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Editori:

Alessandro Del Grosso, Roberta D'Agata
Dipartimento di Scienze Chimiche, Università degli Studi di Catania
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Viale Andrea Doria, 6, 95125 – Catania, Italia

Premio Ambrogio Mazzucotelli

In occasione dell'Incontro di Spettroscopia Analitica (ISA), il Gruppo di Spettroscopia Analitica (GSA) appartenente alla Divisione di Chimica Analitica della Società Chimica Italiana, conferisce il Premio intitolato al Prof. Ambrogio Mazzucotelli, prematuramente scomparso e già aderente al Gruppo, attraverso il quale ha operato per promuovere e valorizzare le ricerche in questo settore della chimica analitica.
Il Premio viene assegnato a giovani studiosi la cui attività di ricerca nel campo della Spettroscopia Analitica risalti particolarmente sia per l'originalità e qualità dei metodi che per la rilevanza dei risultati.

Premio Franco Cariati

In occasione dell'Incontro di Spettroscopia Analitica (ISA), il Gruppo di Spettroscopia Analitica (GSA), appartenente alla Divisione di Chimica Analitica della Società Chimica Italiana, conferisce il Premio intitolato al Prof. Franco Cariati, professore ordinario di Chimica Analitica dal 1982 presso la Facoltà di Scienze dell'Università di Milano, docente di Chimica Analitica e direttore dal 1987 al 1993 del Dipartimento di Chimica Inorganica, Metallorganica e Analitica. Aderente al Gruppo di Spettroscopia Analitica ed organizzatore di alcune delle passate edizioni dell'ISA, il Prof. Cariati ha contribuito a promuovere lo sviluppo della chimica analitica.
Il Premio viene conferito per il miglior contributo orale presentato all'ISA da un/a ricercatore/ricercatrice in termini di rilevanza, originalità e qualità dei risultati presentati.

Invited Lectures

Invited Lecture INV 1

Jakub Dostálek
Single Molecule Detection with Plasmonically Enhanced Readout
Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Invited Lecture INV 2

Patrizio Giacomini
Circulating tumor DNA (ctDNA): clinical applications and outlook on optical biosensors
Fondazione Policlinico Universitario Agostino Gemelli IRCCS, Rome, Italy

Single Molecule Detection with Plasmonically Enhanced Readout

Jakub Dostálek[a,b], Naoto Asai[b], Katharina Schmidt[b], Gizem Aktug[a], Dario Cattozzo Mor[a], Andres de los Santos Pereira[c], Tomas Riedel[c], Andreas Weinhäusel[d]

[a] FZU – Institute of Physics, Czech Academy of Sciences, Na Slovance 1999/2, Prague 182 21, Czech Republic, [b] LiST – Laboratory for Life Sciences and Technology, Viktor Kaplan-Straße 2, Danube Private University, 2700 Wiener Neustadt, Austria, [c] Institute of Macromolecular Chemistry, Czech Academy of Sciences, Prague 162 00, Czech Republic, [d] AIT-Austrian Institute of Technology, Giefinggasse 4, Wien 1210, Austria

Metallic nanostructures support tightly confined surface plasmon modes that are associated with strongly increased electromagnetic field intensity and local density of optical states. Such optical resonances are highly attractive in bioanalytical technologies for probing of chemical and biological species and they frequently serve in plasmonic affinity biosensors as well as in numerous surface enhanced optical spectroscopy methods. Among others, plasmonic nanomaterials finds their applications in amplification of weak fluorescence signals in assays that rely on using of fluorescent labels [1].

In conventional plasmon-enhanced fluorescence (PEF) biosensors, the output optical signal is averaged over an ensemble of target molecular species and optical amplification is used for increasing the signal to noise ratio, which enables improving the analytical performance characteristics such as limit of detection (typically to sub pM concentrations). More recently, we witness efforts to reach ultimate level of detecting individual target molecules. There will be discussed two approaches that combine PEF with additional molecular-based amplification based on rolling circle amplification (RCA) [2] and catalytic hairpin assembly (CHA) [3]. In these methods, target molecules are affinity captured from analyzed liquid sample at the solid sensor surface that is optically probed by confined field of surface plasmons. With the use to fluorescence imaging, the presence of individual target molecules at the sensor surface is associated with bright fluorescent spots generated by local attachment of emitters in their vicinity, either by using long ssDNA chains generated by RCA or based on tethered flexible molecular linker locally triggering CHA. This allows for establishing 'digital' readout of the assay based on direct counting of the target molecules. The importance of design of the biointerface enabling mitigation of unspecific sorption of assay constituents will be highlighted and the implementation of these concepts to assays enabling detection of biomolecules at aM - low fM concentration will be presented in the context of detection of methylated DNA biomarkers.

Acknowledgements: Support from Gesellschaft für Forschungsförderung Niederösterreich m.b.H. project FTI24-G-027 Multiplexed single-molecule plasmonic biosensor for cancer cell-free DNA biomarker, the Austrian Research Promotion Agency (FFG) within the COMET Project "PI-SENS" (Project No 915477) as well as by the Federal Provinces of Lower Austria and Tirol, Czech SoMiCELL (23-05908K), European Commission via project Versilib (101046217, HORIZON-EIC-2021-PATHFINDEROPEN-01), Operational Programme Johannes Amos Comenius financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SENDISO - CZ.02.01.01/00/22_008/0004596) is acknowledged.

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Circulating tumor DNA (ctDNA): clinical applications and outlook on optical biosensors

Patrizio Giacomini[a], *Alessandra Fabi*[a]

[a] *UOSD Medicina di Precisione in Senologia, Fondazione Policlinico Universitario Agostino Gemelli IRCCS, Largo Agostino Gemelli, 8, 00168 Roma*

Two topics will be addressed: (a) ctDNA clinical benefit, now firmly established particularly in advanced cancer, and (b) the contribution of optical biosensing to ctDNA diagnostic testing.

Two examples of ctDNA clinical utility will be provided, both in advanced cancer settings:

- ***therapeutic rescue:*** patients experiencing progression in the absence of approved therapy options *de novo* acquire ctDNA-only, actionable ctDNA variants not seen in tumor tissues. These confer susceptibility to treatment to 30% to 50% of 'untreatable' patients [1, 2].
- ***disease monitoring:*** Response Evaluation Criteria in Solid Tumors (RECIST) provide a simple and elegant binary system based on medical imaging (e.g. CT scans) to determine whether a patient is responding to therapy or undergoing progression. In a breast cancer clinical trial named GIM21, proof-of-principle was provided that ctDNA not only anticipates clinical progression, but predicts its timing in individual patients, e.g. ctDNA complements RECIST (unpublished) in every day oncology practice.

Central to a number of biological applications, optical biosensors may also find application in the two above ctDNA scenarios. Their competitive/unique features include:

- ***sensitivity***: as low as single-molecule detection [3, 4].
- ***speed:*** kinetic measurement, as opposed to endpoint measurement of NGS and dPCR.
- ***robustness:*** pre-analytical cumbersome ctDNA isolation steps, needed for NGS and dPCR, may be skipped, as shown by the group from Catania [3, 4].
- ***multi-analyte capability:*** liquid biopsy at its best is a multi-analyte search, and only biosensors may detect analytes as diverse as ctDNA and circulating proteins. Major HER2 oncogenic properties depend on two parameters: gene amplification and resulting protein overexpression. Assessing them in parallel (HER2-2D) improves disease understanding and identifies breast cancer patient subsets responding to HER2 therapeutic blockade [5].
- ***competitive cost***. This was estimated in two recent EU projects (ULTRAPLACAD and VerSiLib).

Yet, ctDNA biosensors do have limitations:

- ***limited multiplexing ability and laborious assay set up***: although these may be solved in the near future, right now biosensors are ideally suited for clinical conditions in which limited sets of resistance traits recurrently arise under therapeutic pressure. Examples of routine application in colorectal carcinoma, breast cancer and melanoma will be provided.

Regardless, only biosensors can be made point of care and wearable, which soon will become mandatory given the above clinical scenarios of therapeutic rescue and ctDNA monitoring.

