377 (2014).

1C – Simulation of SIMS depth profiles of organic solids by transport diffusion model

N. Tuccitto, G. Zappalà, S. Vitale, A. Torrisi, A. Licciardello

Aims

SIMS depth profiling of organic targets is nowadays achievable thanks to the introduction of cluster beams, which allow the in-depth detection of the typical fragments of the material under investigation well beyond the so–called "static limit". Such capability depends on several physical and chemical processes following the cluster impact, which are nowadays attracting the interest of many researchers.
In this research, we develop a new model for the simulation of SIMS depth profiles, which is able to incorporate the beam-induced reactivity, so leading to a reasonable simulation of depth profiles of polymers and organic solids.

Results

During a dynamic SIMS experiment the sputter beam erodes the uppermost layers of the target reaching deeper and deeper portions of the sample with a velocity (sputtering rate) that depends on the primary beam parameters (current density, energy and type of projectile ion) and on the nature of the target. In the phenomenological model outlined here, the position of the bombarded surface is kept invariant, so that he erosion process is represented as a "travel" of the underlying material toward the surface. The sputtering rate is represented by the travel velocity, $\boldsymbol{v}$, of the target layers travelling towards the surface. When the material moving towards the surface enters the altered layer, it is redistributed by ion-beam mixing, which can be described by a Fick-like diffusivity. [1]
If the beam does not induce reactions in the sample, the partial differential equation describing the evolution of the concentration profile $\boldsymbol{C}(x,t)$ of a certain species in the target during a sputter-profile experiment can be written as:

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\boldsymbol{v} c) \qquad (1)$$

where: C is the concentration of the species composing the target layer, $\boldsymbol{v}$ is the velocity at which the inner material is moving towards the surface (i.e. the sputtering rate), and D (corresponding to the Fick's diffusion coefficient in the diffusion laws) is a function describing the beam-induced alterations in the target. These include all the ion-beam effects leading to the formation of the altered layer (such as ballistic mixing and radiation enhanced diffusion) as well as beam-induced roughening. In the case of samples undergoing beam-induced reactions, the partial differential equation describing the evolution of the concentration C of the species of interest can be written as:

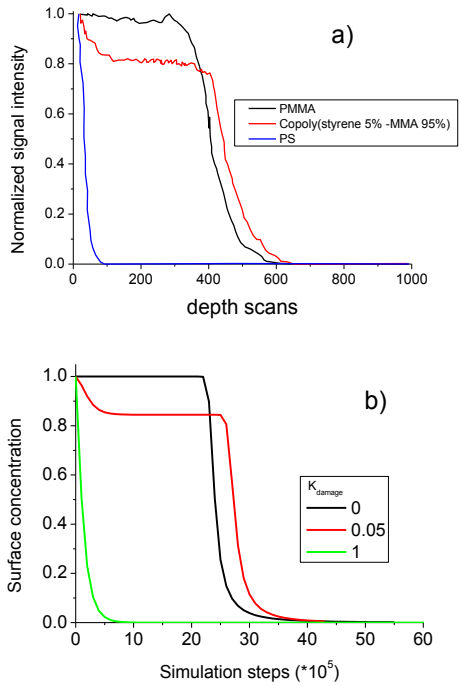
$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\boldsymbol{v} c) + R \qquad (2)$$

where R incorporates all the kinetic equations of the beam-induced reactions occurring in the region involved in the sputtering process.
During a SIMS depth profile experiment on organic samples, the intensity of species characteristic of the original material is often reduced, due to beam-induced damage. A simple case that can be hypothesized is that of a single (beam-induced) reaction taking place in the sample, which produces a decrease of concentration C of the

original molecule with a first order rate law. In such instance the continuity equation that models the entire process becomes:

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) - \nabla \cdot (vC) + \left(- K_{damage}\, C\right) * A \qquad (3)$$

where K_{damage} is the kinetic constant of the damage-producing reaction, and A is a function that takes into account the fact that the reaction is occurring in a limited depth region of the sample



We measured the SIMS depth profiles, obtained by using a C_{60} sputter beam, of several polymers displaying different damage behavior in the same experimental conditions, namely PS, PMMA and a random PS-MMA copolymer (5% styrene-95% MMA). In Figure the experimental depth profiles (1a) are compared with those calculated by means of the transport & reaction model (1b). The simulated profiles were obtained by using the same input parameters (i.e. D, v, sample thickness) with the exception of K_{damage}, which was assumed to be 1.0, 0.05 and 0.0, for polystyrene, poly (styrene-co-MMA) and PMMA respectively. As it is evident from figure, the model is able to reproduce the essential characteristics of the experimental profiles, namely the drop of signal intensity and the decrease of the sputtering yield. This is accomplished by changing just a single parameter (K_{damage},) that is describing the different ion-beam induced chemical behavior of the three systems.

References

[1] Tuccitto, N.; Zappalà, G.; Vitale, S.; Torrisi, A.; Licciardello, A. Journal of Physical Chemistry C. 2016, 120 (17), 9263-9269.

1C – Automated Data Mining of Secondary Ion Mass Spectra

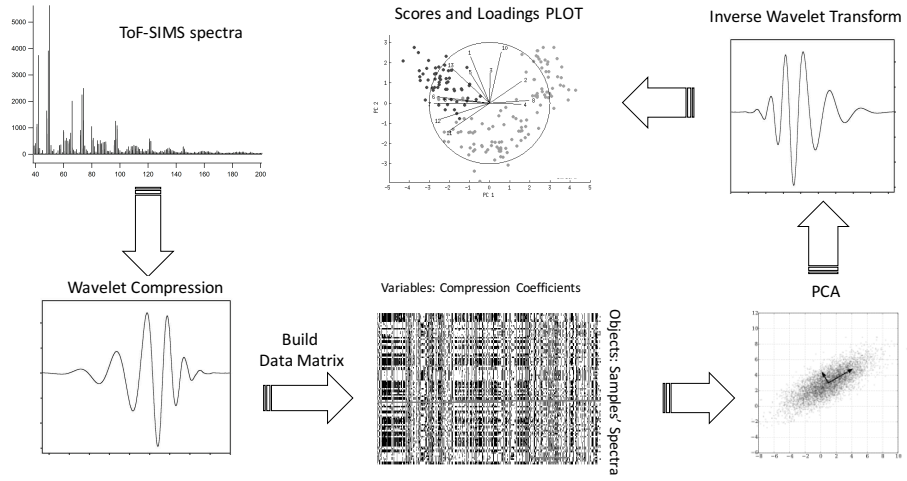
N. Tuccitto, G. Zappalà, S. Vitale, A. Torrisi, A. Licciardello

Aims

Secondary ion mass spectrometry (SIMS) is an important technique for the characterization of materials. However, each set of experiments produces giant raw data files composed by several spectra each containing thousands of peaks that carry the chemical information. The challenge is to perform an ease features extraction from complex polymeric and organic functional materials. We applied the wavelet transform for data compression and noise removal, followed by principal component analysis for feature extraction.

Results

Time of flight secondary ion mass spectrometry (ToF-SIMS) allows the reliable analytical determination of organic and polymeric materials. Since a typical raw data may contain thousands of peaks, the amount of information to deal with is accordingly large, so that data reduction techniques become indispensable for extracting the most significant information from the given data set. We used wavelet-PCA based signal processing of giant raw data acquired during ToF-SIMS experiments. The proposed procedure provides a straightforwardly "manageable" dataset without any binning procedure neither detailed integration. By studying the PCA results detailed and reliable information about the chemical composition of polymeric samples have been gathered.



The approach is based on the use of a "smart" data compression by discrete wavelet transform followed by PCA of the approximation coefficients and the successive wavelet inversed transformation of data. First the spectrum of each sample is compressed to the proper level of approximation by means of the appropriate wavelet function. The selection of the wavelet function and the choice of the acceptable

approximation-level are achieved by means of several quantitative estimators of the compression-quality. The wavelet-based compression procedure is able to reduce each original spectrum-data of 2^N factor, where N is an integer representing the selected approximation level. In such a way, PCA dataset matrix is assembled by using the wavelet approximation coefficients (PCA-variables) calculated at each scan (PCA-objects). Finally, Scores values of the most important Principal Components are plotted besides the reconstructed "pseudo–spectra" after the inverse-wavelet transform applied to the Loadings values. The benefits of performing the multivariate regression or classification analysis on the relevant signal part of the wavelet coefficients are reduced computation resources and time and possibly a better discrimination of most statistically important signals based of the study of the loadings from PCA.
This procedure has already been applied for the investigation of ToF-SIMS depth profiles data. [1,2] We applied such data-treatment on static ToF-SIMS spectra acquired from model polymers-based material deposited onto silicon substrate by means of spin-assembly procedure. The automated procedure allowed to obtain information about the sample, and this information is comparable to those obtained by a detailed classic single peak investigation that may have been performed by a specialist.

References

[1] Tuccitto, N.; Zappalà , G.; Vitale, S.; Torrisi, A.; Licciardello, A. Surface and Interface Analysis, 2016, 48 (6), pp. 317-327.
[2] Cristaudo, V.; Collette, S.; Tuccitto, N.; Poleunis, C.; Melchiorre, L.C.; Licciardello, A.; Reniers, F.; Delcorte, A. Plasma Processes and Polymers. 2016, 13 (11), 1104-1117.

2A – Environmental Assessment of total Reinjection System For Deep High Temperature/High Pressure Geothermal Resources

M.L. Parisi, M. Bravi, G. Manfrida (Univ. Firenze), F. Batini (Magma Energy Italia S.R.L.), R. Basosi

Aims

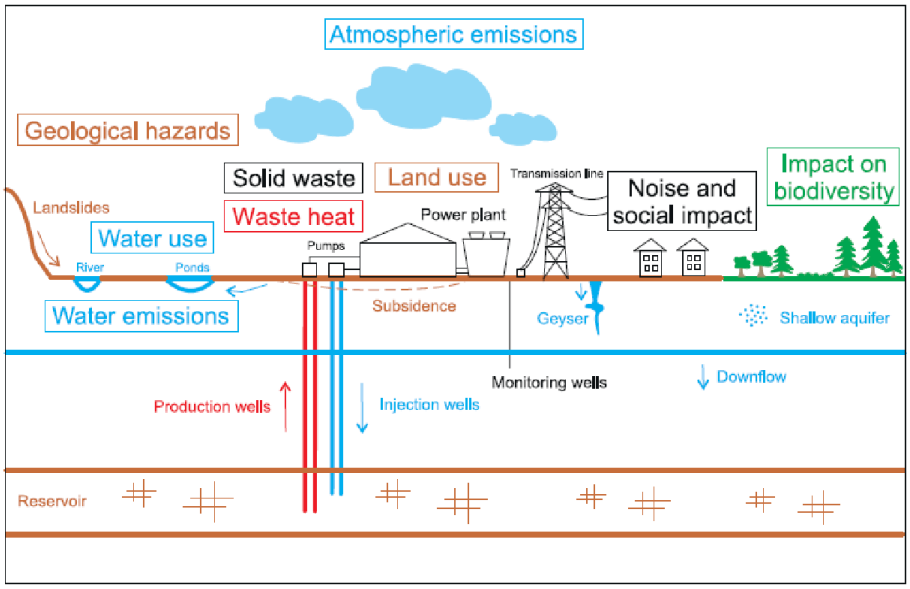
The aim of the project is the life cycle analysis of technological solutions for closed-loop zero emission and total reinjection pilot systems for geothermal energy production from high temperature and high pressure deep-seated sources.

Results

One of the major challenges Europe will face in the coming decades is to make its energy system clean, secure and efficient, while ensuring EU industrial leadership in low-carbon energy technologies. Geothermal energy can strongly contribute to decarbonise the energy system in a sustainable way, to secure energy supply and to complete the energy internal market in line with the objectives of the Strategic Energy Technology Plan (SET-Plan) and of the related energy legislation (notably the Renewable Energy and CCS Directives) and energy policies designed to deliver the 2020 targets and to shape energy market frameworks for 2030 and 2050. The growth of geothermal power production is mainly related to deep (> 3 km) high temperature HT (>250°C) high pressure HP (>70 bar) resources mostly located in fractured hard rock reservoirs. These resources are located in magmatic areas, which are often intensively cultivated or environmentally protected. Geothermal development in such regions can be severely hindered by the perspective of emission of Mon-Condensable Gases (NCG) in the atmosphere. Furthermore, the NCG emissions pose some concern to the effectiveness of geothermal to mitigate climate change. Lack of Social acceptability related to venting of NCG poses a major financial risk and effectively renders many prospective areas with excellent subsurface potential, which are proximal to inhabited areas in Europe, unattractive for development. Total reinjection can avoid emission of NCG, and considerable enhance resource development. However, new resource-efficient and cost-effective concepts and technologies for total reinjection are needed in order to increase the economic and environmental sustainability of geothermal projects with a minimal environmental footprint.

In this context the life cycle analysis methodology is employed in order to perform a systematic and in-depth geo-specific assessment of environmental impacts and burdens (in energy, resources and emissions terms) connected with the technological solutions used for the realization and implementation of a geothermal pilot plant with total reinjection system in the Tuscany region.

The outcomes of such analysis are pivotal to draw the eco-profile of the geothermal system in order to highlight the critical points and hot spots of the process, on one hand, and to make comparisons with other available technologies for the exploitation of the geothermal resource in similar geophysical conditions.



References

Bravi, M.; Basosi, R. "Environmental impact of electricity from selected geothermal power plants in Italy", Journal of Cleaner Production 66, 301-308 (2014).

Ruzzenenti, F.; Bravi, M.; Tempesti, D.; Salvatici, E.; Manfrida, G.; Basosi R. "Evaluation of the environmental sustainability of a micro CHP system fueled by low-temperature geothermal and solar energy", Energy Conversion and Management 78, 611-616 (2014).

Fiaschi, D.; Lifshitz, A.; Manfrida, G.; Tempesti, D. "An innovative ORC power plant layout for heat and power generation from medium-to low-temperature geothermal resources", Energy Conversion and Management 88, 883-893 (2014).

Bayer, P.; Rybach, L.; Blum, P.; Brauchler R. "Review on life cycle environmental effects of geothermal power generation", Renewable and Sustainable Energ Reviews 26, 446-463 (2013).

Kaya, E.; Zarrouk, S.; O'Sullivan, M. "Reinjection in geothermal fields: A review of worldwide experience", Renewable and Sustainable Energy Reviews 15, 1, 47-68 (2011).

2A – Biomass Adsorbent for Removal of Toxic Metal

R. Angelico, G. Palumbo,
R. Campanini (Dept. Phys. University of Bologna, BO, Italy)

Aims

The contamination of water bodies by heavy metals has been the subject of many studies worldwide. Systems such as ion exchange resins, electrochemical process, chemical precipitation and activated carbon have been widely used in the processes of wastewater purification. Such processes could have reduced its costs from the use of alternative and cheaper materials. Materials of natural origin such as seaweed, biological depuration plant sludge, agricultural and industrial wastes are inexhaustible, low-cost and non-hazardous materials, which are specifically selective for different contaminants and easily disposed by incineration. Rice husk (RH) is a low cost (agricultural by-product) bio-adsorbent which has been studied intensively for the removal of various heavy metals and metalloids (such as Pb, Cd, Zn, Ni and As) from both groundwater and surface water. However, no investigations have yet been carried out about the role played by the size and shape of HR particles on the adsorption efficiency for the removal of heavy metals from aqueous solutions.

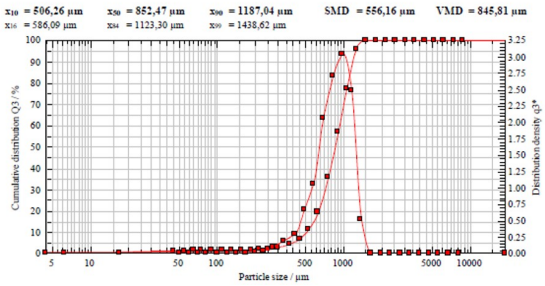
Results

A weighted amount of raw rice husk (RH), generated as agricultural waste material in a rice producing plant located in Northern Italy (Figure 1A), was washed with deionized water and let drying in ventilated oven at 40-50°C. 10 g of washed RH were grounded with a lab mill and subsequently passed through a sieve with a mesh size of 1.0 mm.

A dynamic image analyser, capable to acquire every single particle image of the sample analysed, thus ensuring a perfect statistical representation thanks to the large amount of particles (order of million particles!) analysed in a short time, was used to perform the particle size analysis of the passed RH fraction (Figure 1B).

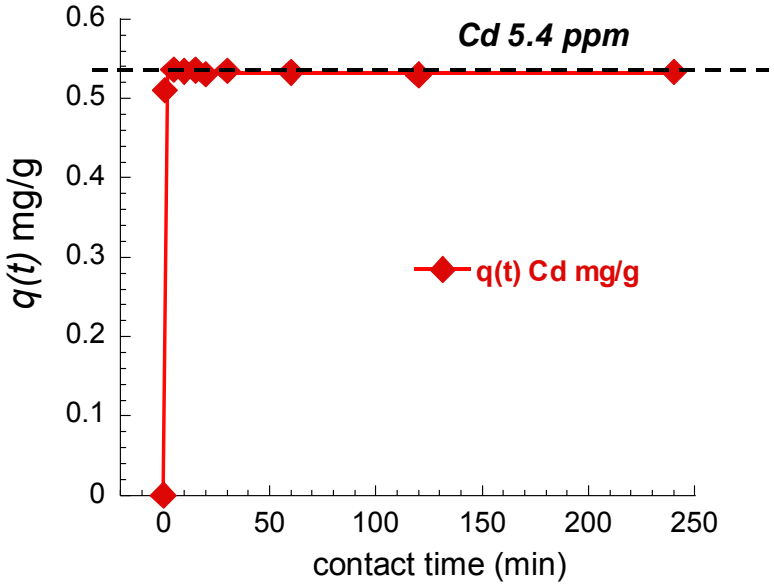
1A

1B



A first indication of the high adsorption efficiency of RH toward Cd was yielded from a series of adsorption tests, where equal amounts of sieved RH (1g each sample) were left in contact with a Cd 5.4 ppm aqueous solution for increasing contact times from 1 to 240 min. Analytical determinations of residual Cd recorded vs time confirmed that

just after t = 5 min, 1 g of RH was able to adsorb 100 % of heavy metal dissolved in 100 ml aqueous solution.



Further experiments are in progress to investigate the equilibrium sorption property of RH and combine several adsorption isotherm models with physicochemical parameters of the adsorbent, such as surface area, average size and shape of particles and chemical composition.

References

Angelico, R.; Palumbo, G.; Torino, V.; Campanini, R. "Adsorption of Cd ions by rice husk: a focus on the physicochemical parameters of the adsorbent", submitted to International Journal of Environmental Research and Development (2016).

Zhang, Y.; Zheng, R.; Zhao, J.; Ma, F.; Zhang, Y.; Meng, Q. "Characterization of H_3PO_4-Treated Rice Husk Adsorbent and Adsorption of Copper(II) from Aqueous Solution", BioMed. Res. Int. 10.1155/2014/496878 (2014).

2A – Synergies in chemical, optical and biological conditions causing the formation of black water blooms

S.A. Loiselle, L. Galgani, C. Rossi, H. Duan (CAS-China), Y. Zhang (CAS – China), R. Ma (CAS – China)

Aims

Excessive production of organic matter in aquatic ecosystems can lead to a phenomena known as black water blooms. These have been associated to fish-kills and the closure of potable water supplies. The frequency and duration of these events has increased in recent decades in rivers, inland lakes and reservoirs, and has often been associated with the decay and release of organic matter (planktonic algae, aquatic macrophytes, sediment release, etc.).

Results

Using optical, chemical and biological approaches, the present series of studies shows the interactions between microbial, chemical, hydrodynamic and optical conditions necessary for black blooms to occur. The study combines field investigations and laboratory mesocosm studies to show that black blooms are caused by a combination of high CDOM (chromophoric dissolved organic matter) absorption, the formation of CDOM-Fe complexes and low backscattering. Mesocosm experiments showed that black bloom conditions occur after 4 days, with a significant increase in the concentrations of Fe2+ and ΣS2-. Total absorption (excluding absorption due to water) at 440nm increased by 30% over this time to 7.3 m-1. In addition, the relative contribution of CDOM absorption to the non-water total absorption increased from 18% to 50%. Regression analyses between chemical and bio-optical data in both field and mesocosm experiments indicated that the concentrations of Fe2+ co-varied positively with CDOM absorption ag(440) ($R2 > 0.70$), and the specific CDOM absorption (ag(440)/DOC). Conditions that favored the development of black blooms were elevated algal or macrophyte biomass and limited water column mixing.

References

Zhang, Y.; Ma, R.; Duan, H.; Loiselle, S.; Zhang, M.; Xu, J. “A novel MODIS algorithm to estimate chlorophyll a concentration in eutrophic turbid lakes”, Ecological Indicators 69, 138-151 (2016).

Duan, H.; Loiselle, S.A.; Li, Z.; Shen, Q.; Du, Y.; Ma, R. “A new insight into black blooms: Synergies between optical and chemical factors”, Estuarine, Coastal and Shelf Science 175, 118-125 (2016).

Jiang, G.; Ma R.; Duan H.; Ma R.; Loiselle S.A. “Remote sensing of particulate organic carbon dynamics in a eutrophic lake (Taihu Lake, China)” Science of The Total Environment 532, 245-254 (2015).

Duan, H.; Ma, R.; Loiselle, S.A.; Shen, Q.; Yin, H.; Zhang, Y. “Optical characterization of black water blooms in eutrophic waters”, Science of The Total Environment, 482–483: 174-183 (2014).

2A – Micro and macroscale drivers of nutrient pollution in freshwater environments in North and South America

S.A. Loiselle, C. Rossi, D. Gasparini, F. Cunha (USP-Brazil), S. Shupe (UFV-Canada), E. Valiente (UNM- Mexico), L. Rocha (UL – Argentina)

Aims

Widespread use of agricultural fertilisers has had a significant impact on freshwater ecosystems across the globe. To identify the extent of these impacts, low cost methods are combined with enagment approaches to train communities to monitor their environment for the degree of impact related to eutrophication.

Results

The present study explored the relationship of nutrient concentrations in 150 streams in 57 hydrological basins in South, Central and North America (Buenos Aires, Curitiba, São Paulo, Rio de Janeiro, Mexico City and Vancouver) with macroscale information available from global datasets and microscale data acquired by trained citizen scientists. New methods to determine average sub-basin phosphate (P-PO4) concentrations were found to be well correlated with sub-basin attributes on both macro and microscales, while the relationships between sub-basin attributes and nitrate (N-NO3) concentrations were limited. A phosphate threshold for eutrophic conditions (>0.1 mg L-1 P-PO4) was exceeded in basins where microscale point source discharge points (eg. residential, industrial, urban/road) were identified in more than 86% of stream reaches monitored by citizen scientists. The presence of bankside vegetation covaried (rho = –0.53) with lower phosphate concentrations in the ecosystems studied. Macroscale information on nutrient loading allowed for a strong separation between basins with and without eutrophic conditions. Most importantly, the combination of macroscale and microscale information acquired increased our ability to explain sub-basin variability of $P\text{-}PO_4$ concentrations. The identification of microscale point sources and bank vegetation conditions by citizen scientists provided important information that local authorities could use to improve their management of lower order river ecosystems.