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Premio Ambrogio Mazzucotelli

Nel corso dell'ISA 2023, il GSA conferisce il Premio Ambrogio Mazzucotelli, dedicato a giovani studiosi la cui attività di ricerca nel campo della Spettroscopia Analitica risalti particolarmente per l'originalità e qualità dei metodi sia per la rilevanza dei risultati.

Presenta la vincitrice
Noemi Bellassai
noemi.bellassai@unict.it

Advances in analytical technologies for sensitive detection of circulating biomarkers in clinical and food samples

Noemi Bellassai[a,b]

[a]*Department of Chemical Sciences, University of Catania, Viale Andrea Doria 6, 95122, Catania, Italy;*
[b]*INBB, Istituto Nazionale di Biostrutture e Biosistemi, Viale delle Medaglie d'Oro, 305, 00136 Roma, Italy*
noemi.bellassai@unict.it

The sensitive detection of circulating biomarkers for early-stage diagnosis and personalised treatments plays a crucial role in controlling disease outbreaks and increasing patient survival rates [1]. Pre-analytical conditions play a crucial role in ensuring the high quality of biospecimen analysis, affecting the reproducibility and specificity in biomarker detection for clinical use purposes. Conventional biomarker analysis protocols involve complex sample handling and time-intensive pre-analytical steps, including analyte extraction, purification, and isolation. Amplification methods are generally required for increasing target molecules to detectable levels, especially at early disease stages or during down-regulation processes, where analyte concentration is extremely low. Moreover, the analysis of real-world samples like plasma or serum can trigger non-specific binding events between analytes and receptors, negatively impacting the outcome results. These challenges, along with the risks of sample contamination and increased analysis costs, highlight significant concerns during the pre-analytical phase [2].
The research primarily aimed to tackle each limiting factor in identifying circulating biomarkers in real-world samples by improving the performance of analytical methods.
Advances in surface plasmon resonance (SPR) biosensors, combined with microfluidic devices and gold nanoparticles, have paved the way for detecting tumour-specific mutations, including single-nucleotide polymorphisms (SNPs), in non-amplified circulating tumour DNA (ctDNA), offering promising avenues for minimally invasive, rapid, and real-time colorectal cancer diagnostics by liquid biopsy [3]. To prevent non-specific adsorption of complex biological components and limit the sample manipulation, a new dual-functional, low-fouling poly-L-lysine (PLL)-based polymer linked to anionic peptide [4] and combined with peptide nucleic acid probes complementary to DNA target sequences, effectively captured the analyte at the attomolar level (~2.5 aM) directly in colorectal cancer patient plasma samples, while preventing unrelated biomolecules' non-specific adsorption [5]. The surface modification also showed great versatility and applicability for circulating protein biomarkers, as lysozyme, in clinical and food fields [6]. Lastly, the integration of superparamagnetic particles (MPs) contributed to streamlining the workflow analysis and improving SNPs detection sensitivity at sub-attomolar levels (~0.5 aM) in real-time measurements, by minimising the matrix effect and requiring only a few microliters of plasma from colorectal cancer patients and healthy donors per single analysis [7].

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Elenco Contributi Orali

O1	**Molecular Imprinting Meets Spectroscopy: A New Frontier in Bioanalytical Sensing** *Davide Sestaioni[a], Simone Ventisette[a], Pasquale Palladino[a], Maria Minunni[b], Simona Scarano[a*]* *[a] Department of Chemistry "Ugo Schiff", University of Florence, via della Lastruccia 3-13, 50019, Sesto Fiorentino, Florence, Italy;* *[b] Department of Pharmacy, University of Pisa, Via Bonanno 6, 56126, Pisa, Pi, Italy*
O2	**Fractal Networks of Nanostructures for Imaging and Sensing** *Maria Josè Lo Faro[a], Antonio Alessio Leonardi[b], Maurilio Galletta[c], Barbara Fazio[c], Francesco Priolo[a], Alessia Irrera[c]* *[a] Dipartimento di Fisica ed Astronomia, Università di Catania, Via Santa Sofia 64, 95123 Catania, Italy;* *[b] Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche, ed Ambientali, Università degli studi di Messina, V.le F. Stagno D'Alcontres 31, 98158 Messina, Italy;* *[c] CNR-IMM Messina, V.le F. Stagno D'Alcontres 31, 98158 Messina, Italy*
O3	**Analytical characterization by spectroscopic techniques of Gellan gum-based hydrogels for cartilage tissue regeneration** *Elvira De Giglio[a], Francesco Busto[a], Stefano Liotino[a], Piero Mastrorilli[b], Stefania Cometa[c]* *[a]Department of Chemistry, University of Bari Aldo Moro, Via Orabona 4, 70126 Bari* *[b]DICATECh Department Politecnico di Bari, Via Orabona 4, 70125 Bari* *[c]Jaber Innovation s.r.l., Via Calcutta 8, 00144 Roma*
O4	**Raman spectroscopy for fingerprinting historical inks: a valuable tool for discriminating logwood recipes** *Adele Ferretti[a], Eva Vermeersch[b], Francesca Sabatini[a,c], Peter Vandenabeele[b,d], Ilaria Degano[a]* *[a]Department of Chemistry and Industrial Chemistry, Università di Pisa, Via G. Moruzzi 13, 56124, Pisa (Italy)* *[b]Raman Spectroscopy Research Group, Department of Chemistry, Ghent University, Ghent (Belgium)* *[c]Department of Earth and Environmental Sciences, University of Milano-Bicocca, Piazza della Scienza 1, 20126 Milan (Italy)* *[d]Archaeometry Research Group, Department of Archaeology, Ghent University, Ghent (Belgium)*
O5	**Spectroscopic characterization of novel cross-linked biopolymeric sodium alginate films with ZnO NSs for food packaging** *Antonica Valeria Montefusco[a,b,c], Miquel Oliver[d], Magdalena Pons[d], Margherita Izzi[a,c], Nicola Cioffi[a,c], Manuel Miró[d], Rosaria Anna Picca[a,c]* *[a]Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Via E. Orabona 4, Bari, Italy; [b]Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, Via E. Orabona 4, Bari, Italy; [c]CSGI (Center for Colloid and Surface Science)- Unità di Bari, 70125 Bari, Italy; [d]FI-TRACE group, Department of Chemistry, University of the Balearic Islands, Carretera de Valldemossa km 7,5, Palma de Mallorca, Spain*

O6	**From Surface to Air: Leveraging Spectroscopy to Monitor Iso-Eugenol Release from Mesoporous Silica** *Anna Laura Tassi[a], Alessia Santiglia[a], Vittoria Guglielmi[a], Laura Santagostini[a]* *[a] Università degli Studi di Milano, Dipartimento di Chimica, Via Camillo Golgi 19, 20133, Milano (MI), Italia*
OS1	**SPONSOR (Shimadzu): Analysis of microplastics with IR technique coupled to Raman in a Microscope** *Andrea D'Alessandro, Spectro & Toc Product Specialist* *Shimadzu Srl, Italy*
O7	**Statistical analysis of bacterial motion as a new methodology to study bacteria/antimicrobial interactions** *Margherita Izzi[a,b], Gavino Bassu[b,c], Adele Castellani[c], Rosaria Anna Picca[a,b], Emiliano Fratini[b,c], Marco Laurati[b,c], Nicola Cioffi[a,b]* *[a] Chemistry Department, University of Bari Aldo Moro, Via Orabona, 4, 70126 Bari, Italy* *[b] Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Via della Lastruccia 3, Sesto Fiorentino 50019, Italy* *[c] Department of Chemistry "Ugo Schiff", Via della Lastruccia 3, Sesto Fiorentino 50019, Italy*
O8	**Decoding Plastic Behavior in Environment through Surface Characterization: an X-ray photoelectron spectroscopy (XPS) study** *Tiziano Di Giulio[a], Elisabetta Mazzotta[a], Cosimino Malitesta[a]* *[a] Laboratorio di Chimica Analitica, Dipartimento di Scienze e Tecnologie Biologiche e Ambientali (Di.S.Te.B.A.), Università del Salento, via Monteroni 73100 Lecce – Italy*
O9	**The optimization of a combined analytical approach for clarifying the cadmium removal mechanism by Sardinian limestone and Carrara marble** *E. Tuveri[a], D. Biggio[a], R. Ottonello[a], M. Cau[a], M. Fantauzzi[a], B. Elsener[a], G. Ennas[a], G. E. Porcedda[a], M. Surracco[b], N. Careddu[b], A. Rossi[a]* *[a] Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Cittadella Universitaria, I - 09042, Monserrato, Cagliari, Italy; [b] Dipartimento di Ingegneria Civile, Ambientale e Architettura, Università di Cagliari, via Marengo, 2, I - 09123 Cagliari, Italy*
O10	**Synthesis and characterization of silver-based nanoantimicrobials included in food-grade polypropylene** *Valerio De Marzo [a], Salvatore Mastromarino[a], Syed Imdadul Hossain[b,c,d], Chiara Purgatorio[e], Annalisa Serio[e], Nicola Cioffi[a,b], Nicoletta Ditaranto[a,b]* *[a] Dipartimento di Chimica, Università degli Studi di Bari, via E. Orabona 4, 70125 Bari, Italy; [b] CSGI – Consorzio Interuniversitario per lo sviluppo dei Sistemi a Grande Interfase, Unità di Bari, c/o Dipartimento di Chimica, Università degli Studi Bari Aldo Moro, via E. Orabona 4, 70126 Bari, Italy;* *[c] Laboratory of Nano-bio and Advanced Materials Engineering (NAME), Jashore University of Science and Technology, Jashore 7408, Bangladesh; [d] Centre for Sophisticated Instrumentation and Research Laboratory (CSIRL), Jashore University of Science and Technology, Jashore 7408, Bangladesh* *[e] Dipartimento di Bioscienze e Tecnologie Agroalimentari e Ambientali, Università degli Studi di Teramo, Via R. Balzarini 1, 64100 Teramo, Italy*