References

Castilla, E.P.; Cunha, D.G.F.; Lee, F.W.F.; Loiselle, S.; Ho, K.C.; Hall, C. "Quantification of phytoplankton bloom dynamics by citizen scientists in urban and peri-urban environments", Environmental monitoring and assessment, 187 (11), 1-11 (2015).

Loiselle, S.A.; Cunha, D.G.F.; Shupe, S.; Valiente, E.; Rocha, L.; Heasley, E.; Belmont, P.P.; Baruch, A. "Micro and Macroscale Drivers of Nutrient Concentrations in Urban Streams in South, Central and North America", PloS one 11 (9), p.e0162684.

2A – LCA of integrated agro-industrial chains for energy and biochemicals production from micro-algae and terrestrial oilseed crops

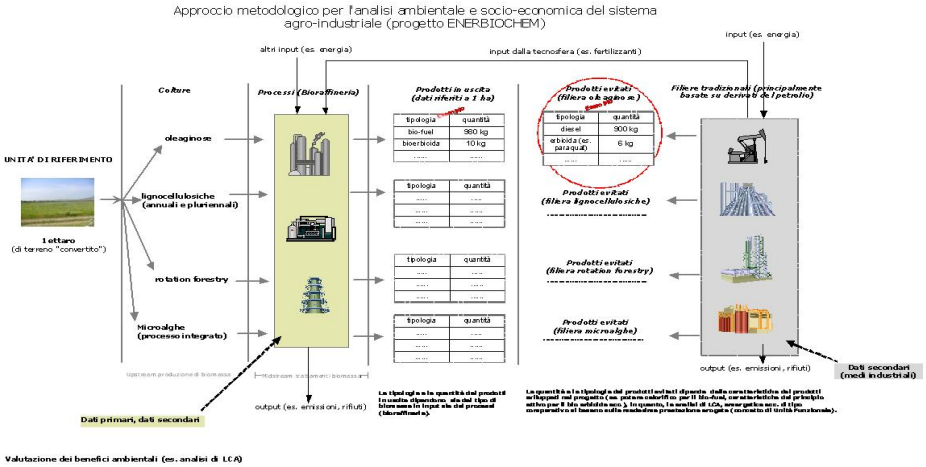
S. Jez, E. Busi, D. Spinelli (Laboratory Manager / R&D unit, Solaris Biotechnology srl), M.L. Parisi, R. Basosi

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.

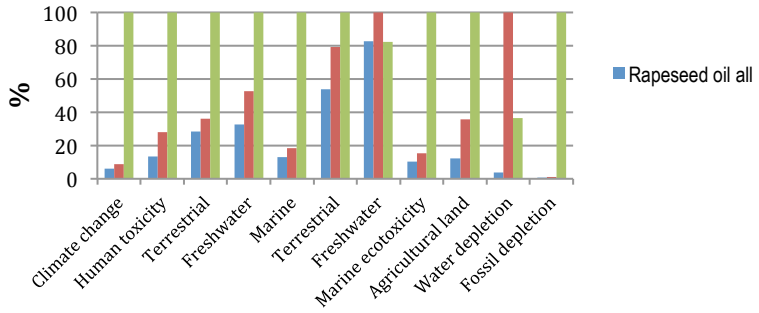
Results

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. Valorisation of residues and by-products through the production of new renewable products are investigate in order to improve the competitiveness of the entire production system. A variety of studies and investigations are carried out on biomass production, transformation processes and optimization of end-products use and recycling of by-products of oilseeds crops, lignocellulosic and autotrophic algae and yeast. 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.

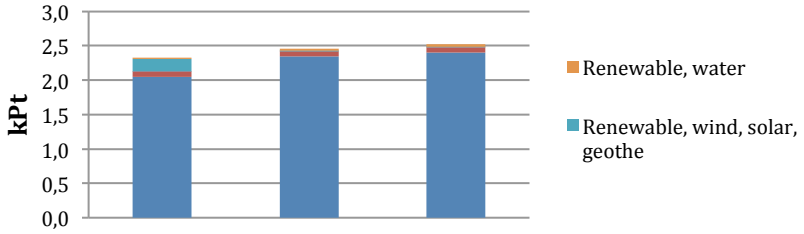


Environmental Impact Indicators (Embodied Energy Analysis (EEA), Energy Accounting (EA) and LCA has been applied to oleaginous crops: sunflower, rapeseed and tobacco. The results, according with our previous studies, show that the major

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. Final results show that despite their high potential as sustainable energy feedstock, micro-algae are not yet competitive with the traditional oil crops in both economic feasibility and environmental impact.
A further important result is that the use of renewable technologies as photovoltaics and biogas self production could increase the competitiveness of micro-algae oil reducing its demand of non-renewable energy sources. This can reduce the costs of production of oil from micro-algae, allowing a cheaper and more efficient production of biofuel or value added crops in remote locations far from sources of electrical power.



Comparison among sunflower oil, rapeseed oil and micro-algae oil production processes (ReCiPe Midpoint (H) V1.04 / Europe ReCiPe H / Characterization).



Comparison with CED Method of three scenarios of algae oil production

References

Spinelli, D.; Jez, S.; Busi, E.; Fierro, A; Basosi, R. "Comparative Life Cycle Assessment study on environmental impact of oil production from micro-algae and terrestrial oilseed crops", Energy Conversion and Management (under revision).
Spinelli, D.; Bardi, L.; Fierro, A.; Jez, S.; Basosi, R. "Environmental analysis of sunflower production with different forms of mineral nitrogen fertilizers", Journal of Environmental Management 129, 302-308 (2013).
Spinelli, D.; Jez, S.; Pogni, R.; Basosi, R. "Environmental and LCA analysis of a biodiesel production line from sunflower in the province of Siena (Italy)", Energy Policy 59, 492-506 (2013).
Spinelli, D.; Jez, S.; Basosi, R. "Integrated Environmental Assessment of sunflower oil production", Process Biochemistry 47, 1595-1602 (2012).

2A – Energy efficiencies and LCA studies on technologically advanced energy devices and grid system

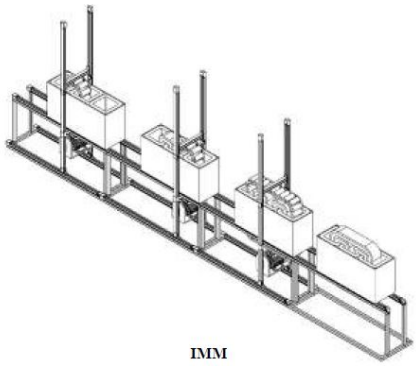
E. Busi, S. Maranghi, M.L. Parisi, R. Basosi

Aims

The project aims to achieve the primary goal of creating all the skills necessary for the manufacture of innovative three-phase distribution transformers (Medium Voltage /Low Voltage).

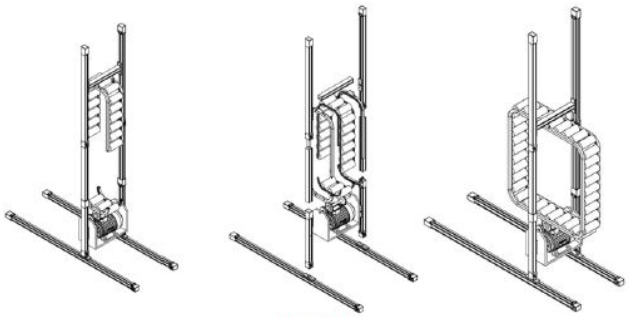
Results

This study wants to insert new types of MV/LV transformers with very high efficiency, not only in the European markets, but also in the American and Asian ones. The transformer which is currently being tested is based on a new concept type of ferromagnetic core, where the innovation lies in the construction of this element starting from a sheet of amorphous ferromagnetic material which, thanks to an automated construction system, manages to be wrapped inside the coils. The current architecture of the electrical system has been defined since its inception thanks to the invention of the transformer: this has allowed the development of electric generators in MT, the transfer in HT and end use both MT (industries) and LV.
The project wants to develop, on the one side an attractive product for the market (three-phase transformer with a continuous core in amorphous material), on the other an industrial process for the transformers realization. The production process will be based on the current machine providing a highly automated system, in which the intervention of an operator is limited to only some stages of preparation of the product. The model of the industrial machine (IMM), is composed of four stations, three reserved for the formation of cores and one for the removal of the completed transformer.



IMM

The three processing stations are functionally identical and consist of the same basic module developed by Newton (PIMM). The production process involves the construction of the three phase transformer in four distinct stages, each characterized by the formation of a specific part of the transformer.



PIMM

Once completed the winding of the three ferromagnetic cores, the transformer can be subjected to a hardening phase if the resin applied on the surfaces if the tapes being the thermosetting resin, the transformer can be placed in an oven to effect polymerization if the resin itself and consolidate thereby between them the coils of the amorphous material.
The production process is completely different from the one currently used for the production of core laminations, and the solution developed will allow the lead partner to introduce a high degree of automation, so that the productivity of its plants can be significantly increased. Currently the production of this type of transformers is done with a low degree of automation, in fact the majority of the construction stages are done manually. The production system that the project intends to develop will guarantee certain costs for the production (having reduced the operators' manual intervention to a minimum), environmental benefits thanks to the use of the LCA (Life Cycle Assessment) and LCC (Life Cycle Costing) methodologies and a potentially improved productivity with time. The process will also help improve the standards of the product compared to the existing production processes, as it will be capable of a real series production.
Other important objectives of the project are the study and optimization of the resin from the chemical point of view, conferring it the specific characteristics required by the project as also in terms of solidification times. Other studies will consider the process of realization of the rolls, in particular the deposition of the resin. The final products of the project will be more samples of the pre-series of the transformer manufactured by the prototype of the production line.

References

Bermada, S.; Rizzo, R.; Sani, L. “Didactic Considerations on Magnetic Circuits Excited by Permanent Magnets”, Ieee Transcation On Education 52/4, 532 (2009).
Ceraolo, M.; Funaioli, M.; Lutzemberger, G.; Pasquali, M.; Poli, D.; Sani, L. “Electrical storage for the Enhancement of Energy and Cost Efficiency of Urban Railroad Systems”, Proceedings of the II International Conference on the Railway Technology, Ajaccio (FR) (2014).
Grossi, N.; Scippa, A.; Sallese, L.; Sato, R.; Campatelli, G. “Spindle speed ramp-up test: A novel experimental approach for chatter stability detection”, International Journal of Machine Tools and Manufacture 89, 224-233 (2015).
Parisi, M.L.; Maranghi, S.; Basosi, R. “The evolution of the dye sensitized solar cells from Grätzel prototype to up-scaled solar applications: A life cycle assessment approach”, Renewable and Sustainable Energy Reviews 39, 124-138 (2014).

2A – Nanomaterials for enzymes immobilization

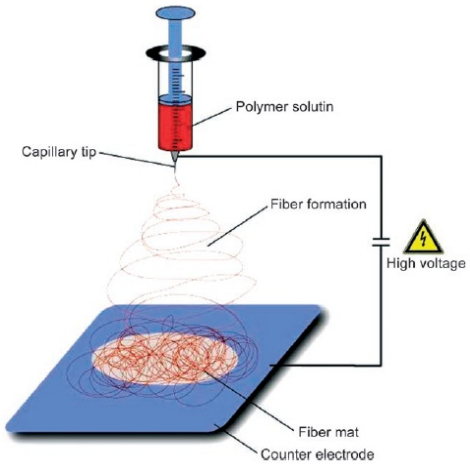
D. Spinelli (Laboratory Manager / R&D unit, Solaris Biotechnology srl), E. Fatarella (Next Technology Tecnotessile), M.C. Baratto, R. Basosi, R. Pogni

Aims

The aim of this research is to address the catalytic properties of different enzymes supported onto nanomaterials 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.

References

Fatarella, E.; Spinelli, D.; Ruzzante, M.; Pogni, R. "Nylon 6 film and nanofiber carriers: preparation and laccase immobilization performance", Journal of Molecular Catalysis B: Enzymatic, submitted (2014).

Spinelli, D.; Fatarella, E.; Di Michele, A.; Pogni, R. "Immobilization of fungal (Trametes versicolor) laccase onto Amberlite IR-120H beads: optimization and characterization", Process Biochemistry 48, 218-223 (2013).

Spinelli, D.; Coppi, S.; Basosi, R.; Pogni R. "Biosynthesis of ethyl butyrate with immobilized Candida rugosa lipase onto modified Eupergit C", Biocatalysis 1, 1-12 (2014).

2A – Visible light activated carbon doped titanium dioxide for cleaning of olive mill wastewaters

F. Lopez, F. Venditti (C. O. S. I. B. Termoli – CB), A. De Leonardis, F. Cuomo, A. Ceglie

Aims

Study of the efficiency of the visible light activated Carbon doped Titanium Dioxide photocatalyst towards the olive mill wastewaters (OMW) compounds.

Results

Carbon doped titanium dioxide (CDT) was tested as catalyst for photodegradation of phenolic compounds of olive mill wastewater (OMW). The activation of the catalyst was triggered by exposure to visible light radiation. The cleaning effectiveness of this catalyst towards the polluted wastewater from olive oil industry was demonstrated by means of HPLC and UV-visible spectroscopy combined with phenol compound determination. The photodegradation activity was tested on systems having different initial concentration of phenols and in the presence of different amounts of CDT. By introducing a suitable parameter, namely the ratio between the amount of catalyst and the amount of total phenols Ti/TPh, it was demonstrated that the proposed degradation method could be scaled up without losing its effectiveness. The OMW decolorization occurring in the presence of CDT particles under visible light radiation is marked enough to be directly appreciated with the naked eye. The decolorization is strongly associated with the removal of phenols. In fact, while bleaching the solutions, CDT successfully removed 70% of the phenols in 24 hours. HPLC analysis demonstrates that CDT was effective in degrading the higher part of the phenols of OMW.

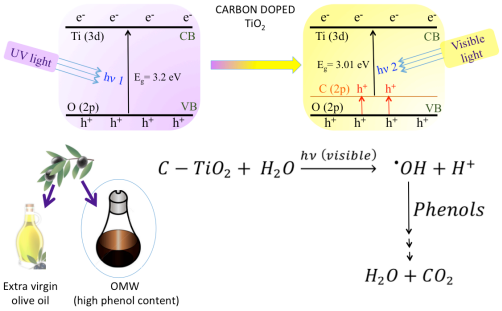


Fig. 1: Above: the difference between TiO_2 and carbon doped TiO_2 in terms of light activation either UV or visible light. The difference of band gap energy from 3.2 to 2.3 eV is also highlighted. Below: OMW from the production of olive oil, the content of phenols and the photo-oxidation reaction obtainable in the presence of CDT is depicted.

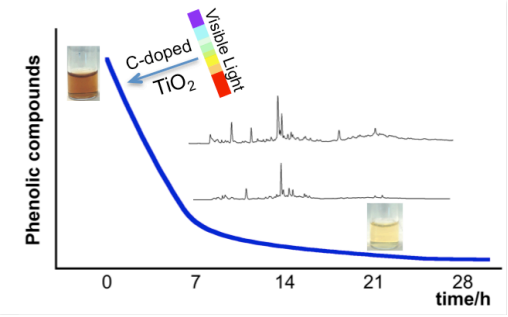


Fig. 2: Whitening of OMW in the presence of visible light activated CDT. HPLC chromatograms refer to the initial OMW phenolic fraction (upper chromatogram) and to the phenolic fraction after 23 hours of treatment. After 23 h almost all the representative phenolic species were removed from the water solution.

References

Cuomo, F.; Venditti, F.; Cinelli, G.; Ceglie, A.; Lopez, F. "Olive mill wastewater (OMW) phenol compounds degradation by means of a visible light activated titanium dioxide-based photocatalyst", Zeitschrift fur Physikalische Chemie 230 (9), 1269-1280 (2016).

Venditti, F.; Cuomo, F.; Ceglie, A.; Avino, P.; Russo, M.V.; Lopez, F. "Visible light caffeic acid degradation by carbon-doped titanium dioxide", Langmuir 31 (12), 3627-3634 (2015).

Cuomo, F.; Venditti, F.; Ceglie, A.; De Leonardis, A.; Macciola, V.; Lopez, F., "Cleaning of olive mill wastewaters by visible light activated carbon doped titanium dioxide", RSC Advances 5 (104), 85586-85591 (2015).

2A – Physico-chemical analysis and characterization of ancient mortars and other archaeological materials

P. Cofrancesco, C. Milanese, A. Girella, G. Trojsi, A. Frisetti, F. Marazzi (Suor Orsola Benincasa University, Napoli)

Aims

The main aim of this project is to investigate, from the physico-chemical point of view, the materials coming from archaeological investigations.

Results

Within the framework of an archaeological and historical survey of the Medieval and Roman buildings of the Medio Volturno River area (in the Italian regions of Molise and Campania) conducted by the Laboratorio di Archeologia Tardoantica e Medievale (LATEM) of the University Suor Orsola Benincasa of Naples, we analyzed and characterized the samples of ancient mortars of about 25 historical sites of the area, dating from the 1st century B.C. to the 14th century A.D., taken from several different kind of buildings, with civil, religious, and military uses. The physico-chemical characterization of the mortars was carried out by X-ray powder diffraction (XRPD) with Rietveld refinement, for the quantitative determination of their mineralogical compositions, with subsequent validation by scanning electron microscopy (SEM) with energy dispersion spectroscopy (EDS). Moreover, thermo-gravimetric measurements (TGA) were performed to determine the water content of the mortars, and microscopic thin sections analyses were made to obtain information about their morphological and basic physical properties. The results of the analyses were mapped by our GIS system (Fig. 2), and compared with geological data of the area of interest to find the relation between the composition of the mortars and the typical minerals present in each area.

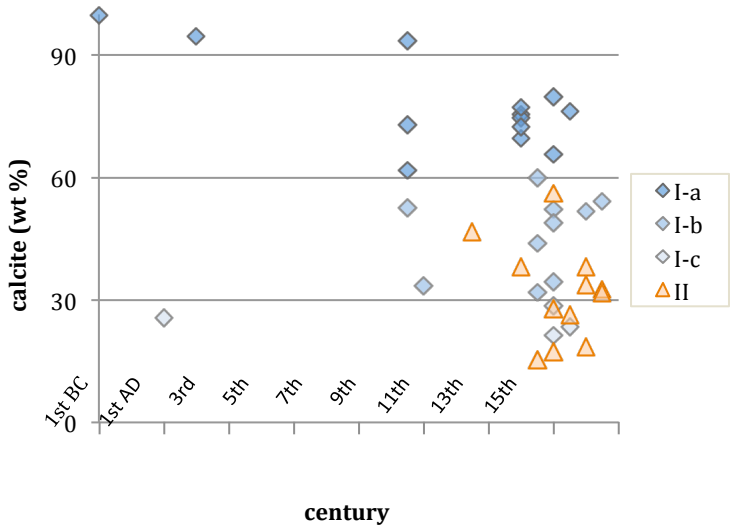


Fig.1

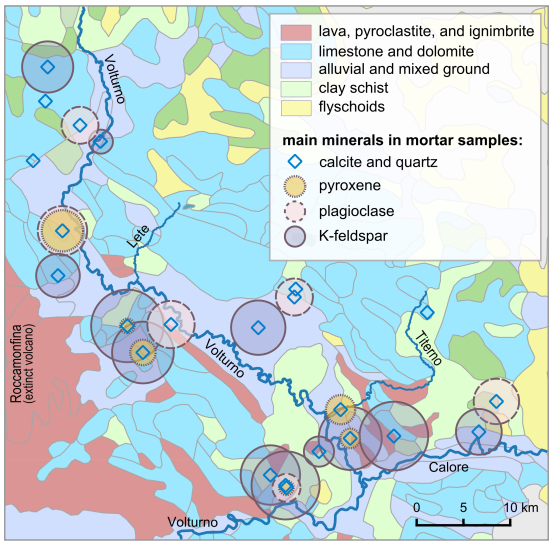


Fig. 2

We also found that, during the classical Roman period, the Vitruvius' suggestion of using "pure carbonate rock" was the standard practice, not only for the binder, but also for the aggregate part of mortars, in particular for public buildings, such as bridges and city walls. On the contrary, during the Middle Ages it was common to use other raw materials with lower percentage of carbonate rocks, such as feldspars and other volcanic minerals, typical of the region Campania areas, rich in volcanic sediments, and also some amorphous materials, such as ground bricks, and glassy volcanic stones. It is also frequent to find poor quality medieval mortars, because of the low quality of the raw materials from one side, and because of the often hurried binder preparation process, resulting in more friable mortars and, consequently, in less durable walls.

References

Cofrancesco, P.; Frisetti, A.; Licchelli, M.; Milanese, C.; Trojsi, G. 1st International Conference on Metrology for Archaeology, Benevento, Italy, October 22-23 2015 “Analysis and characterization of ancient mortars of the Medio Volturno River area”. Oral Presentation.

Cofrancesco, P.; Milanese, C.; Trojsi, G.; Girella, A.; Valsecchi, G.; Bombeccari, M.; Frisetti A. XLIV Congresso della Divisione di Chimica Fisica della SCI, Napoli, Italy, September 20-23 2016 “Ancient mortars from the classical antiquity to the Middle Ages in the Medio Volturno River area”. Oral presentation.

2A – Organogels for the cleaning of artifacts

M.D. Pianorsi, M. Raudino, P. Ferrari, N. Bonelli, D. Chelazzi, R. Giorgi, E. Fratini, P. Baglioni

Aims

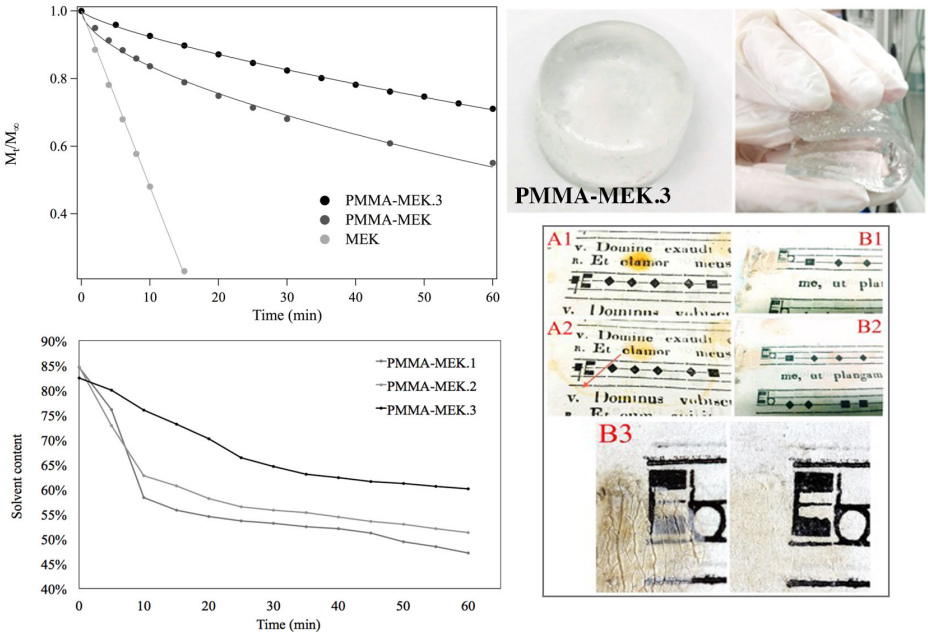
Synthesis and characterization of chemical organogels with tunable properties for the cleaning of artworks.