O11	**A multi-analytical approach for assessing the performance of hydrogen permeation barriers on iron** *Deborah Biggio[a], Bernhard Elsener[a], Marzia Fantauzzi[a], Antonella Rossi[a]* *[a] Department of Chemical and Geological Science, University of Cagliari, Cittadella Universitaria,09042 Monserrato (CA), Cagliari, Italy*
O12	**Investigating sulfur crystal formation in arsenic sulfide pigments by using advanced mobile X-rays methods** *Eva Luna Ravan[a,b], Rosario Andolina[a], Irene Barba Castagnaro[c], Michela Botticelli[a], Costanza Miliani[a], Gianluca Santagati[a,] Claudia Caliri[a] and Francesco Paolo Romano[a]* *[a] ISPC-CNR, Via Biblioteca 4, 95124, Catania, Italy1,2,4-8; [b] Sapienza University of Rome, Piazzale A.Moro 5, 00185 Rome, Italy1; [c] Department of Physics, University of Calabria, Via Ponte Bucci, Cubo 33B, 87036 Rende, CS, Italy*
O13	**An XPS investigation on Neodymium – Chitosan interaction** *Giulio Casula [a], N. Aramu [a], Deborah Biggio [a], Bernhard Elsener [a], Antonella Rossi [a], Marzia Fantauzzi [a]* *[a] University of Cagliari, Department of Chemical and Geological Science, ss 554 bivio per Sestu – 09042, Monserrato, CA, Italy*
O14	**Unravelling Metabolic Alterations in Parental and Drug-Resistant Human Non Small Lung Cancer: from spectroscopic screening to high-resolution transcriptomics** *Emilia Bramanti[a], Giorgia Maroni[b], Eva Cabrera San Millan[b], Ettore Mosca[b], Alice Chiodi[b], Beatrice Campanella[a], Massimo Onor[a], Elena Levantini[b]* *[a] CNR-Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), SS di Pisa, Area della Ricerca di Pisa, Italy; [b] CNR-Consiglio Nazionale delle Ricerche, Istituto di Tecnologie Biomediche (ITB-CNR), SS di Pisa, Area della Ricerca di Pisa.*
O15	**High throughput evanescent-wave biosensor for the early-stage detection of biomarkers in liquid biopsies** *Caterina Dallari[a,b], Laura Perego[b], Lucia Gardini[a,b], Caterina Credi[a,b] and Francesco Saverio Pavone[a,b,c]* *[a] National Institute of Optics (INO), National Research Council (CNR), Sesto Fiorentino 50019, Italy* *[b] European Laboratory for non-linear Spectroscopy (LENS), University of Florence, Florence, Italy* *[c] Department of Physics, University of Florence, Sesto Fiorentino 50019, Italy*
O16	**Co-registered Hyperspectral Imaging System with Multiblock Data Processing for Stratigraphic Investigation of Paintings** *Zelan Li[a], Emilio Catelli, Enmanuel Cruz Muñoz[b], Michele Occhipinti[c], Silvia Prati[a], Alessandro Tocchio[c], Paolo Plebani[d], Davide Ballabio[b], Paolo Oliveri[e], Giorgia Sciutto[a]* *[a] Department of Chemistry "G. Ciamician", University of Bologna, Ravenna Campus, Via Guaccimanni, 42, Ravenna, 48121, Italy; [b] Milano Chemometrics and QSAR Research Group, Department of Earth and Environmental Sciences, University of Milano-Bicocca, P.za della Scienza 1-20126, Milano, Italy; [c] Bruker Nano Analytics, via Conte Rosso 23, 20134, Milano, Italy; [d] Accademia Carrara, Piazza Giacomo Carrara, 82, 2412, Bergamo, Italy; [e] Department of Pharmacy (DIFAR), University of Genova, Viale Cembrano, 4, Genova, 16148, Italy*

O17	**Integrated analytical approach for the characterisation of dyed wool fibers in the oldest Moroccan carpet** *El Jeddaoui Bensalem[a], Fikri Imane[a], Oubelkacem Yacine[a], El Bakkali Abdelmajid[a], Lamhasni Taibi[b], Amechrouq Ali[c], Haddad Mustapha[a], Tomasin Patrizia[d], Nodari Luca[d], Campanella Beatrice[e], Legnaioli Stefano[e], Lorenzetti Giulia[e], Poggialini Francesco[e], Bicchieri Marina[f], Ait Lyazidi Saadia[a]* [a]*Laboratory of Spectrometry, Materials and Archaeomaterials, (LASMAR, URL-CNRST, N°7), University of Moulay Ismail, Faculty of Sciences, Zitoune BP 11201, 50000 Meknes, Morocco.* [b]*National Institute of Archaeology and Heritage Sciences (INSAP), BP 6828, Madinat al Irfane, avenue of Allal El Fassi, Rabat, Morocco.* [c]*Laboratory of Molecular Chemistry and Natural Substances (CMSN), University of Moulay Ismail, Faculty of Sciences, Zitoune BP 11201, 50000 Meknes, Morocco.* [d]*Institute of Condensed Matter Chemistry and Technologies for Energy, National Research Council, (ICMATE-CNR), Corso Stati Uniti 4, 35127, Padua, Italy* [e]*Institute for the Chemistry of Organo Metallic Compounds, National Research Council, (ICCOM-CNR), Via Moruzzi 1, 56124, Pisa, Italy* [f]*Independent researcher*
O18	**From field to data: real-time protein and moisture analysis in wheat using portable spectroscopic sensors and chemometrics** *Manuel Monti [a], Marina Cocchi [b], Alessandro D'Alessandro [c], Caterina Durante [b], Mattia Pietropaolo [b], Lorenzo Strani [b], Barbara Giussani [a]* [a] *Department of Science and High Technology, University of Insubria, Via Valleggio, 9, 22100 Como, Italy.* [b] *Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Via Campi 103, 41125 Modena, Italy.* [c] *Barilla G. e R. Fratelli, Via Mantova 166, 43122 Parma, Italy*
OS2	**SPONSOR (Renishaw): Simultaneous and colocalised Raman and SEM imaging for correlated multimodal analysis** *Riccardo Tagliapietra [a], Jorge Diniz [b], Jennifer Ferguson [b], Pete Johnson [b], Tim Batten [b]* [a]*Renishaw Italy;* [b] *Renishaw United Kingdom*
O19	**The gardener of the Grand Duke: history and analysis of Ms. 462 Hortus Pisanus, Icones variarum plantarum** *Giulia Lorenzetti [a], Claudia Giostrella [b], Vincenzo Palleschi [a], Luca Nodari [c], Patrizia Tomasin [c], Stefano Legnaioli [a]* [a] *ICCOM-CNR, Italy;* [b]*Ministry of Culture SABAP Pisa-Livorno, Italy;* [c] *ICMATE-CNR, Italy*
O20	**Qualitative Study of Apatite and Clays Using IR Spectroscopy: The Case Study of Riparo Gaban** *Alessia Santiglia [a], Anna Laura Tassi [a], Martina Sciortino [b], Annaluisa Pedrotti [b], Laura Santagostini [a], Vittoria Guglielmi[a]* [a] *Department of Chemistry, Università degli Studi di Milano, Via Golgi 19, Milano, Italy;* [b] *Labaaf, Università di Trento, Via Tommaso Gar 14, Trento, Italy*
O21	**Degradation of Silk under the Influence of Dyes and Different Aging Conditions** *Cecilia Campi [a], Emilia Bramanti [b], Ilaria Bonaduce [a], Ilaria Degano [a]* [a] *Department of Chemistry and Industrial Chemistry, Università di Pisa, Pisa, Italy;* [b]*Institute of Chemistry of Organometallic Compounds, CNR, Pisa, Italy*