Results

Gels are particularly useful for the cleaning of works of art, as they allow the controlled delivery of cleaning fluids on solvent-sensitive substrates such as easel paintings. Owing to the presence of covalent cross-links between the polymer chains, chemical gels exhibit mechanical properties that allow their easy handling and their residue-free removal from artistic surfaces after the cleaning intervention.

MMA-based organogels obtained by solubilizing MMA in pure organic solvents (e.g. ethyl acetate, butyl acetate and metyl-ethyl ketone) and using a dimethacrylate cross-linker were prepared for the removal of historical varnishes from canvas painting samples. The macro- and mesoporosity of the gels have been characterized through Scanning Electron Microscopy (SEM) and Small Angle X-ray Scattering (SAXS). Moreover, a new organogel, based on MMA and MEK was specifically designed for the selective removal of aged wax layers from the surface of ancient (solvent-sensitive) inked paper. The new gel formulation was designed in order to improve on previous PMMA-based gels, which lacked the desired retentiveness, for extending their application also to paper substrates. To achieve this improvement, we systematically tuned the amount of cross-linker and monomer-solvent phase ratio used during the free radical polymerization of MMA in the MEK liquid phase, which allowed obtaining organogels with optimal characteristics in terms of retentiveness and mechanical properties (i.e. feasible handling and removal from the treated surface). The increased amount of cross-linker and the different solvent-monomer ratio used in the radical process, resulted in a decreased solvent content and mesoporosity of the gel network. In turn, this led to a slower and more gradual solvent release, both on porous and non-porous surfaces, as compared to the previous formulation (see left panel in figure). The PMMA-MEK organogels were applied on a 19th century inked document (see figure) to remove spots of paraffin wax that hindered the readability and aesthetic appearance of the artifact. The performance of the new systems (PMMA-MEK.3) was compared to that of the previous formulation (PMMA-MEK.1, PMMA-MEK.2). The gel formulation previously developed (which worked well on varnished canvas paintings) led to uncontrolled spreading of MEK and to the formation of tidelines on the paper surface (A1-2 in figure). On the other hand, the new PMMA-MEK.3 system allowed a safer and more gradual release of solvent on the paper surface, which led to the gradual swelling and detachment of the wax contaminant (B1-3 in figure).

After the cleaning intervention, the gel can be removed without leaving polymer residues on the surface as verified by ATR-FTIR.



Overall, this work validated the tunable synthesis of PMMA-based organogels as a process to produce versatile cleaning tools that can be used on different artistic surfaces, decreasing the risks of altering the original properties of the artifacts.

References

Pianorsi, D.; Raudino, M.; Bonelli, N.; Chelazzi, D.; Giorgi, R.; Baglioni, P.; "Organogels for the cleaning of artifacts", Pure Appl. Chem., accepted for publication (2017).

Baglioni, P.; Bonelli, N.; Chelazzi, D.; Chevalier, A.; Dei, L.; Domingues, J.A.L.; Fratini, E.; Giorgi, R.; Martin, M.; "Organogel formulations for the cleaning of easel paintings", Appl. Phys. A 121, 857-868 (2015).

Baglioni, P.; Chelazzi, D.; Giorgi, R. "Nanotechnologies in the Conservation of Cultural Heritage", Springer (2015).

Baglioni, P.; Chelazzi, D. "Nanoscience for the Conservation of Works of Art", RSC Publishing (2013).

2A – Chemical hydrogels for the cleaning of artifacts

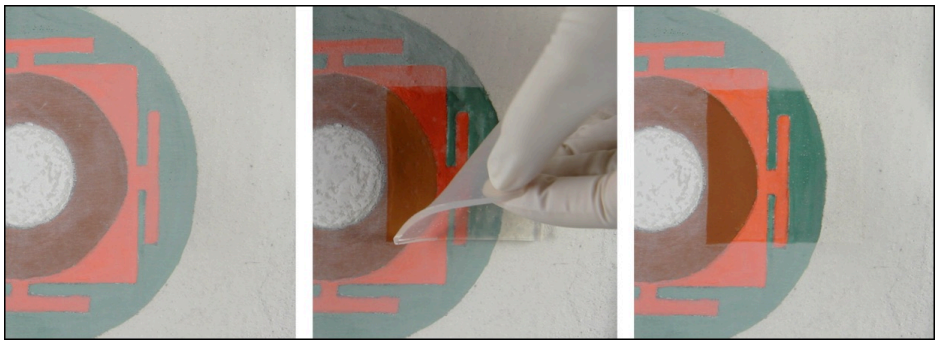
N. Bonelli, E. Fratini, R. Giorgi, P. Baglioni

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.



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

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.

References

Domingues, J.A.L.; Bonelli, N.; Giorgi, R.; Baglioni, P. "Chemical Semi-IPN Hydrogels for the Removal of Adhesives from Canvas Paintings", Appl Phys A 3, 705-710 (2014).
Domingues, J.A.L.; Bonelli, N.; Giorgi, R.; Fratini, E.; Baglioni, P. "Innovative Method for the Cleaning of Water-Sensitive Artifacts: Synthesis and Application of Highly Retentive Chemical Hydrogels", Int J Conserv Sci, Special Issue, 715-722 (2013).
Domingues, J.A.L.; Bonelli, N.; Giorgi, R.; Fratini, E.; Gorel, F.; Baglioni, P. "Innovative hydrogels based on semi-interpenetrating p(HEMA)/PVP networks for the cleaning of water-sensitive cultural heritage artifacts", Langmuir 29, 2746-2755 (2013).
Baglioni, P.; Chelazzi, D.; Giorgi, R.; Poggi, G. "Colloids and Material Science for the Conservation of Cultural Heritage: Cleaning, Consolidation and Deacidification", Langmuir 29, 5110-5122 (2013).

2A – Film forming PVA-based cleaning systems for the removal of corrosion products from historical bronzes

E.I. Parisi, N. Bonelli, E. Carretti, R. Giorgi, P. Baglioni

Aims

Development of plasticized PVA-based polymeric systems loading complexing agents for the safe removal of alteration products from historical Cu-based alloys.

Results

Innovative poly(vinyl)alcohol-based film forming system, specifically devised for the controlled and selective cleaning of copper-based artifacts were developed.

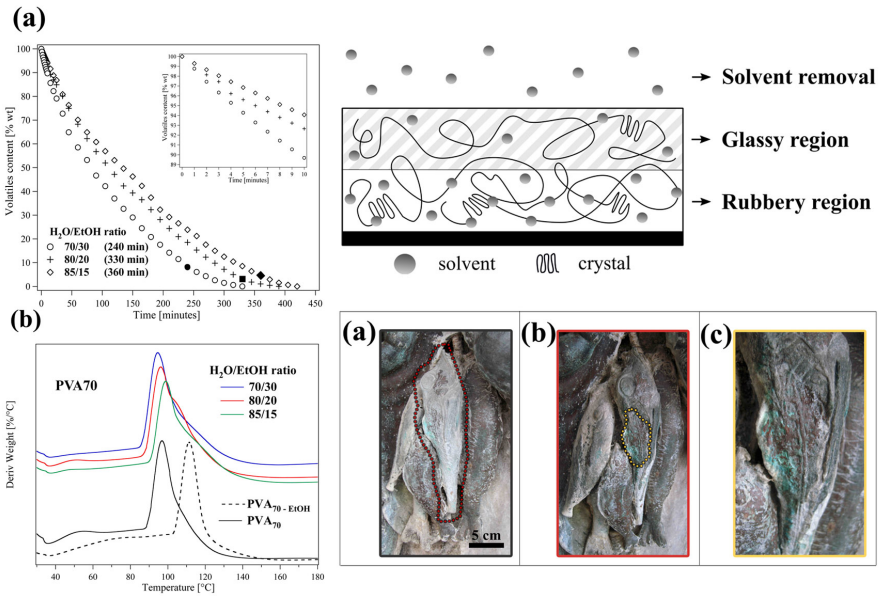
Traditional cleaning procedures of metallic artifacts are commonly performed by mechanical and/or chemical methods. Both these methods present some limits related to both, the poor selectivity and invasiveness of the mechanical procedure, and to the scarce control over the reactions involved in the chemical approach.

In the case of copper-based alloys, the cleaning procedure is particularly delicate, it should aim at the complete removal of the defacing and harmful corrosion products of Cu(II) (copper carbonates, sulphates, chlorides, etc.) but preserving the underlying protective cuprite Cu(I) layer.

The proposed cleaning procedure consists in the application of a PVA-based polymeric solution able to form an elastic film, which can be gently peeled off from the surface upon drying. Plasticizers (different polyols) were added to the solution in order to obtain a final film with suitable mechanical properties to facilitate the peeling action, while the composition of the volatile fraction (water and ethanol) was adjusted in order tune both, the viscosity of the system and the time required for the film to form. Finally, a complexing agent (EDTA, chosen because of its good chelator performances and selectiveness for Cu(II)) was loaded in the polymeric dispersion.

The main advantage of this cleaning system consists in the simultaneous chemical and mechanical action, guaranteed by both, the presence of the complexing agent and the final removal of the film by peeling off.

The physico-chemical characterization of the system was carried out in order to investigate the kinetics of film formation, the variation in mechanical behavior of the system during drying, and the properties of the final polymeric films. The kinetics of film formation were studied by means of gravimetric and thermogravimetric methods (both scanning and isothermal) and rheology (both dynamic and rotational experiments) was used to investigate changes in mechanical behavior during evaporation of the volatile fraction of the system. The final films were characterized by means differential scanning calorimetry (DSC) and ATR-FTIR to evaluate the crystallinity degree, which is correlated to rigidity of the polymeric film. Moreover, the viscoelastic behavior of the system before and after the addition of a complexing agent solution was studied by means of rheological measurements.



The PVA70 formulation, containing 70% of volatiles fraction (55% H_2O and 15% ethanol) showed the best application properties in terms of manipulation (initial viscosity), evaporation kinetics (see left panels in figure, showing the temperatures of evaporation and kinetics of formulations with different water/ethanol ratios) and elasticity of the final film (related to plasticizer content). PVA70 was loaded with 3% w/w EDTA and used for the cleaning of artificially aged Cu-alloy samples and on a real cases study, the "Fontana dei Mostri Marini" by P. Tacca in Florence (see figure, right panel).

References

Parisi, E.I.; Bonelli, N.; Giorgi, R.; Ingo, G.M.; Baglioni, P. "Development of an innovative film-forming cleaning system for the removal of corrosion products from copper-based artifacts", ICOM 2017 (in press).

Baglioni, P.; Chelazzi, D.; Giorgi, R. "Nanotechnologies in the Conservation of Cultural Heritage", Springer (2015).

Baglioni, P.; Chelazzi, D. "Nanoscience for the Conservation of Works of Art", RSC Publishing (2013).

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

R. Giorgi, G. Poggi, D. Chelazzi, 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 tradename is "Nanorestore®", produced at the CSGI laboratory. Nanorestore is the first chemical product based on nanotechnology, made available specifically to the conservator community.
More recently, CSGI have placed on the market a new class of commercial products named "Nanorestore Plus®" that are an updated version of the classic formulation "Nanorestore®". Nanorestore Plus® formulations are composed of calcium hydroxide nanoparticles dispersed in short-chain alcohols such as ethanol and 2-propanol.

References

Chelazzi, D.; Poggi, G.; Jaidar, Y.; Toccafondi, N.; Giorgi, R.; Baglioni, P. "Hydroxide nanoparticles for Cultural Heritage: consolidation and protection of wall paintings and carbonate materials", J. Colloid Interface Sci. 392, 42-49 (2013).
Baglioni, P.; Giorgi, R. "Inorganic nanoparticles for works of art conservation, in Inorganic Nanoparticles: Synthesis, Applications, and Perspectives; Series: Nanomaterials and their Applications", C. Altavilla & E. Ciliberto (eds), CRC Press – Taylor & Francis Group: London (2010).
Giorgi, R.; Ambrosi, M.; Toccafondi, N.; Baglioni, P. "Nanoparticles for Cultural Heritage Conservation: Calcium and Barium Hydroxide Nanoparticles for Wall Painting Consolidation", Chem. Eur. J. 16, 9374-9382 (2010).
Baglioni, P.; Giorgi, R. "Soft and hard nanomaterials for restoration and conservation of cultural heritage", Soft Matter 2, 293-303 (2006).
Giorgi, R.; Chelazzi, D.; Carrasco, R.; Colon, M.; Desprat, A.; Baglioni, P. "The Maya site of Calakmul: "in situ" preservation of wall paintings and limestone by using nanotechnologies", The Object in Context: Crossing Conservation Boundaries, Munich IIC Congress 2006: proceedings, Edited by David Saunders, Joyce H. Townsend and Sally Woodcock, 162-169 (2006).

2A – Nanomaterials for the cleaning and pH adjustment of leather

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

Aims

The development of a combined treatment for the cleaning and pH adjustment of leather.

Results

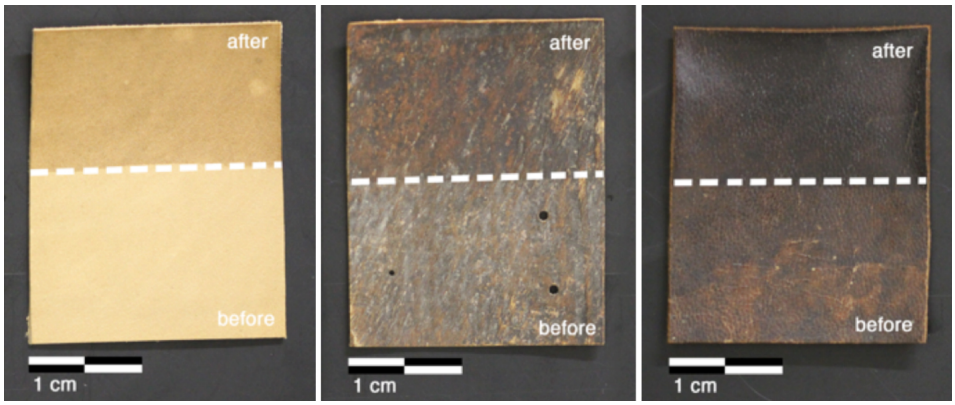
Leather has been used by mankind since ancient times, yet the preservation of this collagen-based material represents a challenge for conservators worldwide. Leather objects are made from mammalian skin and hide, which are then transformed into a material that is resistant to mechanical abrasion, microbial attack and heat. This is achieved through the tanning process, where either vegetable tannins or salts of metals (e.g. chromium, aluminum) are commonly applied to improve the stability of collagen. In particular, tannins have been used since Neolithic time to retard decay, and vegetable tanned leather was indeed one of the most important materials in Western and Mediterranean Europe until the end of the 19th century, when chromium mineral tanning gradually came into use. Tannins form a complex with collagen, mainly through hydrogen bonds between free amino side groups of the collagen protein and hydroxyl groups from the polyphenolic tannin molecules, as well as through hydrophobic bonds.

Leather artifacts in historical collections and archives are often contaminated by soiling, salts, biocontamination or coatings that alter their appearance and readability. Moreover, degradation is promoted by the presence of acidic compounds, either coming from manufacturing processes (tannery) or from the absorption of air pollutants such as sulfur and nitrogen oxides. Acidity increases the rate of hydrolysis of bonds within the collagen structure, reducing the polymer's structural integrity and eventually turning collagen into a gelatin colloidal solution. The tanning agents break down in turn under oxidative and acid hydrolytic conditions, forming products that can promote the degradation of collagen.

Both cleaning and pH adjustment of leather pose a great challenge for conservators, owing to the sensitivity of these materials to the action of solvents, especially water-based formulations and alkaline chemicals. In this study the cleaning of historical leather samples was optimized by confining an oil-in-water (o/w) nanostructured fluid in a highly retentive pHEMA/PVP chemical hydrogel, which allows the controlled release of the cleaning fluid on sensitive surfaces. The chemical gel exhibits optimal viscoelasticity, which facilitates its removal after the application without leaving residues on the object. Nanoparticles of calcium hydroxide and lactate, dispersed in 2-propanol, were synthesized and used to adjust the pH up to the natural value of leather, preventing too high alkalinity which causes swelling of fibers and denaturation of the collagen.

The gel, nanostructured cleaning fluid and nanoparticles dispersions were tested on both modern and historical leather samples. The modern sample was a vegetable tanned (sumac) leather made from calfskin. Leaves from sumac shrub (Rhus coriaria) were among the most important vegetable source for tanning leather. The sample was

tested as received. The first historical sample was the cover of a Luther Bible (1749 AD). The second historical sample was the cover of a Missale Romanum (Roman Missal, 1725 AD). The historical samples exhibited surface deposits of dirt, salts, or waxy (or lipid) materials, which needed to be removed. In the picture, the visual aspect of samples before and after cleaning and pH adjustment is depicted.



The treated samples were characterized using Scanning Electron Microscopy (FE SEM), and infrared spectroscopy (ATR-FTIR). The analytical assessment validated the use of tools derived from colloid and materials science for the preservation of collagen-based artifacts.

References

Baglioni M.; Bartoletti, A.; Bozec, L.; Chelazzi, D.; Giorgi, R.; Odlyha, M.; Pianorsi, D.; Poggi, G.; Baglioni, P.; "Nanomaterials for the cleaning and pH adjustment of vegetable-tanned leather", Appl. Phys. A 122, 114 (2016).

Baglioni, P.; Chelazzi, D.; Giorgi, R.; Poggi, G. "Nanoparticles for the Conservation of Cultural Heritage: Paper and Wood", in Encyclopedia of Surface and Colloid Science, Second Edition; Somasundaran, P., Ed.; Taylor & Francis: New York, 1-16 (2012).

Domingues, J.; Bonelli, N.; Giorgi, R.; Fratini, E.; Gorel, F.; Baglioni, P. "Innovative hydrogels based on semi-interpenetrating p(HEMA)/PVP networks for the cleaning of water-sensitive cultural heritage artifacts.", Langmuir 29, 2746-2755 (2013).

Giorgi, R.; Baglioni, M.; Berti, D.; Baglioni, P. "New Methodologies for the Conservation of Cultural Heritage: Micellar Solutions, Microemulsions, and Hydroxide Nanoparticles", Acc. Chem. Res. 43, 695-704 (2010).

2A – Nanocomposite materials for the consolidation and strengthening of cellulose-based artifacts

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

Aims

Development of a nanocomposite material for the consolidation and concomitant pH adjustment of cellulosic works of art and artifacts.

Results

Two are the main issues need to be solved if the conservation of degraded fibrous material-based artifacts is concerned. Firstly, a mechanical reinforcement of artifacts is usually needed to ensure, for instance in the case of paintings, that the paint layer or decoration keeps its integrity. Moreover, pH buffering is needed to prevent acidic degradation that is inherent to natural materials. It has been recently shown that these two issues are related. As a matter of fact, the acidity of canvases made of natural materials is generally of concern as it can lead to loss of mechanical properties and deterioration of canvases based on natural materials in less than 100 years. The stability of synthetic canvases is even less known than that of canvases of natural origin. This problem dramatically concerns also jute, which becomes quite acidic in a faster way than linen, and paintings done on this type of canvas become more brittle. Therefore, the main areas for which both these issues are very relevant are conservation of modern and contemporary canvas paintings, as well as polymateric works of art using other types of fibrous supports such as paper. In fact, paper is also subjected to the same degradation mechanisms above described.

The application of glue and the attachment of a new canvas on the back of the painting, i.e. the lining, is traditionally used for the consolidation of canvases. However, although inevitable for the most degraded canvases, lining should to be avoided due to its invasiveness, because it hides the original canvas and is very resource-intensive.

Therefore, the goal within the EU Project NANORESTART is to develop materials for the mechanical strengthening of canvases of modern/contemporary paintings. The development and use of nanocellulose in combination with nanoparticles and cellulose derivatives could ensure the consolidation of fiber-based materials using almost entirely natural materials. The choice of these materials is due to the high compatibility of the proposed treatments with the original fibrous support, which is essential from the conservation point of view.

Mechanical tests on not aged and aged reference samples could be used to assess the consolidation efficacy of the proposed consolidation treatments before testing on real case studies.

References

Poggi, G.; Toccafondi, N.; Canton, P.; Giorgi, R.; Baglioni, P. “Calcium hydroxide nanoparticles from solvothermal reaction for the deacidification of degraded waterlogged wood”, Journal of Colloid and Interface Science 473, 1-8 (2016).

Poggi, G.; Toccafondi, N.; Melita, L.N.; Knowles, J.C.; Bozec, L.; Giorgi, R.; Baglioni P. “Calcium hydroxide nanoparticles for the conservation of cultural

heritage: new formulations for the deacidification of cellulose-based artifacts", Appl. Phys. A. 114, 685-693 (2014).
Poggi, G.; Baglioni, P.; Giorgi, R. "Alkaline Earth Hydroxide Nanoparticles for the Inhibition of Metal Gall Ink Corrosion", Restaurator 32, 247-273 (2011).
Poggi, G.; Giorgi, R.; Toccafondi, N.; Katzur, V.; Baglioni, P. "Hydroxide Nanoparticles for Deacidification and Concomitant Inhibition of Iron-Gall Ink Corrosion of Paper", Langmuir 26, 19084-19090 (2010).
Baglioni, P.; Giorgi, R. "Soft and hard nanomaterials for restoration and conservation of cultural heritage", Soft Matter 2, 293-303 (2006).
Giorgi, R.; Chelazzi, D.; Baglioni, P. "Conservation of acid waterlogged shipwrecks: nanotechnologies for de-acidification", Appl. Phys. A: Mater. Sci. Process. 83, 567-571 (2006).
Giorgi, R.; Chelazzi, D.; Baglioni, P. "Nanoparticles of calcium hydroxide for wood conservation. The deacidification of the Vasa warship", Langmuir 21, 10743-10748 (2005).
Giorgi, R.; Dei, L.; Ceccato, M.; Schettino, C.V.; Baglioni, P. "Nanotechnologies for conservation of Cultural Heritage: paper and canvas deacidification", Langmuir 18, 8198-8203 (2002).

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

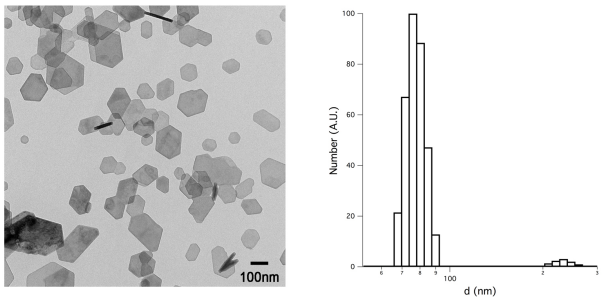
G. Poggi, R. Giorgi, P. Baglioni

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 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 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.
As a results of research efforts in the field of the conservation of paper and wood, CSGI have recently placed on the market a new class of commercial products named "Nanorestore Paper®", designed for the deacidification of cellulose-based materials. Nanorestore Paper® formulations are composed of calcium hydroxide nanoparticles dispersed in ethanol and 2-propanol.

References

Poggi, G.; Toccafondi, N.; Canton, P.; Giorgi, R.; Baglioni, P.; "Calcium hydroxide nanoparticles from solvothermal reaction for the deacidification of degraded waterlogged wood", Journal of Colloid and Interface Science 473, 1-8, (2016).
Poggi, G.; Toccafondi, N.; Melita, L.N.; Knowles, J.C.; Bozec, L.; Giorgi, R.; Baglioni, P. "Calcium hydroxide nanoparticles for the conservation of cultural heritage: new formulations for the deacidification of cellulose-based artifacts", Appl. Phys. A. 114, 685-693 (2014).
Poggi, G.; Baglioni, P.; Giorgi, R. "Alkaline Earth Hydroxide Nanoparticles for the Inhibition of Metal Gall Ink Corrosion", Restaurator 32, 247-273 (2011).
Poggi, G.; Giorgi, R.; Toccafondi, N.; Katzur, V.; Baglioni, P. "Hydroxide Nanoparticles for Deacidification and Concomitant Inhibition of Iron-Gall Ink Corrosion of Paper", Langmuir 26, 19084-19090 (2010).
Baglioni, P.; Giorgi, R. "Soft and hard nanomaterials for restoration and conservation of cultural heritage", Soft Matter 2, 293-303 (2006).
Giorgi, R.; Chelazzi, D.; Baglioni, P. "Conservation of acid waterlogged shipwrecks: nanotechnologies for de-acidification", Appl. Phys. A: Mater. Sci. Process. 83, 567-571 (2006).
Giorgi, R.; Chelazzi, D.; Baglioni, P. "Nanoparticles of calcium hydroxide for wood conservation. The deacidification of the Vasa warship", Langmuir 21, 10743-10748 (2005).
Giorgi, R.; Dei, L.; Ceccato, M.; Schettino, C.V.; Baglioni, P. "Nanotechnologies for conservation of Cultural Heritage: paper and canvas deacidification", Langmuir 18, 8198-8203 (2002).

2A – A stabilizer-free nonpolar dispersion for the deacidification of contemporary art on paper

G. Poggi, R. Giorgi, P. Baglioni

Aims

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

Results

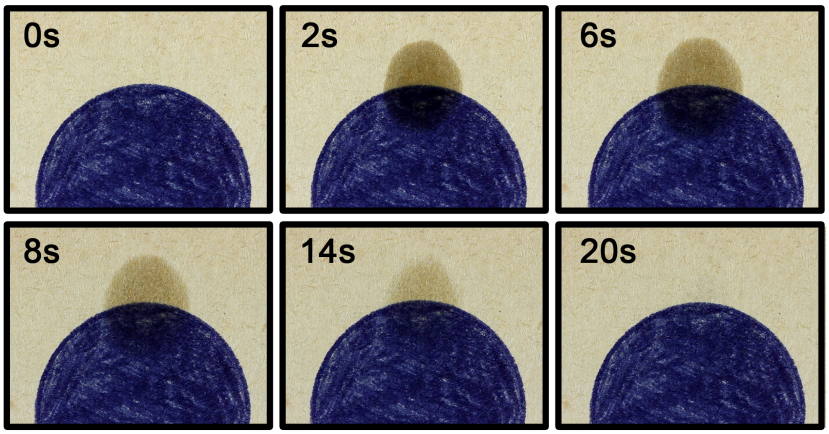
The preservation of cellulose-based works of art is threatened by the presence of acidity within the substrates, native, i.e., due to the papermaking process, or developed upon aging. The depolymerization of cellulose catalyzed by acidic compounds leads to a decrease in the mechanical properties of the artworks. Many strategies for hampering the acid-catalyzed degradation of cellulosic substrates have been developed in the past; unfortunately, few of them can be safely used on contemporary artworks, drawings or archival materials.

The use of paper started to change in the middle of 20th century, moving from a simple support for studies or sketches to being the heart of autonomous works, at time torn, burnt, folded, perforated, twisted or creased. This is the case of Simon Schubert, Kiki Smith or Stefano Arienti artworks. At the same time the world of art has seen the arrival of a large number of new media, such as acrylic and vinyl resins, pressure sensitive adhesives, ballpoint and felt-tip pens and markers. The same pens and markers used by contemporary artists can be found in manuscripts and archival documents. All of these media and techniques are rarely compatible with traditional restorative procedures. This makes the conservation and restoration of the wide field of contemporary drawings and archival documents unexplored. In particular, few are the available deacidification treatments that can be safely used on contemporary drawings or contemporary art on paper, as well as on contemporary documents and manuscripts.

A deacidifying dispersion of calcium hydroxide in cyclohexane has been prepared starting from alkaline nanoparticles obtained via a solvothermal reaction. The most interesting feature of this formulation is that a stabilizer is not required for the preparation of the dispersion, differently from other commercial nonpolar products. Cyclohexane is a colorless, nonpolar, and volatile liquid that allows fast and simple applications by spraying, respectful of the original artist's technique, as shown in the image reported below.

In order to evaluate the efficacy of this $Ca(OH)_2$ nanoparticles dispersion in cyclohexane, mockups were prepared on acidic paper using ballpoint pens.

The protective action arising from the applied treatment was evaluated upon artificial aging, measuring cellulose viscosimetric polymerization degree (DPv), cellulose pyrolysis temperature, samples pH, and colorimetric coordinates. The promising results obtained on mockups led to the application of this innovative formulation on a series of drawings from a private collection, opening the way for the treatment of such an important field of contemporary arts. Reflectance Transformation Imaging (RTI), a computational photographic method that captures the surface shape of artifacts in a noninvasive way, was used to evaluate the compatibility of the newly developed cyclohexane dispersion with burnt, perforated and creased paper.



References

Poggi, G.; Toccafondi, N.; Canton, P.; Giorgi, R.; Baglioni, P. "Calcium hydroxide nanoparticles from solvothermal reaction for the deacidification of degraded waterlogged wood", Journal of Colloid and Interface Science 473, 1-8 (2016).

Poggi, G.; Toccafondi, N.; Melita, L.N.; Knowles, J.C.; Bozec, L.; Giorgi, R.; Baglioni, P. "Calcium hydroxide nanoparticles for the conservation of cultural heritage: new formulations for the deacidification of cellulose-based artifacts", Appl. Phys. A. 114, 685-693 (2014).

Baglioni, P.; Chelazzi, D.; Giorgi, R.; Poggi, G. "Nanoparticles for the Conservation of Cultural Heritage: Paper and Wood", in Encyclopedia of Surface and Colloid Science, Second Edition; Somasundaran, P., Ed.; Taylor & Francis: New York, 1-16 (2012).

Poggi, G.; Baglioni, P.; Giorgi, R. "Alkaline Earth Hydroxide Nanoparticles for the Inhibition of Metal Gall Ink Corrosion", Restaurator 32, 247-273 (2011).

Poggi, G.; Giorgi, R.; Toccafondi, N.; Katzur, V.; Baglioni, P. "Hydroxide Nanoparticles for Deacidification and Concomitant Inhibition of Iron-Gall Ink Corrosion of Paper", Langmuir 26, 19084-19090 (2010).

Baglioni, P.; Giorgi, R. "Soft and hard nanomaterials for restoration and conservation of cultural heritage", Soft Matter 2, 293-303 (2006).

Giorgi, R.; Chelazzi, D.; Baglioni, P. "Conservation of acid waterlogged shipwrecks: nanotechnologies for de-acidification", Appl. Phys. A: Mater. Sci. Process. 83, 567-571 (2006).

Giorgi, R.; Chelazzi, D.; Baglioni, P. "Nanoparticles of calcium hydroxide for wood conservation. The deacidification of the Vasa warship", Langmuir 21, 10743-10748 (2005).

Giorgi, R.; Dei, L.; Ceccato, M.; Schettino, C.V.; Baglioni, P. "Nanotechnologies for conservation of Cultural Heritage: paper and canvas deacidification", Langmuir 18, 8198-8203 (2002).

2A – Amphiphile-based nanofluids for the removal of organic coatings from works of art

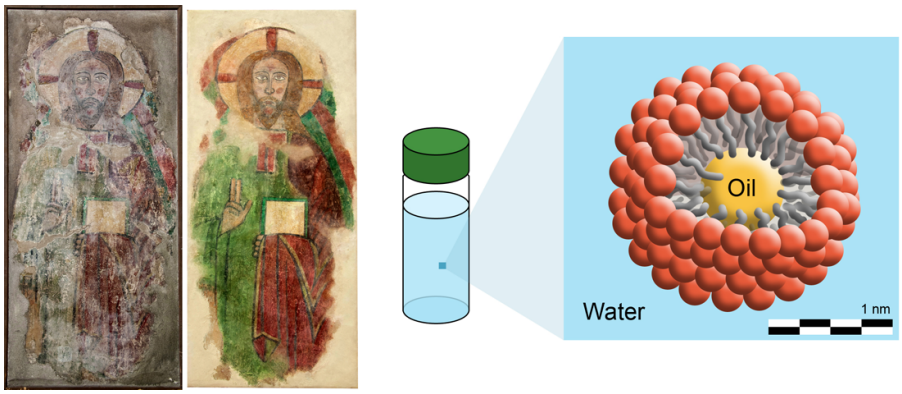
M. Baglioni, D. Berti, E. Carretti, L. Dei, D. Chelazzi, R. Giorgi, P. Baglioni

Aims

Development of innovative, effective, safe and environmentally-friendly systems for the cleaning of painted surfaces.
Improvement of the available formulations with the inclusion of degradable (biodegradable, labile, cleavable) surfactants, which should solve the residues' issue.

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 two decades 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, their use was extended to the removal of organic coatings (synthetic polymers, natural and synthetic varnishes, adhesives, modern paints) from wall paintings, easel paintings, stone, wood, paper and leather.
The main issue that still needs to be addressed with these systems is that surfactants may remain on the treated surfaces as a residue (which, nonetheless, can easily

washed away by rinsing with water). In fact, surfactants are the only non-volatile chemicals included in these formulations. Thus, using surfactants that spontaneously degrade to harmless volatile compounds would be a major advancement of this methodology. We recently moved our focus from ionic surfactants to nonionic alcohol ethoxylates, which possess interesting (bio)degradability properties, and we are currently studying new classes of surfactants, such as cleavable pH sensitive autodegradable surfactants.
Interesting results are being obtained using these innovative surfactants in new nanofluids.
As a result of these research efforts, nanofluids for the cleaning of cultural heritage have been made available to conservators and restorers as commercial products under the trademark of Nanorestore Cleaning®.

References

Baglioni, P.; Chelazzi, D. "Nanoscience for the Conservation of Works of Art", Royal Society of Chemistry (2013).
Baglioni, P.; Chelazzi, D.; Giorgi, R.; Poggi, G. "Colloid and Materials Science for the Conservation of Cultural Heritage: Cleaning, Consolidation, and Deacidification", Langmuir 29, 5110-5122 (2013).
Baglioni, P.; Berti, D.; Bonini, M.; Carretti, E.; Dei, L.; Fratini, E.; Giorgi, R. "Micelle, microemulsions, and gels for the conservation of cultural heritage", Adv. Colloid Interface Sci. 205, 361-371 (2014).
Baglioni, M.; Raudino, M.; Berti, D.; Keiderling, U.; Bordes, R.; Holmberg, K.; Baglioni, P. "Nanostructured fluids from degradable nonionic surfactants for the cleaning of works of art from polymer contaminants", Soft Matter 10, 6798-6809 (2014).
Baglioni, P.; Chelazzi, D.; Giorgi, R. "Nanotechnologies in the Conservation of Cultural Heritage: A compendium of materials and techniques", Springer (2014).
Brajer, I.; Fossé-Le Rouzic, M.; Shashoua, Y.; Taube, M.; Chelazzi, D.; Baglioni, M.; Giorgi, R.; Baglioni, P. "The removal of aged acrylic coatings from wall paintings using microemulsions", Melbourne (2014).
Baglioni, M.; Jàidar Benavides, Y.; Berti, D.; Giorgi, R.; Keiderling, U.; Baglioni, P. "An amine-oxide surfactant-based microemulsion for the cleaning of works of art", J. Colloid Interface Sci. 440, 204-210 (2015).
Baglioni, P.; Carretti, E.; Chelazzi, D. "Nanomaterials in art conservation", Nat. Nanotechnol. 10, 287-290 (2015).

2A – Nanostructured fluids for the conservation of cultural heritage: understanding the mechanism of organic coatings removal

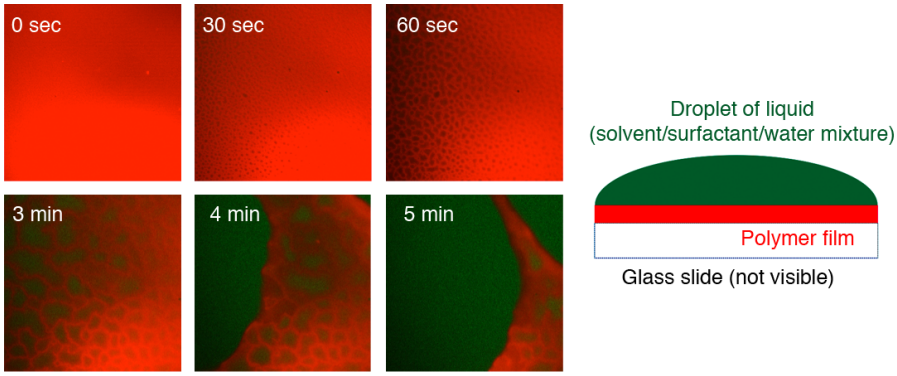
M. Baglioni, D. Berti, C. Montis, M. Raudino, M. Bonini, P. Baglioni

Aims

Understanding the mechanism of interaction between polymer coatings and nanofluids will contribute to improve cleaning formulations in the field of conservation of cultural heritage, and, besides having some scientific relevance from fundamentals standpoint, it may open new perspectives on different applicative fields.

Results

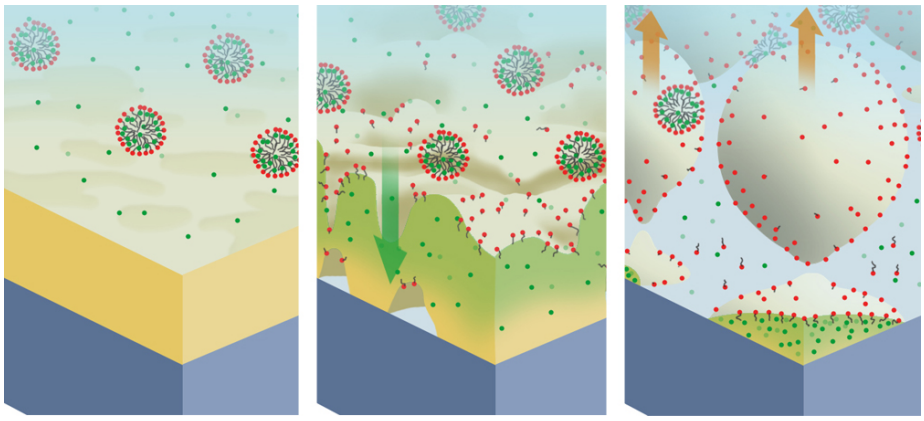
The removal of undesired material from the surface of a work of art is one of the most important and delicate operations in conservation of cultural heritage. In this context, nowadays, neat organic solvents often are not the preferred option, in view of their poor-controlled action, their toxicity and 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.



Most recently, a major effort has been spent in order to investigate the mechanism of polymer removal from porous substrates using 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. Scattering techniques and imaging investigations, such as confocal laser scanning microscopy, are being combined in order to obtain a clearer picture of the cleaning mechanism.

In particular simple ternary mixtures of water/solvent/surfactant at different concentrations were examined, in order to clarify the role of each component in the

formulations, in the interaction with thin films of Paraloid B72 (a ethyl metacrylate/methyl acrylate 70:30 copolymer). Propylene carbonate and methyl ethyl ketone were selected as solvents, while nonionic CiEj surfactants and SDS were considered as surface-active agents.
The results are indeed a step forward in understanding the interaction mechanism between nanofluids and polymeric films at the micro- and nano-scale. A dewetting process is promoted by aqueous nanofluid, which seems to be strongly influenced by the presence, concentration and nature of the surfactant in the cleaning system. The role of micelles or supramolecular aggregates in this context is currently under investigation, as well as the dependence on the thickness of the examined polymer films.



References

Raudino, M.; Selvolini, G.; Montis, C.; Baglioni, M.; Bonini, M.; Berti, D.; Baglioni, P. "Polymer Films Removed from Solid Surfaces by Nanostructured Fluids: Microscopic Mechanism and Implications for the Conservation of Cultural Heritage", ACS Appl. Mater. Interfaces 7, 6244-6253 (2015).
Baglioni, M.; Montis, C.; Berti, D.; Baglioni, P. Manuscript in preparation, to be submitted to Phys. Chem. Chem. Phys. (2017).

2A – Nanofluids and chemical hydrogels for the selective removal of overpaintings and undesired graffiti from street art

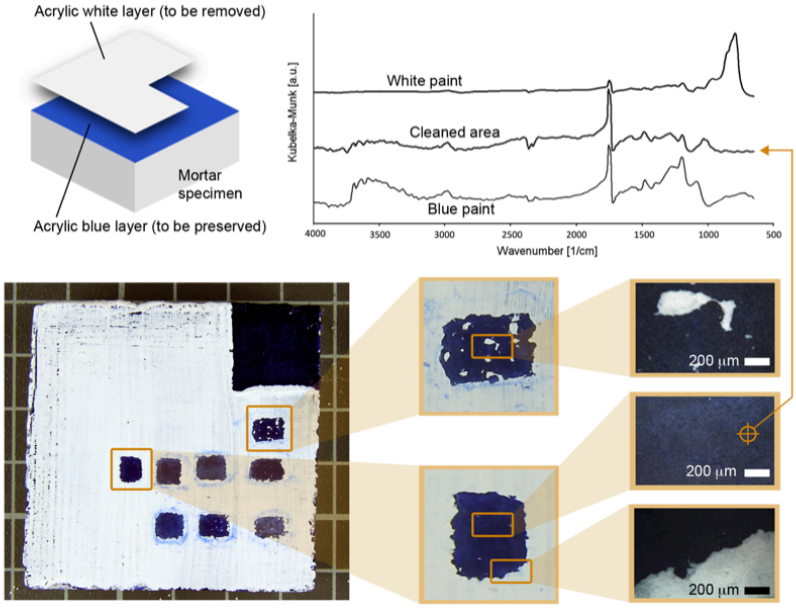
M. Baglioni, R. Giorgi, P. Baglioni

Aims

Removal of graffiti and overpaintings from street art, or, more in general, contemporary art, cannot be performed using available traditional methodologies; therefore selective removal can be achieved combining highly retentive hydrogels and nanofluids.

Results

The removal of graffiti from paintings that must be preserved is a particularly challenging and relatively new issue in conservation of cultural heritage. This is the case of contemporary street art (by unconventional contemporary artists, such as Banksy or Blu) jeopardized by tags, signs and writings. In these conditions, the cleaning action must be extremely selective, as the binder of the undesired paint is likely to have a very similar chemical nature to the one of the underlying original painting.



To this aim, in the frame of an Horizon 2020 EU-funded project named Nanorestart, nanostructured fluids, such as micelles and microemulsions, either neat or combined with highly retentive chemical hydrogels was proposed and it is here reported as a selective and controllable cleaning system for the removal of graffiti and overpaintings from street art. The semi-interpenetrating polymer networks-based hydrogels (SIPN) here proposed are composed by a tridimensional network of

poly(hydroxyehtyl methacrylate)/N,N'-Methylene bisacrylamide (pHEMA/MBA), interpenetrated by a high molecular weight poly(vinyl pyrrolidone) (PVP). These hydrogels have been shown to be particularly suited to limit the cleaning action to the surface layers of the treated area. pHEMA/PVP hydrogels can be loaded with water, some polar solvents, or with aqueous nanostructured fluids (hereafter, shortly, "nanofluids"), composed by eco-friendly, volatile or auto-degradable compounds, which ensure a residue-free and environmentally compatible cleaning intervention. The studied formulations were structurally characterized by means of scattering techniques and their phase diagram was investigated. Then, they were tested on laboratory samples simulating street art paintings covered by graffiti. The samples were prepared by overlapping different paints in various combinations. The paints included in this study include acrylic, vyinl and alkyd binders, while several colors were tested. The outcome of cleaning tests was investigated by means of visual, photographic and microscopic observation, while micro-reflectance FT-IR spectroscopy was performed on the treated area before and after the application of the cleaning systems, in order to gather information about the chemical composition of the surface, searching for possible residues of the removed paint layer. Setting up application times and performing careful and delicate mechanical action were found to be key factors when removing overpaintings having the same binder as the original paint layer. However the removal of acrylic (or vynil) paints from other acrylic (or vynil) paints was achieved with minimum stress for the original paint layer. Microscopic observation and FT-IR analysis of the treated areas confirmed the good results of the cleaning tests.

References

Giorgi, R.; Baglioni, M.; Baglioni, P. Manuscript submitted to Anal. Bioanal. Chem. (2017).

Baglioni, M.; Alterini, M.; Giorgi, R.; Brajer, I.; Shashoua, Y.; Baglioni, P. Manuscript submitted to ICOM CC (2017).

2B – Effect of mechanical energy on solid state synthesis of Ternary Oxides

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

Aims

Through different analytical techniques, the formation reactions of some technologically interesting ternary oxides are followed.

Results

The mechanism of $Bi_4Ti_3O_{12}$ formation starting from the two constituent oxides has been studied. Starting from a physical mixture, a solid-state reaction occurs between the two oxides that leads at ≈700 °C to a mixture of the two ternary oxides $Bi_{12}TiO_{20}$ + $Bi_4Ti_3O_{12}$ along with unreacted precursor oxides. At T ≈ 830 °C $Bi_{12}TiO_{20}$ reacts with TiO_2 forming $Bi_4Ti_3O_{12}$ and, finally, at T ≈ 850 °C, the residual $Bi_{12}TiO_{20}$ undergoes the peritectic reaction that produces $Bi_4Ti_3O_{12}$ plus a liquid phase. However, the formation of $Bi_4Ti_3O_{12}$ is not complete at temperatures as high as 900 °C. Starting from a mechanically activated mixture, the intermediate $Bi_{12}TiO_{20}$ only forms as a minority phase at a lower temperature (T ≈ 550 °C), and then it rapidly reacts to give $Bi_4Ti_3O_{12}$. No trace of the peritectic reaction is found in the case of the activated mixture. The complete formation of $Bi_4Ti_3O_{12}$ can be obtained by 3-h annealing of the activated mixture at T ≥ 650 °C. The heat capacity of the product phase $Bi_4Ti_3O_{12}$ has also been measured in the temperature range 50–300 °C.

Many synthesis procedures have been worked out to prepare $CaSnO_3$. A great deal of them resort to the classical ceramic method that implies a very high temperature treatment (1300-1500°C) of the component oxides mixture. To avoid such high temperature treatment, many alternative routes have been proposed. In this paper stoichiometric mixtures of Ca citrate tetrahydrate and Sn(II) oxalate have been mechanically activated by high energy milling. The reactions taking place in the mixtures during annealing have been studied by coupled TG-DSC measurements, XRPD and diffuse reflectance FT-IR spectroscopy. It has been established that the stage of mechanical activation allows the synthesis to be completed by 3 h-annealing at 850°C.

References

Berbenni, V.; Milanese, C.; Bruni, G.; Girella, A.; Marini A. "Mechanical Activation of the solid – phase reaction between Bismuth citrate and iron(II) oxalate dehydrate to yield $BiFeO_3$", Ceramics International 41(5), 7216-7220 (2015).