O22	**Natural materials Development from Collagen-based Wastes – ArtDECOW: treatment and solubilization methods** *Eleonora Micheli[a], Elena Pulidori[b], Chiara Pelosi[b], Brunella Cipollina[c], Celia Duce[b], Erika Ribechini[b], Leila Birolo[c], Iacopo Corsi[d], Emilia Bramanti[a], Ilaria Bonaduce[b]* *[a] ICCOM-CNR, Italy; [b] Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy; [c] Department of Chemical Science, University of Naples Federico II, Napoli, Italy; [d] Conceria Zabri S.p.A., Fucecchio, Italy* *eleonora.micheli@pi.iccom.cnr.it*
O23	**Advancing Liquid Biopsy: Direct Capture of Circulating Tumor DNA from Plasma with Superparamagnetic Beads** *Alessandro Del Grosso[a], Daria Paladych[b], Roberta D'Agata[a,b], Giuseppe Spoto[a,b]* *[a] Dipartimento di Scienze Chimiche, Università di Catania, Viale Andrea Doria 6, 95122, Catania, Italia; [b] INBB, Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna 19, 00165, Roma, Italia*

Molecular Imprinting Meets Spectroscopy: A New Frontier in Bioanalytical Sensing

*Davide Sestaioni[a], Simone Ventisette[a], Pasquale Palladino[a], Maria Minunni[b], Simona Scarano[a]**

[a] Department of Chemistry "Ugo Schiff", University of Florence, via della Lastruccia 3-13, 50019, Sesto Fiorentino, Florence, Italy;
[b] Department of Pharmacy, University of Pisa, Via Bonanno 6, 56126, Pisa, Pi, Italy
simona.scarano@unifi.it

Smart and innovative materials designed to function as synthetic affinity receptors - replacing traditional antibodies (Abs) - are redefining the frontiers of bioanalytics and biosensing. Despite the progress of modern Abs, their application remains limited by ethical concerns, high production costs, long development times, and poor thermal and operational stability.
Molecularly Imprinted Bio-Polymers (MIBPs), especially those based on endogenous neurotransmitters such as dopamine (DA), norepinephrine (NE), and serotonin (SE), are emerging as powerful alternatives [1-5]. These materials form thin, self-adhesive nanofilms or nanoparticles capable of recognizing biomacromolecules through either whole-protein or epitope imprinting strategies. Their green, one-step synthesis—completed within hours—offers unprecedented advantages in reproducibility, scalability, and environmental sustainability. Recent advancements now open the application of MIBPs to spectroscopy-based analytical platforms, such as (Localized) Surface Plasmon Resonance ((L)SPR), Bio-Layer Interferometry (BLI), and other optical-based techniques. These synthetic receptors enable selective molecular recognition directly at the transducer interface, offering new levels of stability, reusability, and sensitivity—often surpassing traditional biorecognition elements. We present the main milestones in the development of MIBPs for protein sensing, with a particular focus on their integration into label-free and spectroscopic detection systems. Finally, we introduce an automated epitope selection strategy, developed to rationalize and accelerate the imprinting process—overcoming the limitations of conventional trial-and-error approaches and paving the way for next-generation analytical devices.

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Fractal Networks of Nanostructures for Imaging and Sensing

Maria Josè Lo Faro[a], *Antonio Alessio Leonardi* [b], *Maurilio Galletta* [c], *Barbara Fazio*[c], *Francesco Priolo*[a] , *Alessia Irrera*[c]

[a] *Dipartimento di Fisica ed Astronomia, Università di Catania, Via Santa Sofia 64, 95123 Catania, Italy;*
[b] *Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche, ed Ambientali, Università degli studi di Messina, V.le F. Stagno D'Alcontres 31, 98158 Messina, Italy;*
[c] *CNR-IMM Messina, V.le F. Stagno D'Alcontres 31, 98158 Messina, Italy*
mariajose.lofaro@dfa.unict.it

Disordered optical media, known for their strong light scattering, are rapidly emerging as powerful platforms for both fundamental studies and practical applications in imaging, sensing, and energy harvesting. In this scenario silicon nanowires (Si NWs) emerge as interesting materials due to the large silicon industry in microelectronics that may push their interest in large scale applications. The fabrication of 2D fractal array of light-emitting Si NWs has been demonstrated by using thin metal film metal assisted chemical etching, an industrially compatible and cost-effective synthesis that directly start from commercial Si wafer allowing a tunable length, diameter, and morphology of NWs. The light emission of silicon nanowires at room temperature, combined with their fractal morphologies, opens exciting opportunities for photonic applications. Near-infrared silicon-compatible light sources are particularly valuable for photonics and short-range telecommunication technologies.

This work explores a unique class of such materials, random, fractal-like networks of silicon nanowires and silver dendrites, that combine structural disorder with remarkable optical functionality [1]. Using a combination of real-space microscopy and Fourier imaging, we directly visualize Rayleigh scattering, photoluminescence, and weakly localized Raman light in disordered silicon nanowire networks. This direct imaging allows us to probe light transport at the microscopic level, revealing weak localization effects and, notably, coherent Raman light beaming in the out-of-plane direction, something traditionally inhibited in highly scattering media. From the imaging profile of the photoluminescence and Raman signals, it is possible to estimate the diffusion and localization lengths [2] . Similarly, the self-assembled network of silver dendrites presents a highly sensitive and low-cost 3D surface-enhanced Raman scattering (SERS). These dendritic structures exhibit distinct fractal characteristics, with self-similarity and scale invariance across a wide range of length scales. Structural and optical analyses confirm their purity and broad optical resonances, both enhanced by the underlying fractal geometry. We demonstrate the effectiveness of this fractal SERS network by detecting lysozyme in hydration conditions, achieving an impressive enhancement factor of about 2.4×10^6. This highlights the material's potential as a robust biosensing platform [3] . Altogether, our work emphasizes the power of randomness, specifically, the engineered complexity of fractal disordered networks, in enabling novel light manipulation strategies and high-performance applications for gas sensing and biomolecules detections, from proteins to genome recognition without amplification.