Berbenni, V.; Milanese, C.; Bruni, G.; Girella, A.; Marini A. "Synthesis of $Bi_4Ti_3O_{12}$ by high energy milling of Bi_2O_3-TiO_2 (anatase) mixtures", Journal of Thermal Analysis and Caolorimetry 126, 1507-1511 (2016).

2B – New cathode materials for technological applications

D. Capsoni, M. Bini, I. Quinzeni

Aims

Characterization and optimization of the physico-chemical properties of materials for electrochemical applications, to put into evidence the relationships among properties, synthesis method and doping.

Results

We investigated in detail a series of undoped and doped compounds that find application as cathode 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 diffraction data are used to study the structure stability with cell cycling, the cations and doping ions distribution in the cell framework, and to quantify the possible impurity phases formed in the synthesis process. The results, obtained by the combined use of several structural and spectroscopic techniques, are useful to explain the materials properties. The investigated cathodes compounds belong to the Li-Fe/Mn/Co-Si-O and Li-Mn/Ni-O systems. For the preparation of pure and substituted compounds, different synthesis routes were used, to optimize the material properties for its technological application.

Wide interest has been devoted to the study of lithium transition metal ortho-silicates Li_2MSiO_4 (M = Co, Mn, Fe). As cathode materials in Li-ion batteries they offer the possible extraction of two Li ions per formula-unit and a particularly stable anionic framework, thanks to the strong Si-O chemical bonds, thus promoting both higher charge-discharge capacities and longer cycling life. Nevertheless, the presence of different polymorphic forms, the defects formation, and the easy segregation of impurity phases during the synthesis influence the Li diffusion and its intercalation-de-intercalation mechanism, thus affecting the electrochemical performances. In this frame, we investigated the influence of the synthesis procedure on the structure, defects formation and purity of Li_2FeSiO_4, Li_2MnSiO_4, $Li_2Fe_{0.5}Mn_{0.5}SiO_4$ and $Li_2(FeMnCo)SiO_4$ by the combined use of structural, spectroscopic and magnetic techniques. More interestingly, we studied the structural changes of the cathode material during cycling by in-situ and ex-situ X-ray conventional and synchrotron diffraction data. Moreover, we reported, for the first time, the successful preparation of thin films of lithium iron and manganese orthosilicates cathodes, deposited by RF sputtering, to be used in lithium microbatteries. The experimental evidence of the voltage variations during the charge-discharge of Li_2FeSiO_4 has been explained by density functional theory calculations.

Among the high-voltage cathode materials for Li-ion batteries, the Si doped $LiNi_{0.5}Mn_{1.5}O_4$ spinel compound has been prepared and characterized. We demonstrated that the successful substitution of the silicon ions on the tetrahedral site of the cationic framework is obtained for silicon content lower than x=0.15 in $LiNi_{0.5}Mn_{1.5-x}Si_xO_4$. The silicon substitution plays a favourable role in the structure stability and lithium diffusion, thus improving both charge-discharge capacities and cycling performances of the cell.

References

Bini, M.; Ferrari, S.; Ferrara, C.; Mozzati, M.C.; Capsoni, D.; Pell, A.J.; Pintacuda, G.; Canton, P.; Mustarelli, P. "Polymorphism and magnetic properties of Li_2MSiO_4 (M=Fe, Mn) cathode materials", Scientific Reports 3:3452, 1-7 (2013).

Ferrari, S.; Capsoni, D.; Casino, S.; Destro, M.; Gerbaldi, C.; Bini, M. "Electrochemistry of orthosilicate-based lithium battery cathodes: a perspective", Phys. Chem. Chem. Phys. 16, 10353-10366 (2014).

Quinzeni, I.; Ferrari, S.; Quartarone, E.; Capsoni, D.; Caputo, M.; Goldoni, A.; Mustarelli, P.; Bini. M. "Fabrication and electrochemical characterization of amorphous lithium iron silicate thin films as positive electrodes for lithium batteries", J. Power Sources 266, 179-185 (2014).

Kalantarian, M.M.; Oghbaei, M.; Asgari, S.; Ferrari, S.; Capsoni, D.; Mustarelli. P. "Understanding non-ideal voltage behaviour of cathodes for lithium-ion batteries", J. Mater Chem A. 2, 19451-19460 (2014).

Ferrari, S.; Mozzati, M.C.; Lantieri, M.; Spina, G.; Capsoni, D.; Bini, M. "New materials for Li-ion batteries: synthesis and spectroscopic characterization of $Li_2(FeMnCo)SiO_4$ cathode materials", Scientific Reports 6:27895, 1-12 (2016).

Boni, P.F. "Materiali catodici ad alto voltaggio per batterie Li-ione: $LiNi_{0.5}Mn_{1.5}O_4$ drogato Si", 2016 (Univ. Pavia) Master Thesis.

Montagna L. "Il materiale catodico ad alto voltaggio $LiNi_{0.5}Mn_{1.5}O_4$ drogato con Fe e Ga: studio diffrattometrico e microscopico", 2015 (Univ. Pavia) Bachelor Thesis.

2B – Synthesis and characterization of nano-biomaterials

M. Bini, D. Capsoni

Aims

Synthesis and characterization of pure and doped Hydroxyapatites and Zinc ferrites to optimize their biomedical applications.

Results

Due to its compositional similarity to mineral bone, hydroxyapatite (HAp), $Ca_{10}(PO_4)_6(OH)_2$, has been widely investigated for its possible use to promote bone ingrowths when used in orthopedics applications. More studies showed that the traditional HAp materials lacked the ability to induce osteogenesis; this problem can be overcome by proper doping/substitution with different cations on Ca and P sites. In particular, silicon has been demonstrated to be essential to the normal growth and development of bone and cartilage, and can enhance osteoblast proliferation and differentiation, as well as improve collagen production. Also the manganese substitution plays a favorable role in the hydroxyapatite applications. A few is known on the possible role played by Mn/Si co-substitution on the hydroxyapatite performances. Nanocrystalline pure and Mn/Si co-substituted hydroxyapatite were synthesized by different procedures and the samples have been characterized by structural and spectroscopic techniques. The Mn substitution occurs on the Ca(I) crystallographic site of the Hexagonal crystal lattice, while Si ions occupy the P site. SEM analysis confirms that all the samples are of nanometric particle size and the distribution maps of the elements demonstrate that Ca, P, Si and Mn are homogeneously distributed in the samples. The as-synthesized samples were soaked in SBF (simulated body fluid) solution to evaluate their bioactivity. ICP analysis showed a good in-vitro bioactivity and a satisfactory biocompatibility.

A study of magnetic Zinc ferrites nanoparticles has been also undertaken, due to the numerous applications that they can find in various fields such as electronic devices, electrodes for batteries or sensors, as well as in the biomedical field where they can be used as contrast agents (CAs) in magnetic resonance imaging (MRI). Our research focuses on their magnetic hyperthermia application (MHF). The magnetic property of interest for this application is called superparamagnetism, that is present when the nano particles are so small that can be considered as a single magnetic domain. In this frame, we investigated zinc ferrite nano-powders with a nominal composition of $ZnFe_2O_4$. They are magnetic materials with cubic spinel structure and their properties are strongly influenced by the materials' composition and microstructure, which are sensitive to the preparation methodology and also to the doping. Thanks to their superparamagnetism property, particularly prominent when in nanometric dimension, $ZnFe_2O_4$ ferrite nanoparticles are arousing a great interest for magnetic hyperthermia application. In order to improve the magnetic properties of ferrites different methods of synthesis and various types of doping have been tried. The synthesized samples were thoroughly characterized by XRD with Rietveld structural refinement, SEM/EDS, Micro-Raman and FT-IR spectroscopy. The magnetic properties were determined by SQUID magnetometry by collecting hysteresis loops and the magnetization dependence on temperature was determined in zero field cooling and

field cooling regimes. With these characterization techniques, it was shown that the samples obtained are actually nanometric and do not present significant impurities amount. The dopants are easily inserted in the spinel structure and are homogeneously distributed in the nano-particles. The magnetic measurements allowed us to demonstrate that the samples show a pronounced superparamagnetism, that makes them suitable to be employed in MHF.

References

Tondo, C. “Nano ferriti per applicazioni biomediche: l’effetto del drogaggio sulle proprietà strutturali, spettroscopiche e magnetiche”, 2016 (Univ. Pavia), Master Thesis.

Tondo, G. “Idrossiapatiti nanometriche con sostituzione Silicio e Manganese: sintesi e caratterizzazione”, 2016 (Univ. Pavia), Master Thesis.

2C – Chemical Characterization and Antioxidant Properties of Olive Pomaces and Olive Leaves

C. Rossi, G. Tamasi, C. Bonechi, S. Lamponi, A. Donati, A. Magnani

Aims

The study of antioxidant chemical and biological properties are increasing on interest in the last years. The presence of oxidizing species and/or free radicals in foods, reduces its nutritional value and sensory quality due to oxidative reactions in addition to doing damage to human health, for example provoking mutations in DNA. Antioxidants can prevent these reactions via hydrogen atom transfer, electron transfer mechanism or transition metals chelation.

Results

This present study reports the characterization and determination of selected antioxidant properties in olive fruit, extravirgin olive oil (the primary product) and pomace (by-product) samples from the harvesting/production 2013 (one sample, preliminary test), 2014 and 2015. Olive leaves from the pruning process 2013 have been also investigated.

All the samples have been previously lyophilized and extracted via hydroalcoholic mixture ($EtOH/H_2O$, 80/20, v/v). The extracts have been characterized as regards the antioxidant activity through the TEAC (Trolox Equivalent Antioxidant Capacity) and DPPH assays, as well as the analysis of the total polyphenol content (Folin-Ciocalteu method). Selected polyphenols, quercetin, rutin, naringenin, luteolin, epicatechin, kaempferol, and chlorogenic acid, p-coumaric, caffeic and ferulic acid, have been determined quantitatively via HPLC/MS technique. Analysis was ended by analyzing selected metal ions: Na, K, Mg, Ca, Cu, Mn, Zn in the hydroalcoholic extracts as well as in mineralized samples

The hydroalcoholic extracts have been also characterized as regards the viability assay on 3T3 fibroblast cells, showing no toxicity up to 2.5% of extract in the culture medium, while a 5% becomes toxic. This effect can result from the known pro-oxidant activity of polyphenols.

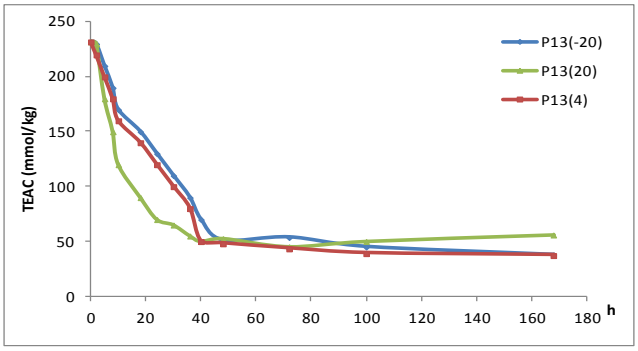


Fig. 1: Kinetic of TEAC values for pomace harvesting 2013 (180 h, P13 lyophilized and extract, EtOH absolute). The extract was kept at different conditions:-20±1, 4±1 e 20±2 °C. Confidence interval, 95%

References

Leopoldini, M.; Russo, N.; Toscano, M. "The molecular basis of working mechanism of natural polyphenolic antioxidants", Food Chem. 125, 288-306 (2011).
Silva, S.; Gomes, L.; Leitão, F.; Coelho, A.V.; Vilas Boas, L. "Phenolic Compounds and Antioxidant Activity of Olea europaea L. Fruits and Leaves", Food Sci. Tech. Int. 12, 385-396 (2006).
Cardoso, S.M.; Guyot, S.; Marnet, N.; Lopes-da-Silva, J.A.; Renard, C.M.G.C.; Coimbra M.A. "Characterisation of phenolic extracts from olive pulp and olive pomace by electrospray mass spectrometry", J. Sci. Food Agric. 85, 21-32 (2005).
Romàn Falcò, I.P.; Teruel, N.G.; Moya, S.P.; Martìn Carratalà M.L. "Kinetic Study of Olive Oil Degradation Monitored by Fourier Transform Infrared Spectrometry. Application to Oil Characterization", J. Agric. Food Chem. 60, 11800-11810 (2012).
El Hajjouji, H.; Fakharedine, N.; Ait Baddi, G.; Winterton, P.; Bailly, J.R.; Revel, J.C.; Hafidi, M. "Treatment of olive mill waste-water by aerobic biodegradation: an analytical study using gel permeation chromatography, ultraviolet-visible and Fourier transform infrared spectroscopy", Bioresour. Technol. 98, 3513-3520 (2007).

The present study has been supported by Regione Toscana financing the project PRAF 2012-2015 Regione Toscana. Strategie di valorizzazione e miglioramento del contenuto di polifenoli nelle olive in Toscana: effetti sulla qualità nutraceutica dell'olio extravergine di oliva e dei formaggi ovini ottenuti dal latte di pecore alimentate con sanse (NutriForOil) (2014-2016).

2C – Chemical characterization of peaches and nectarines

C. Rossi, G. Tamasi, C. Bonechi, G. Leone, A. Donati, A. Magnani

Aims

Chemical characterization of vegetables for food use, and their extracts rich in antioxidant and bioactive components, has increasing attention and efforts on investigating. Particular attention has being devoted to use different and complementary analytical techniques, in order to determine and quantify the key phytochemical compounds. The data can then be interpreted by applying a chemiometric approach.

Results

This study has been conducted on samples of yellow fleshed peaches (Prunus persica L. Batsch; cultivars: RomeStar, ZeeLady) and yellow fleshed nectarines (Prunus persica L. Batsch, var. Nectarina; cultivars: Venus, Nectaross) from two geographic areas of Southern Italy, "Piana di Sibari" and "Piana di Metaponto", located on the Ionian coast of Calabria and Basilicata regions.

The thermogravimetric analysis (TGA) has shown a similar chemical composition of samples having 88±1% water content, 5.4±0.8% sugar content, 1.8±0.2% fibrous content and the remaining 4.8±0.6% associated to minerals. Finally, the rheological analysis revealed a similar consistency of samples (reasonable with a similar maturation stage), and characterized by a greater elastic than viscous component. The measurements of the antioxidant activity (TEAC method) and total polyphenols (Folin-Ciocalteu method) for hydroalcholic pulp extracts, have shown values with comparable trend for the two varieties of nectarine, while in the case of peaches, showed more changeable values. The HPLC-MS analysis of pulp extracts, allowed the identification and quantification of selected polyphenols: chlorogenic and neochlorogenic acid and quercetin glycosides (isoquercetin and rutin), showing a predominant relative distribution of the two hydroxycinnamic acids (Figure 1a), in agreement with the antioxidant activity (and total polyphenols). ^{1}H-NMR spectra revealed the presence of sugars (sucrose, α- and β-glucose, α-xylose, β-D-fructopyranose) among the main constituents of pulp extracts, presenting only minor differences in chemical shift and peaks intensity between samples, in agreement with a very similar chemical composition between peaches and nectarines. The Principal Component Analysis (PCA), obtained by statistical processing of the ^{1}H-NMR data, showed the presence of two outlier samples (ZeeLady-Peach and Nectaross-Nectarine) in agreement with different chemical compositions (particularly high values of hydroxycinnamic acids). Furthermore, Cluster Analysis (CA) showed the grouping of samples on the basis of cultivars (nectarines and peaches) with a 60% significance level. The FTIR-ATR measurements on lyophilized samples of pulps and skins has been also performed, confirming the presence of characteristic bands of -COOH groups of organic acids, -OH groups of sugars, phenols, water, and peptide groups (NH-CO) (Amide bands I, II and III) of proteins. On comparing the skin and pulp FTIR-ATR spectra, more intense absorption bands in the region 1800-1500 cm^{-1} have been found on exocarp samples, attributable to cyanidins, while more intense

absorption bands corresponding to sugars between 1200-800 cm^{-1} have been observed in mesocarp samples. Finally, ToF-SIMS analysis has been carried out, confirming the presence of cyanidin and phosphatidylcholine in the skin of peaches and nectarines, and cyanidin, phosphatidylcholine, oleic acid and coniferyl alcohol in the skin of seeds. The CA obtained from the skins of the seeds, constitutes a viable option for the geographic characterization of peaches and nectarines (Figure 1b).

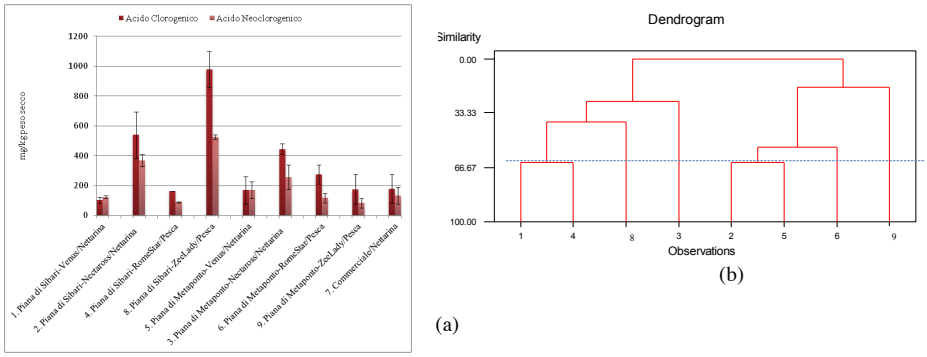


Fig. 1: (a) Relative distribution of hydroxycinnamic acids on hydroalcoolic pulp extracts (HPLC-MS analysis); (b) Cluster analysis from ToF-SIMS data from skin of seed samples.

References

Gil, M.I.; Tomás-Barberán, F.A.; Hess-Pierce, B.; Kader, A.A. "Antioxidant capacities, phenolic compounds, carotenoids, and vitamin C contents of nectarine, peach, and plum cultivars from California", J. Agric. Food Chem. 50, 4976-4982 (2002).

Bureau, S.; Ruiz, D; Reich, M.; Gouble, B.; Bertrand, D.; Audergon, J.M.; Renard, C.M.G.C. "Application of ATR-FTIR for a rapid and simultaneous determination of sugars and organic acids in apricot fruit", Food Chemistry 115, 1133-1140 (2009).

Dunn, W.B.; Bailey, N.J.C.; Johnson, H.E. "Measuring the metabolome: current analytical technologies", The Analyst 130, 606-625 (2005).

Piras, F.M., Dettori, M.F.; Magnani, A. "ToF-SIMS PCA analysis of Myrtus communis L.", Appl. Surf. Sci. 255, 7805-7811 (2009).

The study has been supported by the MiUR, in the framework of the Programma Operativo Nazionale Ricerca e Competitività per le Regioni della Convergenza 2007/2013: PON01_00878 dal titolo "DIRECT FOOD – Valorizzazione delle Produzioni agroalimentari dei Sistemi Locali e di quelli tradizionali del Made in Italy attraverso la gestione integrata delle filiere e di canali innovativi produttore-consumatore".

2C – A multidisciplinary project for the study of historical landscapes: new archaeological and physicochemical data from the "Colline Metallifere" district

A. Donati, V. Volpi, L. Dallai

Aims

The aim of this work is to present some results obtained by a combined-multidisciplinary approach to the study of a territory located in the southern part of Tuscany, the "Colline Metallifere" district. In this paper we are focusing particularly on the use of chemical analyses (pXRF) on crucial historical areas. The considerable amount of information retrieved and the unquestionable value of the data obtained by the pXRF analyses are now opening new fields to the use of the portable instrument.

Results

In the last years the Colline Metallifere district (southern Tuscany) has become a multidisciplinary study area in which a combined archaeological, geological, and environmental approach is providing new interesting evidences for the reconstruction of historical landscapes. Extensive surveys on territorial samples have been carried out to define the main aspects of mining exploitation and metal production; the data collected have been processed with the aim of defining a broad picture of the territory both from an archaeological, geological and environmental perspective.

In order to get the maximum amount of useful information, a combination of underground surveys, fieldworks and XRF analyses on fluvial sediments and soils explored the technical aspects of the production and the environmental impact of ancient mines. From the different case studies combined archaeological and physico-chemical data (pXRF in particular) are gruadually building up a solid database that is helping in defining the historical outlines of the Colline Metallifere landscape.

In the case study of Montieri village the environmental data collection helped to define, on a smaller scale, the topographic limits of a large slag area, very well known from historical descriptions, nowadays partly covered by the standing town of Montieri. The slags are the result of the ore extraction and metallurgical processes that went on around Montieri's village during the Medieval period. The place, as said above, has been in fact in that historical phase an important mining and metallurgical center, and numerous silver mines are still partly visible in the surrounding hills and have been identified by the archaeological surveys.

To estimate the extent of this pile of slag with an initial level of topographical approximation, a large-scale screening was conducted on the river sediments, using the natural leaching process of contaminated soil as a guide. In the case in hand, lead was used as the "tracer" element; indeed, lead is very closely connected with silver

extraction (production from silver-bearing galena). Along the streams it was made a systematic stream sediment sampling for the laboratory analysis through the Atomic Absorption Spectroscopy (AAS) technique.
Results from the analyses showed a high concentrations of Pb on the central rivers compared with the peripheral ones. This indicates that the contamination originated from an area approximately definable (1A). The subsequent level of refinement has included chemical measurements of the soil; this has led us to define with greater precision the area where the slag probably accumulated. The area that can be calculated on the basis of these figures is around 7,500 $mt^2$with a depth of around 4 mt in the southern extremity to a few dozen cm in the northern extremity (1B).
This research is important to determine some important chemical feature for a better understanding of the local historical mining context. In particular it is crucial to find out on the one hand some productive characteristics that can help in defining the amount of mineral worked and, consequently, of metal produced. On the other hand, behind the archaeological aspect, it is useful to verify the spread of contamination and to understand to what extent the presence of metallurgical slags has affected the local environment, providing general indications on the toxic elements speciation in the area.

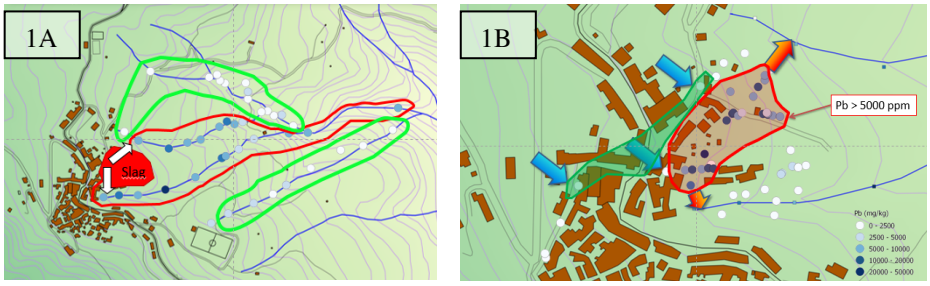


Fig. 1: A) Montieri's vector topographic map. It shows the results of Atomic Absorption Spectroscopy (AAS) analysis of Pb distribution in the river sediments. The darkness of blue color is proportional to the concentrations of Pb. B) The concentration of lead in soil slag heap. The polygon represent the waste area.