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Analytical characterization by spectroscopic techniques of Gellan gum-based hydrogels for cartilage tissue regeneration

Elvira De Giglio[a], *Francesco Busto*[a], *Stefano Liotino*[a], *Piero Mastrorilli*[b], *Stefania Cometa*[c]

[a]*Department of Chemistry, University of Bari Aldo Moro, Via Orabona 4, 70126 Bari*
[b]*DICATECh Department Politecnico di Bari, Via Orabona 4, 70125 Bari*
[c]*Jaber Innovation s.r.l., Via Calcutta 8, 00144 Roma*
elvira.degiglio@uniba.it

Cartilage tissue repair following trauma, rheumatoid arthritis or osteoarthritis is a key focus of research in biomedical sciences. Due to their high-water content and intrinsic biocompatibility, hydrogels are effective tools for addressing cartilage tissue damage, as they mimic the characteristics of native tissue. Gellan gum (GG) was selected for forming hydrogels, due to its high biocompatibility, low cytotoxicity, and a cartilage-like structure. Bioactive molecules can be added to the hydrogel composition to overcome the poor GG mechanical properties or lack of bioactivity[1]. We proposed the incorporation of lignin[2], calcined MgAl-layered double hydroxides (LDH_c) loaded with a *Boswellia serrata* extract (BSE)[3], or tannic acid (TA). Lignin enhanced GG chondrogenic potential and imparted the necessary mechanical properties for printable hydrogels designed for cartilage defect repair. BSE mainly consists of boswellic acids (BAs) which exhibit anti-inflammatory effects. The limited BSE water solubility was overcome by incorporating it into LDH_c to enhance its bioavailability. TA, a gallic ester of D-glucose, is known for its antioxidant properties and ability to act as a crosslinking agent through hydrogen or ionic bonds. Incorporation of TA as a natural crosslinker into GG hydrogels improved their antioxidant, anti-inflammatory, and antibacterial properties, making them promising for cartilage tissue repair. Spectroscopic characterizations of the hydrogels, by XPS, FT-IR/ATR, SS-NMR, provided fundamental information on the interaction between GG and bioactive molecules; some examples are reported in Figure 1. XPS analysis of the C1s signals for the lignin-loaded hydrogels revealed the presence of lignin, as indicated by an additional peak at 284.4 eV, corresponding to carbon atoms in aromatic rings. FT-IR/ATR analysis of the BSE-loaded sample showed the carboxylic C=O stretching band ascribable to BAs at 1699 cm^{-1}. In the CP/MAS ^{1}H-^{13}C NMR spectrum of TA-loaded hydrogel, the meta- and para-carbon signals of the digalloyl fractions of TA resulted slightly shifted to lower fields, indicating the presence of hydrogen bonds between the phenolic groups of TA and the hydroxyl ones of GG. Overall, our investigations demonstrated that spectroscopic analyses can supply valuable insights into structure, composition, and properties of the developed hydrogels.

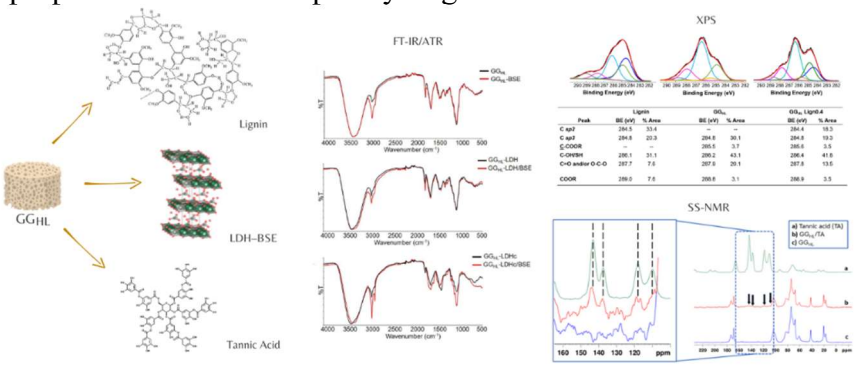

Fig 1: Spectroscopic characterizations of Gellan gum-based hydrogels

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Raman spectroscopy for fingerprinting historical inks: a valuable tool for discriminating logwood recipes

Adele Ferretti[a], Eva Vermeersch[b], Francesca Sabatini[a,c], Peter Vandenabeele[b,d], and Ilaria Degano[a]

[a]*Department of Chemistry and Industrial Chemistry, Università di Pisa, Via G. Moruzzi 13, 56124, Pisa (Italy)*
[b]*Raman Spectroscopy Research Group, Department of Chemistry, Ghent University, Ghent (Belgium)*
[c]*Department of Earth and Environmental Sciences, University of Milano-Bicocca, Piazza della Scienza 1, 20126 Milan (Italy)*
[d]*Archaeometry Research Group, Department of Archaeology, Ghent University, Ghent (Belgium)*
adele.ferretti@phd.unipi.it

The spread of logwood bark (*Heamatoxylum Campechianum* L.) in Europe as a dyestuff dates back to the 16th century. However, its incorporation into ink formulations only began in the 18th century, firstly as an additive in iron gall inks (iron gall logwood inks) and later as the main component (logwood inks). Renowned for their broad spectrum of achievable colours and their non-corrosive impact on paper, logwood inks have been used by many artists, for instance by Vincent van Gogh in his drawings [1]. While their spectroscopic behaviour has been already investigated in the literature [2,3], the direct correlation between these features and the specific molecular composition of the inks remains unexplored, along with the potential synergy between spectroscopic and chromatographic techniques.

This study explored the potential of Raman spectroscopy as a primary tool to investigate the composition and to perform a differentiation of historical logwood inks. Several 19th–20th century ink recipes, which varied in terms of inorganic salt content, additives, and oxidation times, were recreated following historical procedures. The Raman spectra of the ink's mock-ups were dominated by characteristic bands related to –COH bending, C=O stretching, and aromatic C=C stretching. Crucially, we observed spectral shifts in these vibrational modes that correlated strongly with the specific inorganic components of the ink recipes. Al-, Al/Cu-, Fe-, and Cr-based formulations exhibited unique spectral fingerprints, enabling their non-destructive differentiation. This capacity for *in situ*, contactless discrimination of ink types is promising for the examination and preservation of historic manuscripts and artworks.

To complement the spectroscopic data and enhance the interpretation of spectral differences, targeted chromatographic analysis (LC-DAD-HRMS) was applied. This enabled us to confirm the presence of key organic compounds such as hematein derivatives and G-compounds, never or seldom reported in the literature before. Moreover, the integration of Raman spectral features with selective chromatographic findings provided insights into the oxidation pathways of hematoxylin in different ink's formulations, by enabling us to introduce an analytical protocol able of discovering the secrets behind historical technologies [4].

The proposed method is valuable in forensic and heritage science, where the composition of inks can offer crucial insights into the origin and authenticity of documents or artworks.

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Spectroscopic characterization of novel cross-linked biopolymeric sodium alginate films with ZnO NSs for food packaging

Antonica Valeria Montefusco[a,b,c], Miquel Oliver[d], Magdalena Pons[d], Margherita Izzi[a,c], Nicola Cioffi [a,c], Manuel Miró[d], Rosaria Anna Picca[a,c]

[a]Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Via E. Orabona 4, Bari, Italy; [b]Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, Via E. Orabona 4, Bari, Italy; [c]CSGI (Center for Colloid and Surface Science)- Unità di Bari, 70125 Bari, Italy; [d]FI-TRACE group, Department of Chemistry, University of the Balearic Islands, Carretera de Valldemossa km 7,5, Palma de Mallorca, Spain;
a.montefusco@phd.poliba.it

One of the most pressing problems in the 21st century is the environmental pollution and, in particular, that caused by plastics. While on the one hand plastics offer versatile properties such as lightness, transparency and resistance, on the other hand their high stability makes natural degradation difficult. For this reason, alternative solutions to conventional polymers for food packaging development are needed. However, risk assessment of (nano)materials and emerging innovative packaging to be used in the food area is still in its infancy. In this work, we have considered the case of biocomposite films made of sodium alginate (SA), extracted from brown algae, and crosslinked with Ca^{2+} ions, as food coatings. Crosslinked SA (Alg) can be further modified by incorporating antimicrobial zinc oxide nanostructures (ZnO NSs) [1,2]. Spectroscopic (ATR-FTIR, XPS) and optical characterization confirmed successful embedding of NSs. Furthermore, sample microwave digestion in acidic media followed by ICP-OES analysis allowed determining zinc content in 0.3%$_{w/w}$ and 0.15% $_{w/w}$ ZnO NSs-modified Alg films. A flow system exploiting a sequential injection analysis (SIA) for the automatic evaluation over time of the release of zinc from the composites in simulated gastric fluid [3] was specifically developed for risk assessment of accidentally ingested packing films. The dynamic approach mimicking human digestion was coupled to inline spectrophotometric detection using Zincon [4] to determine bioaccessible zinc. The SIA method was fully validated by mass balance confirmation by comparing the bioaccessible plus residual Zn content against the total Zn in the original film.
It was found that the daily intake for the accidental ingestion of 400 mg of 0.3%$_{w/w}$ ZnO NSs/Alg film is around 37 mg Zn, which is below the tolerable zinc intake level as determined for adults [5].