References

Dallai, L.; Donati, A.; Volpi, V.; Bardi, A. "Archaeological and physicochemical approaches to the territory: on-site analysis and multidisciplinary databases for the reconstruction of historical landscapes", CAA 2015. Proceedings of the 43rd Annual Conference on Computer Application and Quantitative Methods in Archaeology, 177-185 (2015).
Dallai, L.; Bianchi, G.; Donati, A.; Trotta, M.; Volpi, V. "Le analisi fisico-chimiche territoriali ed 'intra-sito' nelle Colline Metallifere: aspetti descrittivi, 'predittivi' e prima interpretazione storica dei dati", VII congresso nazionale di archeologia Medievale, 389-394 (2015).
Benvenuti, M.; Bianchi. G.; Bruttini, J.; Buonincontri, L.; Chiarantini, L.; Dallai, L.; Di Pasquale, G.; Donati, A.; Grassi, F.; Pescini, V. "Studyng the Colline Metallifere mining area in Tuscany: an interdisciplinary approach", IES Yearbook, 261-287 (2014).

2C – Identification of catalytic protein radicals in LRET mechanism of peroxidases and variants

M.C. Baratto, A. Sinicropi, R. Basosi, R. Pogni

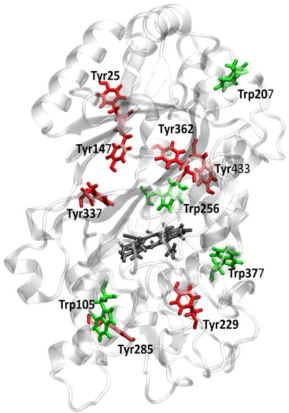
Aims

A combined spectroscopic and computational approach, together with site-directed mutagenesis studies, enabled to identify and characterise catalytic different protein radicals formed through LRET pathways in novel peroxidases.

Results

Peroxidases, a lignin-degrading system, are able to oxidize high redox potential aromatics via exposed protein radicals. 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). The role of protein radical intermediates in the catalytic cycle was studies by multifrequency EPR and identified in the Trp164 site in the *P. eryngii* VP. In a new Lignin Peroxidase (LiP), recently found in the *Trametopsis cervina*, it was found that the conserved catalytic tryptophan lacks and it 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. A new peroxidase, DyP dye-decolorizing peroxidase has been recently tested and characterised. DyPs are widely distributed in fungi, bacteria and archea. The terms "dye-decolorizing" derives from the ability to decolorize and degrade xenobiotic anthraquinone and azo dyes. The catalytic mechanism of DyPs is similar to that of classical peroxidases, where the resting enzyme undergoes a two-electron oxidation by hydrogen peroxide to Compound I (CpI). The activated enzyme is then reduced back by two substrate molecules to the resting state via the Compound II. Different from other fungal peroxidases in the distal side arginine and aspartic residues contribute to the heterolytic cleavage of H_2O_2 to form CpI. AauDyP possesses seven Tyr and four Trp residues as potential sites to active different long range electron transfer pathways (LRET).

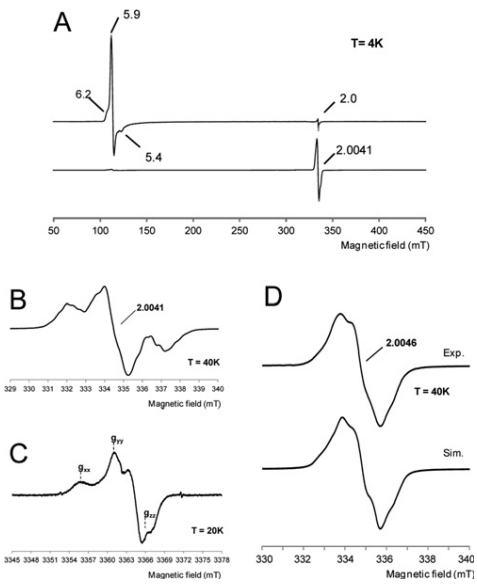
To oxidise bulky substrates, a LRET pathway was also suggested for AauDyP. Simulations using PELE (Protein Energy Landscape Exploration) software provided several binding-energy optima for anthraquinone-type Reactive Blue 19 near the aromatic residues and the heam access channel. Subsequent QM/MM calculations showed a higher tendency of TrP-377 than other exposed heam-neighbouring residues to harbour a catalytic protein radical. The existence of such radical was shown by low temperature EPR on the H_2O_2-activated DyP, being identified a mixed tryptophanyl/tyrosyl radical with a multifrequency EPR approach. The signal was dominated by TrP-377 neutral radical contribution which



Heme prosthetic group (gray), Trp (green), and Tyr (red) residues in AauDyP (4W7J pdb code).

disappeared in the W377S variant and included a tyrosyl contribution assigned to Tyr-337 after analysing the W377S spectra.

A pure tryptophanyl radical EPR signal is detected at pH 7 in contrast with the mixed signal observed at pH 3. The presence of a second tyrosine radical /Tyr 147) is deduced by a multifrequency EPR study of a variety of simple and double-directed variants at different freezing times after their activation by H_2O_2. Such results point out that subsidiary long electron-transfer pathways enter into operation when the main pathway is removed by directed mutagenesis, with catalytic efficiencies progressive decreasing. Finally, self-reduction of the Trp377 neutral radical is observed when reaction time (before freezing) is increased in the absence of reducing substrates (from 10 to 60 s). Interestingly, the tryptophanyl radical is stable in the Y147S/Y337S variant, indicating that these two tyrosine residues are involved in the self-reduction reaction.



EPR spectra of WT DyP and its W377S variant(**A**) X-band EPR spectra of WT DyP at pH 3 before (top) and after (bottom) the addition of H_2O_2 (and rapid freezing). (**B** and **C**) Narrow scan X-band (v =9.39 GHz) and W-band (v =94.29 GHz) respectively of the radical species. The positions of the three g-tensor components of the tyrosyl contribution are indicated. (**D**) X-band EPR spectrum of the radical intermediate formed in the W377S variant paired with its better simulation (Sim).

References

Baratto, M.C.; Sinicropi, A.; Linde, D.; Sáez-Jiménez, V.; Sorace, L.; Ruiz-Duenas, F.J.; Martinez, A.T.; Basosi, R.; Pogni, R. "Redox-Active Sites in Auricularia auricula-judae Dye-Decolorizing Peroxidase and Several Directed Variants: A Multifrequency EPR Study", Journal of Physical Chemistry B 119, 13583-13592 (2015).

Linde, D.; Pogni, R.; Cañellas, M.; Lucas, F.; Guallar, V.; Baratto, M.C.; Sinicropi, A.; Sáez-Jiménez, V.; Coscolín, C.; Romero, A.; Medrano, F.J.; Ruiz-Dueñas, F.J.; Martínez, A.T. "Catalytic surface radical in dye-decolorizing peroxidase: A computational, spectroscopic and site-directed mutagenesis study", Biochemical Journal 465, 253-262 (2015).

Miki, Y. et al. "Formation of a tyrosine adduct involved in lignin degradation by Trametopsis cervina lignin peroxidase: A novel peroxidase activation mechanism", Biochemical Journal 452, 3, 575-584 (2013).

Miki, Y. et al. "Crystallographic, Kinetic, and Spectroscopic Study of the first Ligninolytic Peroxidase presenting a Catalytic Tyrosine", J. The Journal of Biological Chemistry 286, 15525-15534 (2011).

Bernini, C. et al. "EPR parameters of amino acid radicals in P. eryngii versatile peroxidase and its W164Y variant computed at the QM/MM level", Physical Chemistry Chemical Physics 13, 5078-5098 (2011).

2C – Biotechnological applications of oxidases

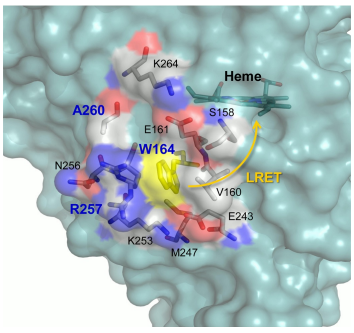
M.C. Baratto, R. Basosi, R. Pogni

Aims

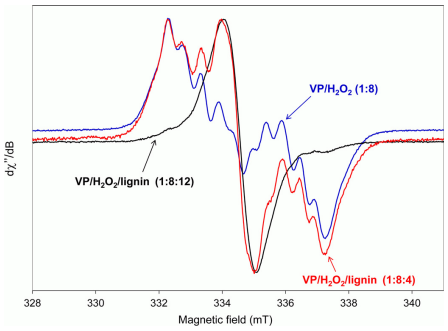
Different oxidases (versatile peroxidase, dye peroxidase, laccase) are understudy for biotechnological applications in the presence of different substrates like lignin polymer and its derivatives, industrial dyes in order to test their double functions: depolymerisation and synthesis of new materials.

Results

Versatile peroxidase (VP) is a high redox-potential peroxidase of biotechnological interest that is able to oxidize phenolic and non-penolic aromatics, Mn(II) and different dyes. The ability of VP from Pleurotus eryngi to oxidize water soluble lignins (softwood and hardwood lignosulfonates) was demonstrated by the combination of directed mutagenesis and spectroscopic techniques. In addition direct electron transfer between the peroxidase and the lignin macromolecules was kinetically characterised using stopped-flow spectrophotometry. VP variants were used to show that the reaction strongly depends on the presence of the solvent-exposed tryptophan residue (Trp164). Moreover, the tryptophanyl radical detected by EPR spectroscopy of H_2O_2-activated VP (being absent from the W164S variant) was identified as catalytically active because it was reduced during lignosulfonate oxidation, resulting in the appearance of a lignin radical. Size-exclusion chromatography showed an increase of the molecular mass of the modified residual lignin, especially for the (low molecular mass) hardwood lignosulfonate, revealing that the oxidation products tend to recondense during the VP treatment.



Environment of the exposed catalytic tryptophan acting as starting point for LRET to heme in VP.



EPR spectra of the reactions of VP with H_2O_2 (at molar ratio 1:8), and of VP with H_2O_2 and softwood lignosulfonate at two different molar ratios (1:8:4 or 1:8:12).

The mechanisms of industrial dye transformation by versatile peroxidase from Bjerkandera adusta were elucidated. The EPR analysis on two copper-containing dyes, reactive violet 5 (azo) and reactive blue 72 (phthalocyanine) after enzymatic decolorization showed the cleavage of the azo bond in azo dyes and the total disruption of phthalocyaninic ring in the phthalocyanine dyes. The role of the catalytic Trp172 in the dye transformation by long-range electron transfer pathway was confirmed and also an oxidation mechanism was proposed.

Furthermore the catalytic properties of a VP from Bjerkandera adusta through the chemical modification of the protein surface with free-radical forming Trp residues has been investigated and a new high redox potential laccase POXA1b from Pleurotus ostreatus and its variant have been produced and characterised spectroscopically. Thanks to their characteristics (chemical derivatization and high redox potential) both these last systems seem to be good candidate for biotechnological applications.

References

Sáez-Jiménez, V.; Baratto, M.C.; Pogni, R.; Rencoret, J.; Gutiérrez, A.; Santos, J.I.; Martínez, A.T.; Ruiz-Dueñas, F.J. "Demonstration of lignin-to-peroxidase direct electron transfer: A transient-state kinetics, directed mutagenesis, EPR, and NMR study", Journal of Biological Chemistry 290, 23201-23213 (2015).

Baratto, M.C.; Juarez-Moreno, K.; Pogni, R.; Basosi, R.; Vazquez-Duhalt, R. "EPR and LC-MS studies on the mechanism of industrial dye decolorization by versatile peroxidase from Bjerkandera adusta", Environ. Sci. Pollut. Res. 22, 8683-8692 (2015).

Sánchez-Alejandro, F.; Juarez-Moreno, K.; Baratto, M.C.; Basosi, R.; Vazquez-Duhalt, R. "Tryptophan-surface modification of versatile peroxidase from Bjerkandera adusta enhances its catalytic performance", Journal of Molecular Catalysis B: Enzymatic 124, 45-51 (2016).

Macellaro, G.; Baratto, M.C.; Piscitelli, A.; Pezzella, C.; Fabrizi De Biani, F.; Palmese, A.; Piumi, F.; Record, E.; Basosi, R.; Sannia, G. "Effective mutations in a high redox potential laccase from Pleurotus ostreatus", Appl. Microbiol. Biotechnol. 98, 4949-4961 (2014).

2C – A comparative study of chromatographic matrices for affinity chromatography of CRM197

A. Stefan, M. Boiani, L. Longanesi, A. Hochkoeppler

Aims

In this study we showed a comparison of three matrices suitable for the purification and refolding of recombinant CRM197 by metal chelating affinity chromatography.

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). Our previous studies indicated the possibility to overexpress the protein in *Escherichia coli* by using an artificial sequence associated with a short oligonucleotide encoding a hexa-histidine tag. Accordingly, a metal chelating affinity chromatography (IMAC) was used for its purification. We firstly used a standard matrix consisting of agarose beads (HiTrap Chelating Sepharose HP, GE Healthcare Life Sciences) and we always found a higher recovery of CRM197his under denaturing than under refolding conditions. We decided to compare this standard matrix with two different commercial matrices, a macroporous silica matrix (Protino Ni-IDA, Macherey-Nagel) and the synthetic Profinity IMAC resin based on polymeric UNOsphere beads (Bio-Rad). The same extraction procedure, identical quantity of bacterial cultures (300 mL) and comparable amount of protein (from 32 to 37 mg) were used to compare the matrices. Firstly, the purification was performed under denaturing conditions using 6 M urea. Table 1 reported the binding capacity and the recovery for each matrix. The agarose-based matrix seems to bind all proteins loaded on the column but the elution profile was broad and diluted along the elution gradient. The maximum protein recovery was 43-44 %. Contrarily, the silica and polymeric matrices showed a narrower elution profile with a comparable recovery yield of 54-55 % and the recombinant protein was eluted in a small volume of buffer (7-8 mL) with a final concentration of 2.3-2.4 mg/mL.

Table 1. Affinity chromatography of CRM197his under denaturing conditions

Matrix	*Input (mg)*	*Flow through (mg)*	*Elution (mg*	*Elution (mL)*	*Recovery (%)*
HiTrap Chelating Sepharose	37	-	16.2	28	44
Protino Ni-IDA	32	8.5	17.2	8	54
Profinity IMAC	33.3	6.9	18.3	7	55

Afterwards, we compared the efficiency of the on-column refolding process using the same three matrices. After loading the sample and washing the column, the urea was removed by two inverse gradients (from 6 to 2 M and from 2 to 0 M urea in 50 mM Tris-HCl pH 7.5, 500 mM NaCl, 1% Triton X-100) before the elution with a linear gradient of imidazole. Preliminary assays with the agarose-based resin showed a very

low yield of recovery (never more than 10 %). When we used the Profinity polymeric matrix, the initial refolding yield was low (13 %), and a high amount of CRM197his was lost inside the flow through during the loading step (Fig. 1(A)(C)). However, when the protein sample was loaded onto the column and the flow-through was reloaded (1 cycle, B), the final recovery increased to 31%, yielding to 9-10 mg of renaturated protein (about 30-32 mg/L). Moreover, as visible in SDS-PAGE (Fig. 1(D)), the band related to CRM197his was detectable in only 5-6 eluted fractions containing 300-340 mM imidazole.

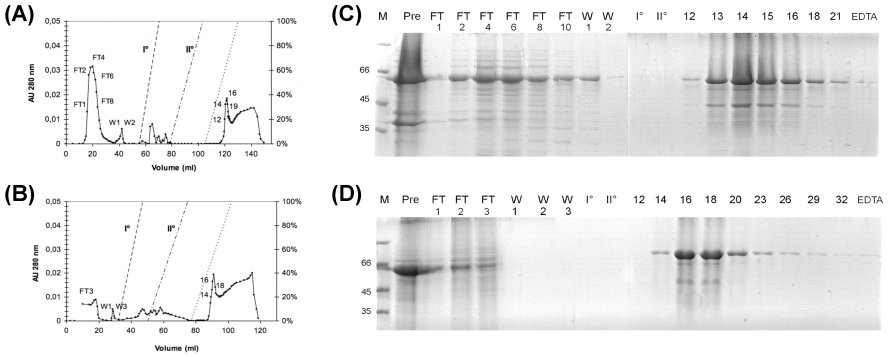


Fig. 1: Purification and refolding of CRM197his by using the Profinity IMAC resin. Chromatographic profiles of the refolding process without (A) or with (B) reloading the flow-through onto the column. (C), (D) SDS-PAGE analysis related to process (A) and (B).

Finally, in order to verify the correct refolding of CRM197his purified with the Profinity IMAC matrix (with recycle), we performed a DNase assay based on agarose gel electrophoresis (data not shown). We found that the on-column refolding procedure allows the recombinant protein to be properly refolded and active.

References

Uchida, T.; Pappenheimer, A.M. Jr.; Greany, R. "Diphtheria toxin and related proteins. I. Isolation and properties of mutant proteins serologically related to diphtheria toxin", J Biol Chem 248, 3838-44 (1973).

Stefan, A.; Conti, M.; Rubboli, D.; Ravagli, L.; Presta, E.; Hochkoeppler, A. "Overexpression and purification of the recombinant Diphtheria Toxin variant CRM197 in Escherichia coli", J Biotechnol 156, 245-252 (2011).

Gaberc-Porekar, V.; Menart, V. "Perspectives of immobilized-metal affinity chromatography", J Biochem Bioph Methods 49, 335-360 (2001).

Singh, S.M.; Panda, A.K. "Solubilization and refolding of bacterial inclusion body proteins", J Biosci Bioeng 99, 303-310 (2005).

2C – Enzyme-containing paints inhibit the growth of marine microorganisms

L. Panizza, P. Frisenda, A. Stefan, M. Francese, A. Madeo, E. Martelli, A. Hochkoeppler

Aims

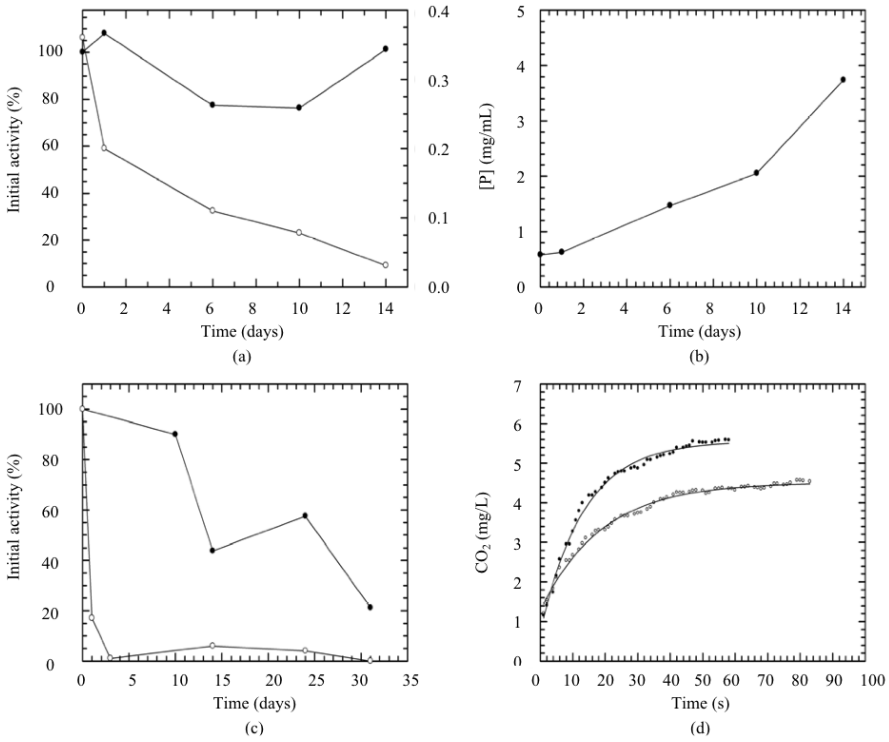
A new strategy to prevent the biofouling of water-submerged surfaces is presented here. In particular, we show that carbonic anhydrase from *Methanosarcina thermophila* can be entrapped into polyacrylic paints.

Results

In conventional practice, paints containing antimicrobial chemicals, e.g. copper, Zinc pyrithion, chlorothalonil, or Sea-Nine are used to delay the fouling of water-submerged surfaces. However, considering the environmental impact of traditional antimicrobials, alternative antifouling strategies were recently considered. Interestingly, enzyme-containing paints were patented as antifouling agents and, recently, encapsulated enzymes were used to prevent biofouling. A major problem concerning the addition of enzymes to antifouling paints is the presence of organic solvents, whose use generally inactivates the enzymes.

Here we present a radically new, acting at a distance, antifouling strategy, i.e. the physical inhibition of microbial colonization of water-submerged surfaces. We show here that the CO_2 released by paint-entrapped carbonic anhydrase is an effective mean to prevent the fouling of water-submerged surfaces. The use of carbonic anhydrase seems ideal to water environments, due to the natural presence of carbonated salts, leading to the production of CO_2, preventing biofouling. Further, CO_2 can feature biocide effects on the fouling organisms present on the water-submerged surface of manufactures, but is devoid of eco-toxicological effect.

First, we investigated the overexpression levels of *Methanosarcina thermophila* carbonic anhydrase (Cam) in *Escherichia coli* (data not shown). Therefore we decided to evaluate the stability of Cam at 54 °C. Surprisingly, 14 days after the onset of the thermal treatment, Cam did fully retain its initial activity (Figure 1a). The thermal treatment triggered the aggregation and sedimentation of *E. coli* proteins; therefore, the specific activity of Cam did consistently increase over the time interval considered (Fig. 1b). When we tested the stability at room temperature in seawater, Cam did perform well, retaining about 20 % of its initial activity after 30 days (Fig. 1c). Finally we tested the CO_2-releasing activity of fiberglass slides (25 cm^2) painted with enzyme-free or enzyme-containing polystyrene resin (Fig. 1d). To obtain enzyme-containing slides, lyophilized carbonic anhydrase from *Methanosarcina thermophila* was dissolved into polystyrene resin (Crilat D120S, Vinavil, Milano, Italy), and the paint accordingly prepared was uniformly distributed over fiberglass slides previously treated with an appropriate primer (Marine Primer, Attiva Marine by Bartolomeo Boero, Genova, Italy). Enzyme-free slides were prepared using the same procedure and a polystyrene resin devoid of carbonic anhydrase.



To assay enzyme activity, the slides were half-immersed into a vessel containing 200 mM Tris buffer (pH 7.6). A CO_2-sensitive electrode was then dipped into the vessel, and reactions were started by the addition of 5 mM $NaHCO_3$.
Remarkably,we detected net CO_2 release from the enzyme-containing slides at a rate equal to 68 ± 34 µg/L·s (Fig. 1d), corresponding to 1.55 ± 0.77 µM/s.
We indeed reasoned that the release of CO_2 by the paint-entrapped enzyme would physically and chemically inhibit the colonization of water-submerged surfaces by microorganisms. In particular, we expected that a CO_2-releasing surface would physically (mechanically) hamper the adsorption of microorganisms, whose the growth would be chemically inhibited by the concomitant increase in CO_2 concentration.

References

Kristensen, J.B.; Meyer, R.L.; Laursen B.S.; Shipovskov, S.; Besenbacher, F.; Poulsen, C.H. "Antifouling enzymes and the biochemistry of marine settlement", Biotechnol Adv 26, 471-481, (2008).
Alber, B.E.; Ferry, J.G. "A carbonic anhydrase from the archeon *Methanosarcina thermophila*", Proc. Natl. Acad. Sci. USA 91, 6909-6913, (1994).
Bellas, J. "Prediction and assessment of mixture toxicity of compounds in antifouling paints using the sea-urchin embryo-larval bioassay", Aquat Toxicol 88, 308-315, (2008).

2C – The multifaceted benefits of protein co-expression in *Escherichia coli*

A. Stefan, A. Ceccarelli, E. Conte, A. Montòn-Silva, A. Hochkoeppler

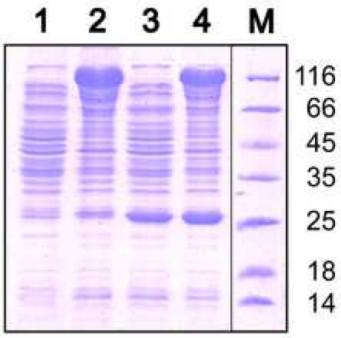
Aims

Here we report on the usefulness of protein co-expression in *Escherichia coli* that is a powerful alternative to the reconstitution *in vitro* of protein complexes, and is of help in performing biochemical and genetic tests *in vivo*.

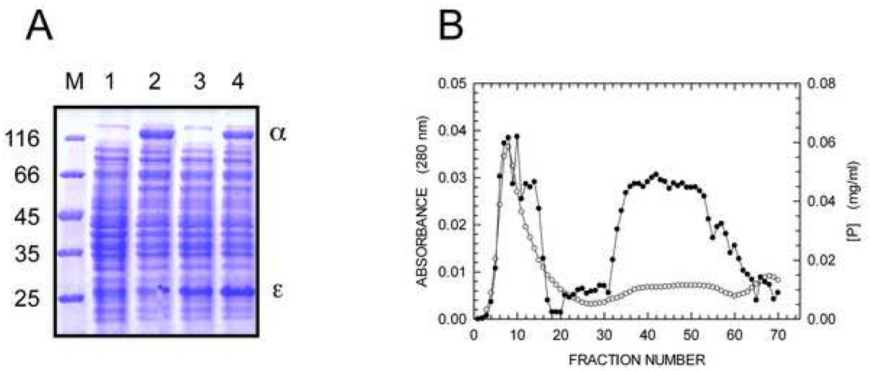
Results

Two main strategies of protein co-expression in *E. coli* can be pursued: i) the use of a single plasmid to host the different genes to be overexpressed; ii) the use of multiple plasmids in single cells to co-express the target proteins. This first approach is quite simple, however, the use of a single plasmid to co-express different proteins faces two major difficulties: i) the molecular mass of the vector increases with the number of hosted genes, limiting the number of co-expressed proteins; ii) when multiple genes are cloned under the control of a single promoter, polarity can decrease the expression of the genes distal from the promoter. We recently constructed the pGOOD plasmid compatible to the pBAD vector; in fact, pGOOD features a p15A origin of replication, a tetracycline-resistance cassette and *lac*-derived regulatory elements. Therefore, co-expression of protein complex is strictly dependent on the addition to the *E. coli* culture medium of both IPTG and arabinose, triggering overexpression from pGOOD and pBAD, respectively. Interestingly, protein co-expression can efficiently solve difficulties linked to the poor solubility of a protein complex subunit. In addition, in *vivo* protein complementation tests can be performed, and the protein co-expression can be also use to tune mutation frequency in *E. coli*. Here we illustrate some examples of each case study by using the pGOOD-pBAD couple.

Example 1: co-expression of α and ε subunits of E. coli DNA polymerase III catalytic core. Cells were grown in the absence of inducers, in the presence of arabinose only, of IPTG only, or in medium supplemented with both arabinose and IPTG (lane 1-4):



Example 2: co-expression can also be used to perform inter-species complementation tests. To evaluate the competence of *Deinococcus radiodurans* polymerase III α subunit (α*Dr*) in binding *E. coli* ε subunit, we have cloned into the pBAD vector a synthetic gene coding for α*Dr* and we have co-transformed *E. coli* with pBAD-α*Dr* and pGOOD-ε. Figure A shows the SDS-PAGE of total protein extracts isolated from cells not induced (lane 1), or induced to overexpress αDr, ε, or αDr and ε (lanes 2-4, respectively). A gel filtration column, loaded with soluble proteins, was used to evaluate complex formation (B, chromatogram empty circles).



Example 3: co-expression of the wild-type and mutagenic ε subunit of *E. coli* DNA polymerase III allows to tune the mutation frequency of the bacterial host. Mutator strains, featuring mutation frequencies higher than their wild type counterparts, are of interest in biotechnology. Protein co-expression can be used to obtain a better control of mutator strains. To this aim, we co-transformed *E. coli* with pBAD-ε and pGOOD1-εD12A, in order to induce the expression of the wild-type and the mutagenic D12A variant of ε with arabinose and IPTG, respectively. As a phenotypic test, we determined the appearance of β-glucosidase activity, which is cryptic in wild-type *E. coli*. When cells were induced to express the D12A mutagenic variant, β-glucosidase activity was acquired in ca. 20 generations (data not shown).

References

Hochkoeppler, A. "Expanding the landscape of recombinant protein production in *Escherichia coli*", Biotechnol. Lett. 35, 1971-1981 (2013).

Bressanin, D.; Stefan, A.; Dal Piaz, F.; Cianchetta, S.; Reggiani, L.; Hochkoeppler, A. "Proteolysis of the proofreading subunit controls the assembly of *Escherichia coli* DNA polymerase III catalytic core", Biochim. Biophys. Acta 1794, 1606-1615 (2009).

Conte, E.; Landolfi, G.; Vincelli, G.; Stefan, A.; Hochkoeppler, A. "pGOODs: new plasmids for the co-expression of proteins in *Escherichia coli*", Biotechnol. Lett. 33, 1815-1821 (2011).

2C – Oleuropein degradation by olive leaf protein extract

A. De Leonardis, V. Macciola, F. Cuomo, G. Cinelli, F. Lopez

Aims

Use of olive leaves as low cost source of substances for interesting biotechnological application.

Results

The enzymatic activity of raw protein olive leaf extract has been investigated in vivo, on olive leaf homogenate and, in vitro with pure oleuropein and other phenolic substrates. At least two types of enzymes were found to be involved in the degradation of endogenous oleuropein in olive leaves. As for the in vitro experiments, the presence of active polyphenoloxidase and β-glucosidase was determined by HPLC and UV–Visible spectroscopy. Interestingly, both the enzymatic activities were found to change during the storage of olive leaves. Specifically, the protein extracts obtained from fresh leaves showed the presence of both the enzymatic activities, because oleuropein depletion occurred simultaneously with the formation of the oleuropein aglycon, 3,4-DHPEA-EA. In comparison leaves subjected to the drying process showed a polyphenoloxidase activity leading exclusively to the formation of oxidation products responsible for the typical brown coloration of the reaction solution.

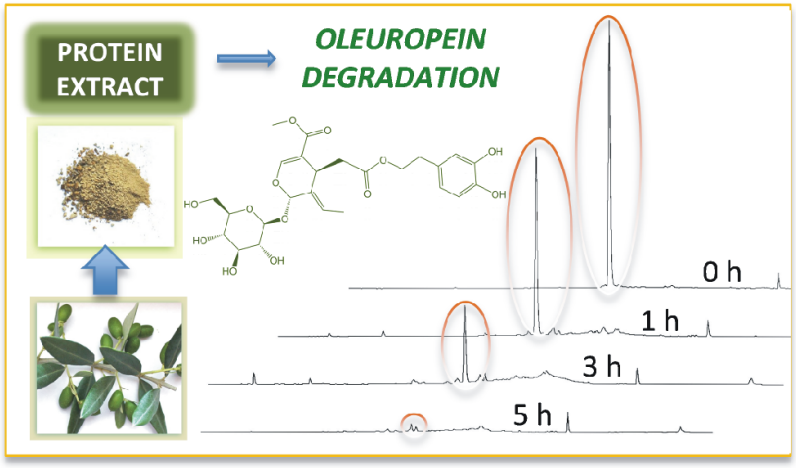


Fig. 1: Representation of the olive leaves protein extract (left) and HPLC chromatograph of the oleuropein hydrolysis within 5 hours (right).

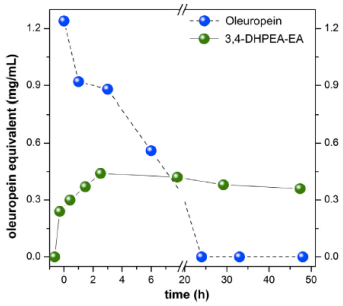


Fig. 2: Oleuropein hydrolysis and 3,4-DHPEA-EA formation produced by raw protein extract from fresh olive leaves at 60°C.Concentrations were measured by HPLC analyses.

References

De Leonardis, A.; Macciola, V.; Cuomo, F.; Lopez, F. "Evidence of oleuropein degradation by olive leaf protein extract", Food Chemistry 175, 568-574 (2015).

2C - Thermodynamics Properties and Photodegradation Kinetics of Indocyanine green in aqueous solution

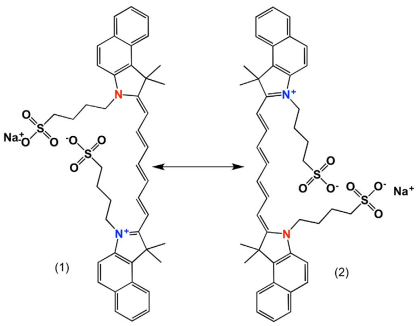
F. Di Nezza, G. Guerra, C. Costagliola, L. Zeppa, L. Ambrosone

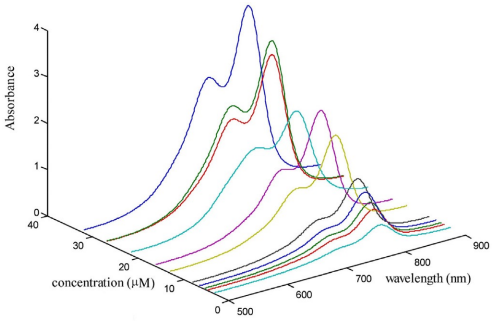
Aims

Indocyanine green (ICG) was approved by the Food and Drug Administration as an agent to evaluate hepatic function, cardiac output and for ophthalmic angiography. ICG has to be administrated in the form of aqueous solutions. However, in aqueous solutions ICG undergoes trans- formations as aggregations and degradation. Such changes result in discoloration decreased light absorption, decreased fluorescence and a shift in the wavelength of maximum absorption. The purpose of the paper is to obtain chemical and physical information about ICG in order to design with less risk possible canalostomy intervention. Therefore the degradation kinetics of the dye when the solution is irradiated with white light has also been studied.

Results

Recently we proved that an aqueous solution of ICG, comprising viscoelastic chondroitin sulfate and sodium hyaluronate, is an effective contrast medium in viscocanalostomy interventation. In this paper our research is focused on dye-dye attractive forces which are generated in aqueous solutions. In aqueous solution of ICG solute-solute interactions, which induce the formation of molecular aggregates such as dimers or n-mers, are highly favored. The fluorescence intensity as a function of the dye concentration shows a maximum. Spectrophotometric results indicate that the dimerization reaction rapidly reaches equilibrium. A new approach was used to calculate the equilibrium constant for the dimerization reaction. The value obtained is comparable to those obtained with different methods on safranine and thionine. ICG exposed to white light degrades. The degradation kinetics is monitored spectrophotometrically and results interpreted on the basis of a direct model. The moving arc strategy is employed to evaluate the evolution speed of the degree of conversion. The method does not provide information about the molecular mechanism, but the lifetime and the apparent reaction order of overall kinetics is fully determined. We are confident that the equations obtained can be of any practical use in planning surgery for glaucoma.





References

Di Nezza, F.; Guerra, G.; Costagliola, C.; Zeppa, L; Ambrosone L. "Thermodynamic properties and photodegradation kinetics of indocyanine green in aqueous solution", Dyes and Pigments 134, 342-347 (2016).

Zeppa, L.; Ambrosone, L.; Fortunato, M.; Costagliola, C. "Soluzione acquosa per rendere visibile mediante metodica fotografica il canale di schlemm e le vie di deflusso dell'umore acqueo e metodo diagnostico che utilizza detta soluzione", Italian Patent (12444PTIT).

Zeppa, L.; Ambrosone, L.; Guerra, G.; Costagliola, C. "Using canalography to visualize the in vivo aqueous humor outflow conventional pathway in human", Jama Opthalomol. 132 (11), 1281 (2014).

2C – In Vivo Near-Infrared Fluorescence Imaging of Aqueous Humor Outflow Structures

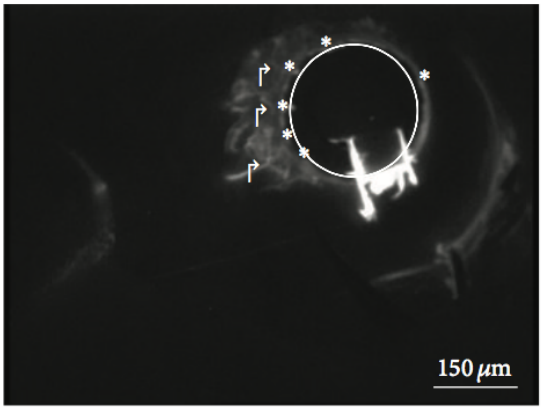
L. Zeppa, L. Ambrosone, G. Guerra, M. Fortunato, C. Costagliola

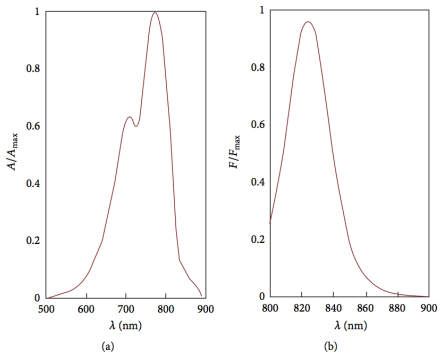
Aims

The aim of this study has been to visualize the aqueous out how system in patients a ected by primary open angle glaucoma. A solution of indocyanine green (ICG) plus high viscosity viscoelastic solution was injected into the Schlemm canal (SC) during surgery in 10 glaucomatous patients undergoing canaloplasty.

Results

Soon a er injection of the dye, there was impregnation of the borders of the scleral ap due to partial re ux caused by the intrachannel resistance; progression of the dye along the SC starting from the site of injection was then visualized. In some eyes, the filling proceeded along 360 degrees whereas in others only a portion of the canal was visualized. In 3 patients, the percentage of lling was 70%, whereas in the remaining 7 patients this percentage decreased up to 50%. A correlation between SC lling and number of CCs visualized was observed. It is possible that an obstruction of the canal was present in such eyes. e lling of the collector channels occurred only in correspondence of the patent portions of the SC. However, even in presence of a patent SC over 360 degrees, the filling of the collector channels was not simultaneously visualized in all four quadrants. Furthermore, the collector CCs closer to the site of injection did not necessarily ll up before the farther ones.





References

Zeppa, L; Ambrosone, L; Fortunato, M; Costagliola, C. “Soluzione acquosa per rendere visibile mediante metodica fotografica il canale di Schlemm e le vie di deflusso dell'umore acqueo e metodo diagnostico che utilizza detta soluzione”, Patent 12444PTIT (2013).

Zeppa, L.; Ambrosone, L.; Guerra, G.; Fortunato, M.; Costagliola C. “In Vivo Near-Infrared Fluorescence Imaging of Aqueous Humor Outflow Structures”, J. Ophthalmology Article ID 8706564, 6 http://dx.doi.org/10.1155/2016/8706564 (2016).

2C – Physico-Chemical Properties of Pharmaceutical Systems

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

Aims

The research activity in the pharmaceutical field concerns the development of 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, strategies to improve the solubility and the dissolution rate of drugs. In particular, in the years 2014-2016 the efforts have been directed towards the preparation and the characterization of co-crystals and of electrospun fibers to enhance or to control the drug release.

Results

Solubility represents an important challenge for formulation of drugs, because the therapeutic efficacy of a drug depends on the bioavailability and ultimately on its solubility. Low aqueous solubility is one of the main issues related with formulation design and development of new molecules. Many drug molecules present bioavailability problems due to their poor solubility. For this reason there is a great interest in the development of new systems able to enhance the dissolution of poorly water-soluble drugs.

We prepared co-crystals of bumetanide, a diuretic and natriuretic active principle, with 4-amino benzoic acid. The synthesis was performed both by wet and dry grinding. The co-crystal formation was investigated with a wide range of techniques, including solid-state NMR, IR, XRD, microscopy and thermal analysis. Wet and dry grinding procedures led to different co-crystal polymorphs. In particular, the dry method gave a co-crystal by powder amorphization and subsequent crystallization. DFT calculations at B3LYP/6-31+G(d,p) level of theory shed light on the H-bond scheme at the basis of co-crystals formation. Both the co-crystals showed improved solubility and dissolution rate with respect to the drug alone. This could guarantee a faster absorption and a better bioavailability of the active principle.

Electrospun fibers loaded with budesonide have been fabricated and characterized with the aim of controlling the drug release in the gastrointestinal tract. Budesonide is a non halogenated glucocorticosteroid drug, highly effective in the treatment of some inflammatory bowel diseases with local action throughout ileum and colon. At this aim, Eudragit® S 100, a polymer soluble at pH>7, commonly used for enteric release of drugs, has been successfully spun into ultrafine fibers loaded with budesonide at 9% and 20 % (w/w) using the electrospinning process. The physico-chemical characterization by scanning electron microscopy, X-ray diffraction, FT-IR spectroscopy and thermal analyses indicated the amorphous nature of budesonide in the electrospun systems. Dissolution rate measurements using a pH-change method showed negligible drug dissolved at pH 1.0 and sustained release at pH 7.2. Therefore, the pharmaceutical systems proposed, made of fibers, represent an effective method for drug targeting to terminal ileum and colon with the aim of improving the local efficacy of this drug.

We prepared fibers containing perphenazine, an insoluble model drug, by the electrospinning method, in order to increase its water solubility. Two hydrophilic polymers, polyvinylpyrrolidone (Plasdone® K29/32) and polyvinyl caprolactam-polyvinyl acetate-polyethylene glycol graft copolymer (Soluplus®) were used.
The physico-chemical characterization suggests that the drug loaded in the fibers is in the amorphous state. Both polymeric carriers are effective to promote the drug dissolution rate in water, where this active is insoluble, due to the fine dispersion of the active into the polymeric matrices, obtained with this production technique. In fact, the dissolution profiles of the fibers, compared to the simple physical mixture of the two components, and to the reference commercial product Trilafon® 8 mg tablets, show that a strong enhancement of the drug dissolution rate can be achieved with the electrospinning technique.

References

Bruni, G.; Maietta, M.; Berbenni, V.; Mustarelli, P.; Ferrara, C.; Freccero, M.; Grande, V.; Maggi, L.; Milanese, C.; Girella, A.; Marini, A. "Mechanochemical synthesis of bumetanide–4-aminobenzoic acid molecular cocrystals: a facile and green approach to drug optimization", Journal of Physical Chemistry B 118, 9180-9190 (2014).
Bruni, G.; Maggi, L.; Tammaro L.; Canobbio A.; Di Lorenzo R.; D'Aniello S.; Domenighini C.; Berbenni, V.; Milanese, C.; Marini, A. "Fabrication, physico-chemical, and pharmaceutical characterization of budesonide-loaded electrospun fibers for drug targeting to the colon", Journal of Pharmaceutical Sciences 104, 3798-3803 (2015).
Bruni, G.; Maggi, L.; Tammaro L.; Di Lorenzo R.; Friuli V.; D'Aniello S.; Maietta M.; Berbenni, V.; Milanese, C.; Girella A.; Marini, A. "Electrospun fibers as potential carrier systems for enhanced drug release of perphenazine", International Journal of Pharmaceutics 511, 190-197 (2016).

2C – Phospholamban (PLN) regulation of sarco/endoplasmic reticulum Ca-ATPase (SERCA)

F. Tadini-Buoninsegni, S. Smeazzetto, M.R. Moncelli
(Department of Chemistry "Ugo Schiff", University of Florence)

Aims

Investigation of the interaction mechanism between Phospholamban (PLN) and sarco/endoplasmic reticulum Ca-ATPase (SERCA).

Results

SERCA promotes muscle relaxation by pumping Ca^{2+} ions from the cytoplasm into the sarcoplasmic reticulum lumen. The activity of SERCA in cardiomyocytes is regulated by a small membrane protein, PLN. It is known that PLN exists as a monomer and homopentamer, both of which are critical for normal cardiac function and can interact with SERCA. Previous studies have shown that recombinant wild-type PLN can form a cation selective ion channel in different biomimetic membranes [1–4].

In the present study we evaluated the effects of PLN on the ATP-dependent Ca^{2+} translocation by SERCA by performing pre-steady state current measurements on a solid supported membrane (SSM, Figure 1A). Proteoliposomes incorporating SERCA and PLN were adsorbed on a SSM and then activated by ATP concentration jumps. The charge obtained by numerical integration of the ATP-induced current transient is attributed to an electrogenic event corresponding to the translocation and release of bound Ca^{2+} upon ATP phosphorylation within the first enzyme cycle [5].

Our results indicate that PLN interferes with ATP-dependent Ca^{2+} translocation by SERCA. By fitting the translocated charges at various Ca^{2+} concentrations using the Hill function, we compared the $K_{0.5}$ and cooperativity coefficient values (Figure 1B). A higher $K_{0.5}$ value was observed in the presence of PLN with respect to the value determined for proteoliposomes containing SERCA only. This result suggests that PLN decreases SERCA calcium affinity. Moreover, in the case of co-reconstituted SERCA/PLN proteoliposomes high $K_{0.5}$ and cooperativity values were obtained with simultaneous ATP and Ca^{2+} concentration jumps, while a much higher $K_{0.5}$ and loss of cooperativity were observed with Ca^{2+} jumps in the presence of ATP.

Therefore, SERCA inhibition by PLN occurred under different substrate conditions. The choice of substrate conditions is important to promote particular conformational states of SERCA. Overall, our observations support the concept that PLN can establish an inhibitory interaction with at least two SERCA conformational states, thereby decreasing the calcium affinity of the enzyme.

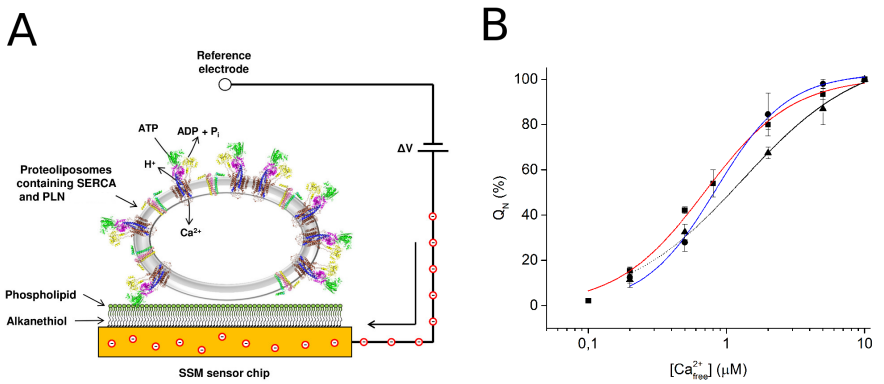


Fig. 1A: SSM technique. Schematic diagram of a proteoliposome incorporating SERCA and PLN adsorbed to a SSM and subjected to an ATP concentration jump.
Fig. 1B: Co-reconstituted SERCA and PLN proteoliposomes activated by ATP and Ca^{2+} concentration jumps. Normalized charges related to simultaneous ATP (100 μM) and free Ca^{2+} (various concentrations) jumps (circles; blue line). Normalized charges related to free Ca^{2+} (at different concentrations) jumps in the presence of 100 μM ATP (triangles; black line). Normalized charges related to ATP concentration jumps on proteoliposomes containing SERCA+PLN in the presence of different Ca^{2+} concentrations (squares; red line). The lines represent curve fitting of the experimental data using the Hill equation. Error bars represent SEM of at least four independent measurements.