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From Surface to Air: Leveraging Spectroscopy to Monitor Iso-Eugenol Release from Mesoporous Silica

Anna Laura Tassi[a], *Alessia Santiglia*[a], *Vittoria Guglielmi*[a], *Laura Santagostini*[a]

[a]*Università degli Studi di Milano, Dipartimento di Chimica, Via Camillo Golgi 19, 20133, Milano (MI), Italia*
annalaura.tassi@unimi.it

This study aims to develop an air purification system using essential oils or pure terpenes, like iso-eugenol, as natural biocides, combined with MCM-41 mesoporous silica. Iso-eugenol, a compound found in essential oils from cinnamon bark, nutmeg, and ylang-ylang, has shown a low Minimal Inhibitory Concentration (MIC) against *E. coli*, demonstrating high antimicrobial activity at very low concentrations [1]. Unlike the complex profiles of essential oils, iso-eugenol, as a pure compound, provides accurate dosing and reliable, consistent performance.
In this study, the adsorption of pure iso-eugenol onto mesoporous silica was examined at various concentrations, beginning from an initial 1%, informed by promising microbiological test outcomes. Notably, isoeugenol was both physisorbed or covalently bonded to the silica surface through a post-grafting process [2], to evaluate the different efficiency of the two processes. Then, head-space gas chromatography coupled with flame ionization detection (HS-GC-FID) was employed to monitor both the adsorption and desorption processes. Desorption experiments revealed the recovery capacity of iso-eugenol, offering valuable insights into the efficiency of the desorption mechanism.
To fully understand the modifications occurring on the silica surface and its interaction with the pure compound, Near-Infrared (NIR) spectroscopy was employed. NIR spectroscopy is sensitive to the overtones and combinations of vibrations, particularly from OH groups that are prominent on materials like MCM-41, so that this technique could detect changes in the molecular environment of these groups, such as the formation of new bonds (e.g., hydrogen bonds), and track how essential oils affect the surface characteristics, including polarity, porosity, and the exposure of hydroxyl groups [3].
The combination of HS-GC-FID and NIR spectroscopy presents a robust, multidimensional approach for analysis. While GC delivers detailed quantitative analysis of the released compound, NIR spectroscopy enables real-time, non-destructive monitoring of surface changes throughout the adsorption, desorption, and post-grafting processes. This dual technique provides comprehensive insights into the adsorption kinetics, release mechanisms, and surface dynamics, offering critical information for the optimization of materials intended for the controlled release of essential oils.

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Statistical analysis of bacterial motion as a new methodology to study bacteria/antimicrobial interactions

Margherita Izzi[a,b], *Gavino Bassu*[b,c], *Adele Castellani*[c], *Rosaria Anna Picca*[a,b], *Emiliano Fratini*[b,c], *Marco Laurati*[b,c], *Nicola Cioffi*[a,b]

[a] *Chemistry Department, University of Bari Aldo Moro, Via Orabona, 4, 70126 Bari, Italy*
[b] *Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Via della Lastruccia 3, Sesto Fiorentino 50019, Italy*
[c] *Department of Chemistry "Ugo Schiff", Via della Lastruccia 3, Sesto Fiorentino 50019, Italy*
margherita.izzi@uniba.it

The uncontrolled spread of infectious diseases has accelerated the development of advanced materials and bioactive surfaces designed to limit microbial transmission. In this context, our material philosophy focuses on imparting bioactivity against microorganisms through the controlled release of metallic ions from particles that are safely embedded and retained within polymeric matrices. Despite the use of such bioactive surfaces is well-established, the precise mechanisms of action remain partially unclear, particularly given that multiple action mechanisms can occur simultaneously. A thorough investigation of surface properties and bioactivity is therefore essential for the development of eco-friendly materials, while also helping to mitigate the risk of antimicrobial resistance through precise dose–response control.

To this end, we investigated the early-stage interaction between inorganic antimicrobial agents and *Bacillus subtilis*, with a focus on ZnO-based bioactive surfaces. Specifically, the short-time motility of bacteria on ZnO-based bioactive surfaces was inspected by laser scanning confocal microscopy (LSCM), proposing an innovative statistical method to study the bacteriostatic/bactericidal activity of antimicrobials. ZnO nanostructures (NSs) were synthesized via a scalable, aqueous-phase electrochemical method [1]. To modulate morphology, two stabilizing agents - Sodium Dodecyl Sulfate (SDS) and Poly-Diallyl-Dimethyl-Ammonium chloride (PDDA) - were employed. These inorganic antimicrobials were then incorporated into three different polymer matrices (polyethylene oxide, polylactic acid, and poly-vinyl-methyl-ketone) to develop nanocomposite coatings with tunable Zn^{2+} ion release profiles, enabling controlled bioactivity. Comprehensive surface characterization was carried out using UV-Vis spectroscopy, Fourier-transform infrared (FTIR) spectroscopy, X-ray photoelectron spectroscopy (XPS), and both scanning and transmission electron microscopy (SEM/TEM). To establish a quantitative dose–effect relationship, we assessed the impact of Zn^{2+} ion release on the motility of Bacillus subtilis using particle tracking analysis of LSCM images [2], which enabled a dynamic evaluation of bacterial behavior shortly after contact with the antimicrobial surfaces. Mean squared displacement (MSD) analysis showed a shift from run-and-tumble motion to sub-diffusive behavior upon Zn^{2+} exposure. Combined with live/dead imaging, the single-cell tracking method provided a robust statistical framework for correlating ion release with bacterial viability and motility.

To our knowledge, few studies have addressed the impact of metal-based antimicrobials on bacterial motility. This integrated analytical approach offers a powerful tool for distinguishing between bacteriostatic and bactericidal effects, supporting the rational design of antimicrobial coatings with spatiotemporally controlled activity.

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Decoding Plastic Behavior in Environment through Surface Characterization: an X-ray photoelectron spectroscopy (XPS) study

Tiziano Di Giulio[a], *Elisabetta Mazzotta*[a], *Cosimino Malitesta*[a]

[a] *Laboratorio di Chimica Analitica, Dipartimento di Scienze e Tecnologie Biologiche e Ambientali (Di.S.Te.B.A.), Università del Salento, via Monteroni 73100 Lecce – Italy;*
tiziano.digiulio@unisalento.it

Plastics, known for chemical resistance and versatility, are pervasive in daily life, widely used from cosmetics to food packaging. Excessive plastic use has led to environmental release, particularly in water bodies and, thus, in marine ecosystems[1]. These materials, resilient but susceptible to fragmentation, generate microplastics (MPs) and nanoplastics (NPs), strongly impacting aquatic organisms[2]. Understanding plastic fate upon fragmentation is challenging due to unclear degradation timescales and dynamic processes. Nonetheless, addressing the environmental impact of plastic materials requires navigating these complexities.
This study[3] employs X-ray Photoelectron Spectroscopy (XPS) to analyze plastic samples subjected to degradation processes with the aim to gain insight on the relevant chemical processes and disclosing fragmentation mechanisms. Two model plastics, namely polystyrene (PS) and polyethylene (PE), have been selected and analyzed before and after artificial UV-radiation-triggered weathering, under simulated environmental hydrodynamic conditions, for different time intervals. The object of the study is to identify and quantify chemical groups possibly evidencing the occurrence of hydrolysis and oxidation reactions, which are at the basis of degradation processes determining macroplastic fragmentation. XPS data on experimentally weathered particles have been compared with ones obtained on marine microplastics for investigating the occurring degradation processes. Changes in chemical bond structures with weathering have been revealed by XPS involving the increase of chemical moieties (hydroxyl, carbonyl and carboxyl functionalities) which can be correlated with hydrolysis and oxidation phenomena, representing some of the most important degradation processes responsible for macroplastic fragmentation.