References

Kovacs, R.J.; Nelson, M.T.; Simmerman, H.K.; Jones, L.R. "Phospholamban forms Ca^{2+}-selective channels in lipid bilayers", J. Biol. Chem. 263, 18364-18368 (1988).

Smeazzetto, S.; Saponaro, A.; Young, H.S.; Moncelli, M.R.; Thiel, G. "Structure-function relation of phospholamban: modulation of channel activity as a potential regulator of SERCA activity", PLoS One 8, e52744 (2013).

Smeazzetto, S.; Sacconi, A.; Schwan, A.L.; Margheri, G.; Tadini-Buoninsegni, F. "Binding of a monoclonal antibody to the phospholamban cytoplasmic domain interferes with the channel activity of phospholamban reconstituted in a tethered bilayer lipid membrane", Langmuir 30, 10384-10388 (2014).

Smeazzetto, S.; Tadini-Buoninsegni, F.; Thiel, G.; Berti, D.; Montis, C. "Phospholamban spontaneously reconstitutes into giant unilamellar vesicles where it generates a cation selective channel", Phys. Chem. Chem. Phys. 18, 1629-1636, (2016).

Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Fendler, K. "Charge transfer in P-type ATPases investigated on planar membranes", Arch. Biochem. Biophys. 476, 75-86 (2008).

2C – Interaction of antitumor drugs with P-type ATPases

F. Tadini-Buoninsegni, S. Smeazzetto, M.R. Moncelli
(Department of Chemistry "Ugo Schiff", University of Florence)

Aims

Mechanism of interaction of antitumor compounds with P-type ATPases. Role of P-type ATPases in anticancer treatment.

Results

P-type ATPases are a large and varied family of membrane transporters that couple the energy provided by ATP hydrolysis to the active transport of various ions across biological membranes. A specific feature of P-type ATPases is the formation of a phosphorylated intermediate state during their catalytic cycle.

The ion transport mechanism of P-type ATPases has been investigated by electrophysiological measurements on solid supported membranes (SSM) [1]. The SSM consists of a hybrid alkanethiol/phospholipid bilayer supported by a gold electrode. Proteoliposomes or native membranes (vesicles or fragments) incorporating the ATPase can be adsorbed on a SSM and activated by a rapid substrate concentration jump. The substrate jump induces charge movement across the transport protein, and a current transient can be detected by the SSM method [1].

We evaluated the inhibitory effects of the antitumor drug cisplatin on the pumping activity of sarcoplasmic reticulum (SR) Ca^{2+}-ATPase and Na^+,K^+-ATPase by employing the SSM-based electrophysiological method. We performed ATP concentration jumps in the absence (control measurement) or in the presence of cisplatin and recorded the relative current signals.

In the case of SR Ca^{2+}-ATPase, we found that cisplatin strongly interferes with translocation of Ca^{2+} ions upon ATP phosphorylation (Fig. 1). We evaluated the concentration dependence of the cisplatin inhibitory effect and we found an IC_{50} value of 1.3μM, indicating that cisplatin acts as a high affinity Ca^{2+}-ATPase inhibitor. It is worth mentioning that an IC_{50} value of ~ 1μM was also reported for the anticancer ruthenium (III) complex KP1019, which was found to affect ATP-dependent calcium translocation by SR Ca^{2+}-ATPase [2].

We also observed an inhibitory effect of cisplatin on the pumping activity of Na^+,K^+-ATPase (Fig. 2). However, in the case of Na^+,K^+-ATPase inhibition by cisplatin an IC_{50} value of 11μM was found, suggesting that cisplatin acts as a less potent inhibitor towards Na^+,K^+-ATPase as compared to SR Ca^{2+}-ATPase.

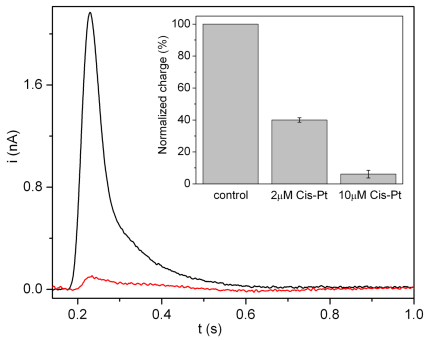


Fig. 1: **Effect of cisplatin on SR Ca^{2+}-ATPase**. Current transients induced by ATP concentration jumps in the absence (control measurement, black line) or in the presence of 5μM cisplatin (red line). Inset: Normalized charges in the absence or in the presence of cisplatin (2μM and 10μM). The error bars represent S.E. of three independent measurements.

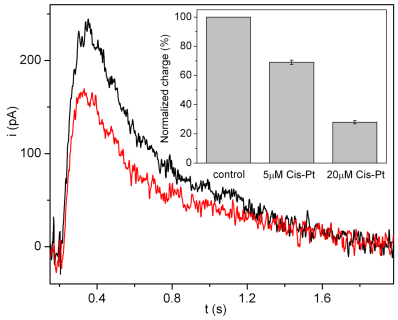


Fig. 2: **Effect of cisplatin on Na^+,K^+-ATPase**. Current transients induced by ATP concentration jumps in the absence (control measurement, black line) or in the presence of 5μM cisplatin (red line). Inset: Normalized charges in the absence or in the presence of cisplatin (5μM and 20μM). The error bars represent S.E. of three independent measurements.

Recently, the SSM technique was employed to investigate Cu^+ ion movement in bacterial (*LpCopA*) [3] and human Cu^+-ATPases (*ATP7A* and *ATP7B*) [4]. In particular, we demonstrated that cisplatin and oxaliplatin can activate ATP7A and ATP7B, whose normal function is to catalyze active transport of Cu^+ across cellular membranes, and undergo ATP-dependent translocation in a fashion similar to that of Cu^+ [5]. We also found that the Pt-related charge movement is dependent on formation of a phosphorylated intermediate, as well as conformational adjustments analogous to those required for Cu-related charge translocation.

References

Tadini-Buoninsegni, F.; Moncelli, M.R.; Peruzzi, N.; Ninham, B.W.; Dei, L.; Lo Nostro, P. "Hofmeister effect of anions on calcium translocation by sarcoplasmic reticulum Ca^{2+}-ATPase", Sci. Rep. 5, 14282 (2015).

Sadafi, F.Z.; Massai, L.; Bartolommei, G.; Moncelli, M.R.; Messori, L.; Tadini-Buoninsegni, F. "The anticancer ruthenium(III) complex KP1019 interferes with ATP dependent Ca^{2+} translocation by sarco-endoplasmic reticulum Ca^{2+}-ATPase (SERCA)", ChemMedChem 9, 1660-1664 (2014).

Mattle, D.; Zhang, L.; Sitsel, O.; Pedersen, L.T.; Moncelli, M.R.; Tadini-Buoninsegni, F.; Gourdon, P.; Rees, D.C.; Nissen, P.; Meloni, G. "A sulfur-based transport pathway in Cu^+-ATPases", EMBO Rep. 16, 728-740 (2015).

Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Pilankatta, R.; Lewis, D.; Inesi, G. "ATP dependent charge movement in ATP7B Cu^+-ATPase is demonstrated by pre-steady state electrical measurements", FEBS Lett. 584, 4619-4622 (2010).

Tadini-Buoninsegni, F.; Bartolommei, G.; Moncelli, M.R.; Inesi, G.; Galliani, A.; Sinisi, M.; Losacco, M.; Natile, G.; Arnesano, F. "Translocation of platinum anticancer drugs by human copper ATPases ATP7A and ATP7B", Angew. Chem. Int. Ed. Engl. 53, 1297-1301, (2014).

2C – Glutathione, glutathione disulfide and *S*-glutathionylated proteins in cell cultures

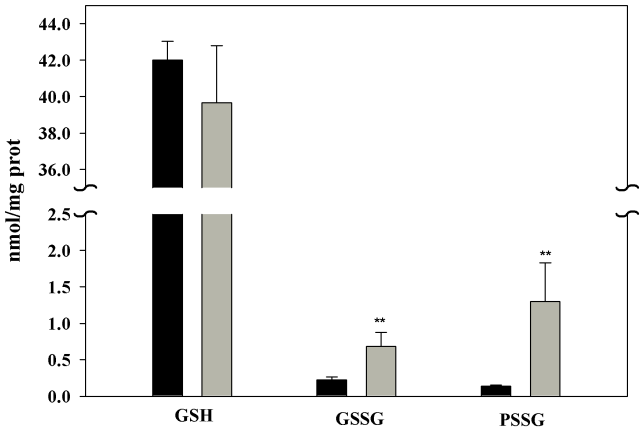
D. Giustarini, F. Galvagni, A. Tesei, A. Farolfi, M. Zanoni, S. Pignatta, A. Milzani, I.M. Marone, I. Dalle-Donne, R. Nassini, R. Rossi

Aims

To develop and validate a new protocol to measure glutathione (GSH), glutathione disulfide (GSSG) and *S*-glutationylated proteins (PSSG) in a large series of cell lines.

Results

We demonstrate that the major artifact occurring during thiol and disulfide analysis in cultured cells is represented by glutathione disulfide (GSSG) and *S*-glutathionylated proteins (PSSG) overestimation due to artificial oxidation of glutathione (GSH) during sample manipulation, and that this methodological problem can be solved by the addition of N-ethylmaleimide (NEM) immediately after culture medium removal. Basal levels of GSSG and PSSG in different lines of cultured cells were 3-5 and 10-20 folds higher, respectively, when the cells were processed without NEM. NEM pre-treatment prevented also the artificial reduction of disulfides that occurs during the pre-analytical phase when cells are exposed to an oxidant stimulus. In fact, in the absence of NEM, after medium removal, GSH, GSSG and PSSG levels restored their initial values within 15-30 min, due to the activity of reductases and the lack of the oxidant. The new developed protocol was used to measure the thiol-disulfide redox status in 16 different line cells routinely used for biomedical research both under basal conditions and after treatment with disulfiram, a thiol-specific oxidant (0-200 μM concentration range). Disulfiram (Antabuse®) is a drug used to treat chronic alcoholism since it induces an extremely adverse reaction when taken in the presence of alcohol by inhibition of acetaldehyde dehydrogenase and is currently being studied as a treatment for cocaine dependence, for its antiprotozoal activity, in cancer therapy and as a treatment in HIV. It possesses a reactive disulfide bond, which reacts readily with both protein and low-molecular mass thiols forming mixed disulfides, disulfides and dithiocarbamates.



Study of the protective effect of NEM. BAEC were treated (black bars) or not (gray bars) with 5 mM NEM. Cells were then lysed by TCA addition and analyzed for the content of GSH, GSSG and PSSG by HPLC. **p<0.01 vs NEM treatment. Data are the mean ± SD, n = 3.

Our data indicate that in most cell lines, treatment with disulfiram affected the levels of GSH and GSSG only at the highest concentration. On the other hand, PSSG levels increased significantly also at the lower concentrations of the drug and the rise was remarkable (from 100 to 1000 folds at 200 μM concentration) and dose-dependent for almost all the cell lines. These data support the suitability of the analysis of PSSG in cultured cells as a biomarker of oxidative stress.

References

Giustarini, D.; Galvagni, F.; Tesei, A.; Farolfi, A.; Zanoni, M.; Pignatta, S.; Milzani, A.; Marone, I.M.; Dalle-Donne, I.; Nassini, R.; Rossi, R. "Glutathione, glutathione disulfide and *S*-glutathionylated proteins in cell cultures", Free Radic Biol Med 89, 972-981 (2015).

2C – Graphene/Nanoparticles hybrid system for the controlled immobilization of biomarkers for early diagnosis of neurodegenerative diseases

C. Lofrumento, M.R. Martina, G. Caminati

Aims

Aim of the research project is the design and fabrication of novel hybrid nanostructures as diagnostic platforms for the determination of biomarkers for the very early stage of neurodegenerations, such as Alzheimer's disease.
The nanostructures result from a combination of ordered and compact arrays of metal nanoparticles veiled with graphene derivatives. The external layer is functionalized with proper receptors of the selected biomarker, immobilized with the fine tuning of its surface density and molecular conformation on the sensor transducer.

Results

We fabricated monolayer assemblies of silver nanocubes (AgNCs), by means of the Langmuir-Blodgett (LB) technique, as a convenient nanostructural basal layer upon which, one-atom-thick GO sheets with lateral dimensions of few microns were deposited. The adsorption process was followed by a Quartz Crystal Microbalance (QCM) with dissipation monitoring that provided mass-density, thickness and elasticity values for the GO layer at saturation. A sketch of the resulting structures is reported in figure 1.

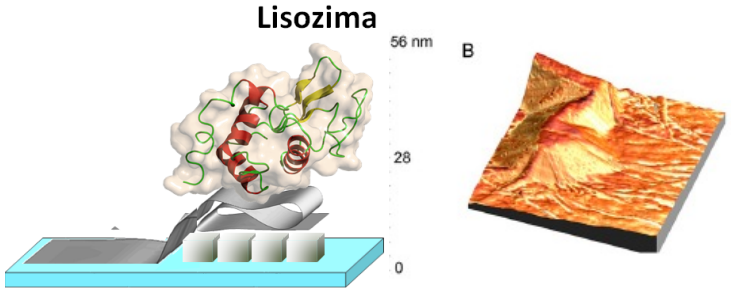
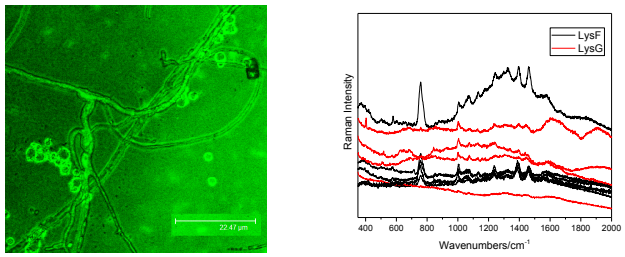


Fig. 1: Cartoon of the proposed sensors platform and Atomic Force Microscopy image of the system

The novel nanostructure was used for the detection of fibrillated lysozyme, as model biomarker for amyloid diseases. The adsorption of native and fibrillated lysozyme on the nanosensors was investigated as a function of bulk protein concentration with a variety of techniques: QCM, Confocal Laser Scanning Microscopy and Atomic Force Microscopy to obtain the surface density and thickness of the lysozyme. CLSM allowed to visualize the morphology of the aggregated fibrils whereas spatially resolved fluorescence spectra of Thioflavine T and Congo Red, used as fluorescence probes for the β-sheet structure, allowed to correlate the morphology of the fibrils with the secondary structure of the protein. Finally, we performed Surface Enhanced Raman Spectroscopy (SERS) analysis on the same samples for the identification of specific signals of secondary structure of native and fibrilled lysozyme (figure 2).



a) (b)

Fig. 2: (a) Lysozyme fibrils observed by CLSM and (b) SERS spectra of globular lysozyme (red line) and fibrillar lysozyme (black line)

The proposed nano-platform represents a valuable substrate for the accurate differentiation between the globular and the fibrillar structures of lysozyme. QCM results combined with SERS analysis allowed for the determination of subnamolar concentration of Lysozyme and to discriminate between the toxic and native form of the protein.

References

Banchelli, M.; Tiribilli, B.; de Angelis, M.; Pini, R.; Caminati, G.; Matteini, P. "Controlled Veiling of Silver Nanocubes with Graphene Oxide for Improved Surface-Enhanced Raman Scattering Detection", ACS Appl. Mater. Interfaces 8, 2628-2634 (2016).

Tramonti, V.; Martina, M.R.; Lofrumento, C.; Dei, L.; Matteini, P.; Caminati, G. "Graphene oxide/silver nanoparticles hybrid layers for SERS detection of amyloid proteins". In preparation.

Author Index

A

Al Katib M. · 131
Ambrosone L. · 179, 247, 249
Angelico R. · 87, 89, 121, 123, 188

B

Baglioni M. · 210, 218, 220, 222
Baglioni P. · 105, 107, 109, 111, 113, 152, 154, 156, 160, 161, 202, 204, 206, 208, 210, 212, 214, 216, 218, 220, 222
Balducci E. · 133
Baratto M.C. · 93, 131, 135, 196, 235, 237
Barbero F. · 163
Bartolini A. · 161
Basosi R. · 91, 131, 135, 173, 175, 177, 186, 192, 194, 196, 235, 237
Batini F. · 186
Berbenni V. · 97, 224, 251
Bergese P. · 158
Bernini C. · 173, 175
Berti D. · 158, 160, 161, 163, 218, 220
Bini M. · 225, 227
Boiani M. · 239
Bonechi C. · 125, 127, 129, 169, 171, 229, 231
Bonelli N. · 202, 204, 206
Bonini M. · 105, 220
Bonucci A. · 133
Borocci, S. · 165
Bravi M. · 186
Brun P. · 101
Bruni G. · 97, 224, 251
Bufalo G. · 179
Busi A. · 194
Busi E. · 192, 194

C

Caltagirone C. · 138, 140
Caminati G. · 115, 259
Campanini R. · 188
Capone A. · 125
Capsoni D. · 225, 227
Carretti E. · 206, 218
Castagliuolo I. · 101
Castroflorio B. · 160
Ceccarelli A. · 243
Ceglie A. · 123, 136, 138, 198
Chelazzi D. · 202, 208, 210, 212, 218
Cimmino L. · 179
Cinelli G. · 245
Cofrancesco P. · 97, 99, 200
Collodel G. · 129
Colombo C. · 87
Consumi M. · 127
Conte E. · 243
Costagliola C. · 247, 249
Cugia F. · 95, 180
Cunha F. · 191
Cuomo F. · 136, 138, 179, 198, 245

D

Dallai L. · 233
Dalle-Donne R. · 257
De Leonardis A. · 198, 245
De Santis A. · 144
Dei L. · 218
Dettin M. · 101
Di Cola E. · 165
Di Nezza F. · 179, 247
Donati A. · 125, 127, 129, 169, 171, 229, 231, 233
Duan H. · 190

F

Facchini A. · 177
Falsini S. · 165
Farolfi A. · 257
Fatarella E. · 93, 196
Ferrari P. · 202
Ferraro G. · 154, 156
Foletti A. · 171
Fortunato M. · 249
Francese M. · 241
Fratini E. · 107, 109, 111, 113, 154, 156, 202, 204
Frisenda P. · 241
Frisetti A. · 200

G

Gaboardi M. · 97
Galgani L. · 190

Galvagni F. · 257
Gasco P. · 163
Gasparini D. · 191
Gelli R. · 105
Gentile L. · 121
Giamblanco N. · 101
Giorgi R. · 202, 204, 206, 208, 210, 212, 214, 216, 218, 222
Girella A. · 97, 99, 200, 224, 251
Giustarini D. · 257
Gonzalez-Paredes A. · 163
Guerra G. · 247, 249
Gümüşderelioğlu M. · 101

H

Hatzixanthis K. · 163
He J.Z. · 87
Hochkoeppler A. · 239, 241, 243

I

In M. · 165

J

Jez S. · 192

K

Karakeçili A.G. · 101

L

Lamponi S. · 127, 229
Leone G. · 125, 127, 231
Lindman B. · 136
Lippolis V. · 140
Liu Y. · 113
Lofrumento C. · 259
Loiselle S.A. · 190, 191
Longanesi L. · 239
Lopez F. · 136, 138, 198, 245
Luchini A. · 147
Luciani G. · 148
Lupetti P. · 125

M

Ma R. · 190
Macciola V. · 245
Madeo A. · 241
Magnani A. · 125, 129, 169, 171, 229, 231
Magnani G. · 97
Mamusa M. · 163
Manfrida G. · 186
Mangia A. · 123
Maranghi S. · 91, 194
Marazzi F. · 200
Marini A. · 97, 99, 224, 251
Marletta G. · 101, 103, 150
Marone I.M. · 257
Martelli E. · 241
Martin, A. · 99
Martina M.R. · 115, 259
McArthur M. · 163
Medda L. · 95, 180
Mendozza M. · 160
Messina G.M.L. · 101, 150
Miguel M.G. · 136
Milanese C. · 97, 99, 154, 200, 224, 251
Milzani A. · 257
Mohammadpourasl S. · 173
Moncelli M.R. · 253, 255
Monduzzi M. · 95, 140, 180
Montis C. · 158, 160, 163, 220
Montòn-Silva A. · 243
Moretti E. · 129
Morris C.W. · 163
Murgia S. · 138, 140

N

Nairi V. · 95
Nassini R. · 257
Ninham B.W. · 180

P

Paduano L. · 142, 144, 146, 147
Palumbo G. · 87, 188
Panizza L. · 241
Parisi E.I. · 206
Parisi M.L. · 91, 131, 177, 186, 192, 194, 206
Parsons D.F. · 180
Perfetti M. · 142
Pezzella A. · 148

Pianorsi M.D. · 202, 210
Pignatta S. · 257
Piludu M. · 95
Poggi G. · 208, 210, 212, 214, 216
Pogni R. · 93, 131, 133, 135, 196, 235, 237
Pontiroli D. · 97

Q

Quinzeni I. · 225

R

Ranieri G.A. · 121
Rapisarda A. · 101
Raudino M. · 152, 202, 220
Rausa R. · 154
Resta C. · 161
Riccò M. · 97
Ridi F. · 99, 105, 107
Ripoli M. · 123
Ristori S. · 165
Rocha L. · 191
Rosati F. · 125
Rossi C. · 125, 127, 129, 169, 171, 190, 191, 229, 231
Rossi M. · 156
Rossi O. · 89, 121
Rossi R. · 257
Rueda Noriega M. · 99
Russo Krauss I. · 146
Russo M.V. · 146
Ruyra A. · 163

S

Sacco P. · 123
Salis A. · 95, 180
Salvatore A. · 160
Sanz Moral L.M. · 99
Scala A. · 177
Selvolini G. · 152
Sfuncia G. · 103
Shupe S. · 191
Sinicropi A. · 91, 173, 175, 235
Sitia L. · 163
Smeazzetto S. · 253, 255
Sogos V. · 95
Spinelli D. · 192, 196
Stefan A. · 239, 241, 243

T

Taddei M. · 173
Tadini-Buoninsegni F. · 253, 255
Tamasi G. · 125, 127, 129, 169, 171, 229, 231
Teltayev B. · 89
Tempesti P. · 105, 161
Tesei A. · 257
Tonelli M. · 107
Tovar Rodriguez J. · 109, 111, 113
Trojsi G. · 200
Tuccitto N. · 103

V

Valiente E. · 191
Valori L. · 177
Varcamonti M. · 148
Venditti F. · 198
Vitiello G. · 147, 148
Volpi V. · 233

W

Wheeler G. · 163

Y

Yurtsever M.Ç. · 101

Z

Zanoni M. · 257
Zeppa L. · 247, 249
Zhang Y. · 190
Ziche M. · 125