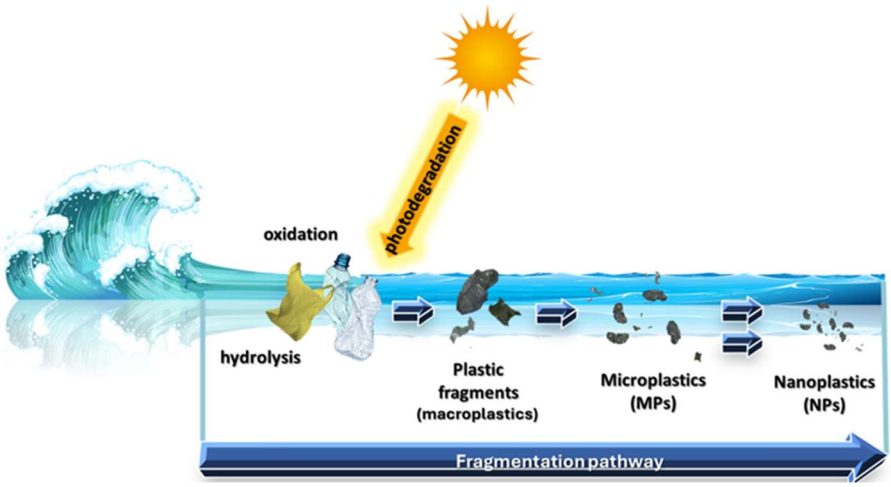

Figure 1: The effect of the fragmentation process: from everyday plastic items to dispersed micro- and nano-plastics.

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The optimization of a combined analytical approach for clarifying the cadmium removal mechanism by Sardinian limestone and Carrara marble

E. Tuveri[a], D. Biggio[a], R. Ottonello[a], M. Cau[a], Marzia Fantauzzi[a], B. Elsener[a], G. Ennas[a], G. E. Porcedda[a], M. Surracco[b], N. Careddu[b], A. Rossi[a]

[a] Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari, Cittadella Universitaria, I - 09042, Monserrato, Cagliari, Italy; [b] Dipartimento di Ingegneria Civile, Ambientale e Architettura, Università di Cagliari, via Marengo, 2, I - 09123 Cagliari, Italy
enrica.tuveri@unica.it

According to Italian regulation, natural stone scraps are classified as special waste [1], and its disposal represents a cost for dimension stone industries [2]. Recent studies demonstrated the efficiency of the marble scraps as a sorbent for removing lead [3] and manganese [4] from model solutions that simulate polluted waters. This project aims to optimize the analytical approach to recycle marble scraps deriving from marble blocks processing and test them as "sorbent" for cadmium in polluted waters. The removal efficiency of commercial $CaCO_3$ microfine dusts (38-45 μm) sourced from two marble and limestone quarries (Carrara and Orosei), is investigated. Sorption tests were in a closed vessel, where 1.0000 g of marble or limestone waste was suspended in 0.10 dm^3 of various model solutions containing cadmium concentrations ranging from 0.5 mg/dm^3 to 10 mg/dm^3. The research examined how cadmium concentration and contact time influence cadmium removal. By combining X-ray photoelectron spectroscopy (XPS) for the characterization of the calcite particles after the contact and inductively coupled plasma optical emission spectroscopy (ICP-OES) before and following the contact of calcite with Cd-containing solutions, the study demonstrates the effectiveness of marble scraps in removing Cd and elucidate the removal mechanisms. The results, obtained on commercial $CaCO_3$ [5], showed that the residual concentration of Cd^{2+} is always below the legal limit of surface water (0.02 mg/dm^3) after the contact with calcite as shown in Figure 1. XPS allows the speciation of cadmium that results to be precipitated as cadmium carbonate on the surface of the microfine dusts. [1,6]. In addition, the synergistic analytical approach was implemented for determining cadmium on $CaCO_3$ microfine dusts and it appears well-suited for an accurate quantification of cadmium removal by marble scraps. The accuracy, the limit of detection and the limit of quantification and the linearity range will be presented and discussed.

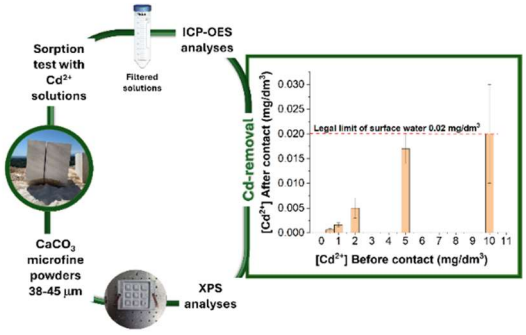

Figure 1: This plot shows the concentration of cadmium after contact with the calcite and how to obtain this data.

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Synthesis and characterization of silver-based nanoantimicrobials included in food-grade polypropylene

Valerio De Marzo[a], *Salvatore Mastromarino*[a], *Syed Imdadul Hossain*[b,c,d], *Chiara Purgatorio*[e], *Annalisa Serio*[e], *Nicola Cioffi*[a,b], *Nicoletta Ditaranto*[a,b]
valerio.demarzo@uniba.it

[a] *Dipartimento di Chimica, Università degli Studi di Bari, via E. Orabona 4, 70125 Bari, Italy;* [b] *CSGI – Consorzio Interuniversitario per lo sviluppo dei Sistemi a Grande Interfase, Unità di Bari, c/o Dipartimento di Chimica, Università degli Studi Bari Aldo Moro, via E. Orabona 4, 70126 Bari, Italy;* [c] *Laboratory of Nano-bio and Advanced Materials Engineering (NAME), Jashore University of Science and Technology, Jashore 7408, Bangladesh;* [d] *Centre for Sophisticated Instrumentation and Research Laboratory (CSIRL), Jashore University of Science and Technology, Jashore 7408, Bangladesh* [e] *Dipartimento di Bioscienze e Tecnologie Agroalimentari e Ambientali, Università degli Studi di Teramo, Via R. Balzarini 1, 64100 Teramo, Italy*
valerio.demarzo@uniba.it

This work, in the frame of the PON PNR 2015-2020 research project One Health-One Welfare-One World (Innovations in Dairy and Meat Supply Chains for Health Welfare and Environment), aims at the preparation of innovative and low environmental impact food-packaging with antimicrobial properties. In this study, silver-based antimicrobial nano systems supported on montmorillonite (AgNPs-MMT) were synthesized and characterized, and finally embedded in a food-grade polypropylene matrix as additives to inhibit microbial growth while increasing the *shelf-life* of the products. AgNPs-MMT were synthesized by exploiting a simple reduction reaction of $AgNO_3$ in 2-propanol by NaOH reported in literature [1]. The protocol was adapted to support the NPs on MMT, studying the effect of the relative amount of silver salt and MMT on the final nanomaterials.
The characterization of the nanoparticles, bare and MMT-supported, was carried out by UV-Vis Diffuse Reflection Spectroscopy (UV-Vis DRS), Fourier Transformed Infrared Spectroscopy in Attenuated Total Reflectance mode (FTIR-ATR), and x-ray Photoelectron Spectroscopy (XPS) techniques. FTIR-ATR results highlighted the presence of Ag in the nanomaterials [2], while the plasmonic peak between 300 and 350 nm in UV-vis spectra confirmed the formation of AgNPs. The data obtained from XPS spectroscopy allowed the surface chemical characterization and Ag speciation in all the nanomaterials, showing the presence of both Ag(0) and Ag oxides [3].
The optimized AgNPs-MMT were embedded in food-grade polypropylene provided by CartonPack S.p.A., project partner company, and subjected to antimicrobial tests to verify their activity against different pathogenic strains (both gram-positive and negative) involved in food contamination. First results, obtained by means of the ISO 22196 procedure [4], demonstrated the complete inhibition (about 99.9%) of the gram-positive bacterium *Listeria monocytogenes* ATCC 7644 on the Ag-MMT-PP composites at different %AgNPs. The results so far obtained showed that the inclusion of silver nanoparticles gave polypropylene significant antimicrobial properties, thus making it a promising candidate for food packaging applications. Further antimicrobial tests on gram-negative bacteria are in progress, as well as the composites characterization.

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A multi-analytical approach for assessing the performance of hydrogen permeation barriers on iron

Deborah Biggio[a], *Bernhard Elsener*[a], *Marzia Fantauzzi*[a], *Antonella Rossi*[a]

[a] *Department of Chemical and Geological Science, University of Cagliari, Cittadella Universitaria,09042 Monserrato (CA), Cagliari, Italy*
deborah.biggio@unica.it

Green hydrogen is considered one of the most promising sustainable energy carriers, as it can be easily generated by water electrolysis using electricity from renewable sources. The hydrogen storage tanks or pipelines are typically made of steels. However, it is well-known that hydrogen diffusion into steel can lead to hydrogen embrittlement (HE), reducing the ductility and formability of the steel [1,2]. HE can be prevented by depositing a hydrogen permeation barrier (HPB) coating on the steel surface. Electroless NiP coating known for its very good anti-corrosion properties is currently of interest because some results have reported a low hydrogen permeability [3].
The aim of the work is to characterize the NiP-coated iron samples with a multi-analytical approach by combining in-situ electrochemical tests and ex-situ surface analytical techniques. Permeation tests were carried out following the ASTM G148-97 and the ISO 17081:2014 as guidelines for developing an analytical method aiming to reproducible measurements of hydrogen permeation with the Devanathan-Stachursky electrochemical cell. Morphology and chemical composition of the samples were investigated by optical microscopy (OM), portable X-ray fluorescence spectroscopy (pXRF) and by X-ray photoelectron spectroscopy (XPS) (Figure 1a): no iron signals from the substrate were detected supporting the absence of through-thickness coating porosity. The results obtained on NiP-coated iron show that, after passivation, the current at the detection side remains constant lower than 1 µA, and thus, no hydrogen could be detected (Figure 1b): the permeation reduction factor (PRF) value is found to be > 80. The NiP coating seems to be a promising hydrogen permeation barrier.

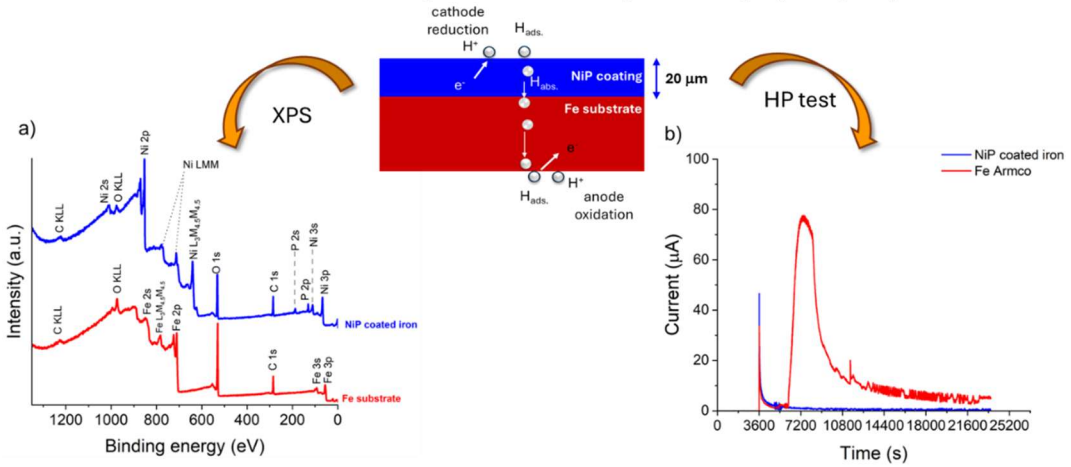

Figure 2: a) Survey spectra of iron substrate (red line) and of 20 µm NiP coated iron (blue line); b) HP tests performed on NiP coated iron (blue line) and Fe Armco (red line). Current (µA) vs time (s)curve measured using the detection cell. Exposed surface 6.9 cm^2.

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Investigating sulfur crystal formation in arsenic sulfide pigments by using advanced mobile X-rays methods

Eva Luna Ravan[a,b], Rosario Andolina[a], Irene Barba Castagnaro[c], Michela Botticelli[a], Costanza Miliani[a], Gianluca Santagati[a,] Claudia Caliri[a] and Francesco Paolo Romano[a]

[a] ISPC-CNR, Via Biblioteca 4, 95124, Catania, Italy; [b] Sapienza University of Rome, Piazzale A.Moro 5, 00185 Rome, Italy; [c] Department of Physics, University of Calabria, Via Ponte Bucci, Cubo 33B, 87036 Rende, CS, Italy; evaluna.ravan@uniroma1.it

Naturally occurring arsenic sulfide minerals have been employed as artists' pigments since antiquity. Among them, realgar (As_4S_4) and orpiment (As_2S_3) were widely used to produce red-orange and yellow hues, respectively. Initially, they were mixed with a polysaccharide-based binder (e.g., gum arabic), and later in egg tempera or linseed oil formulations. Arsenic-bearing minerals are intrinsically unstable and undergo progressive degradation, eventually losing their characteristic yellow or orange appearance. To explore the feasibility of using non-invasive mobile X-ray techniques to investigate, in situ, the physicochemical stability and degradation of these pigments, we prepared simplified paint layers containing pure pigment and medium, following historical recipes. We employed a set of advanced X-rays based techniques developed at the XRAYLab of ISPC-CNR in Catania, including mobile 2D micro-XRF, XRPD mapping, and 3D confocal XRF, to thoroughly characterize the morphological, structural, and chemical changes occurring in degradation processes. In addition, the investigation was supported by complementary lab-based SEM and micro-Raman analysis. Painted mock-ups were subjected to controlled environmental conditions, applying different artificial aging protocols that varied temperature (T), relative humidity (RH), light exposure, and pH. Beyond the well-documented degradation products of arsenic-based pigments, this study revealed the formation of sulfur crystals on the surface of orpiment and realgar mock-ups aged under specific conditions. This phenomenon has been infrequently reported in the field [1]. Typically, the degradation of orpiment or realgar results in the conversion of sulfur into hydrogen sulfide (H_2S), sulfates, or organosulfur compounds [2]. Despite this, recent research has demonstrated that elemental sulfur release from crystalline orpiment is considerably influenced by alkaline pH, elevated dissolved oxygen concentrations, and increased temperature [3]. We observed this phenomenon at the Museo Egizio Torino, during a MOLAB campaign for the non-invasive investigation of the Book of the Dead of Kha. In areas painted with orpiment we have detected a significant presence of sulfur aggregates which were not spatially correlated with arsenic.
These findings provide new insights into the degradation pathways of arsenic sulfide pigments and highlight the necessity of further research to understand the implications of sulfur formation in archaeological and historical painted artworks.

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An XPS investigation on Neodymium – Chitosan interaction

Giulio Casula[a], N. Aramu[a], Deborah Biggio[a], Bernhard Elsener[a], Antonella Rossi[a], Marzia Fantauzzi[a]

[a] *University of Cagliari, Department of Chemical and Geological Science, Monserrato, CA, Italy*
giulio.casula@unica.it

This work presents an X-ray photoelectron spectroscopy investigation on Nd^{3+} ions sorption by chitosan from model solutions. Chitosan is derived from deacetylation of chitin from a waste biomass; thus, its exploitation is in line with the principles of the "circular economy". Chitosan samples are characterized by XPS as pressed powder in an aluminium cuvette. Then, the powders were suspended for 3 hours in the model Nd-containing solutions under constant stirring (Figure 1). Following the contact, chitosan was filtered, and the XPS survey spectra are reported in Figure 1. The spectra showed that the intensity of Nd 3d signals increases with increasing Nd^{3+} concentration in the solution. The high-resolution Nd $3d_{5/2}$ signal overlaps with O KLL signal (Figure 1) resulting in a complex peak shape. It is necessary the identification of the component that can be assigned to Nd $3d_{5/2}$ and those that belong to the O KLL envelop. CasaXPS software was used to solve the spectra in its components using Gaussian/Lorentzian (GL30) product functions. The chemical shift of the photoelectron peaks provides information on the chemical state of the elements, and allow determining how neodymium is bonded to chitosan through the $-NH_2$ groups; in fact, N 1s component found at 401.2 (0.1) eV in chitosan samples shifted to 400.5 (0.1) eV due to the interaction with neodymium, and its at% increases from 1.9% to 3%. Moreover, a new component ascribed to the charge transfer from amine sites to neodymium atoms is found at 402.0 eV [1,2]. The O 1s peak seems to be not involved in the bond. The spectrum of the O KLL obtained on the chitosan before the interaction with Nd^{3+} ion was thus considered as reference and its components are subtracted from the total signal allowing us to identify the Nd $3d_{5/2}$ component. The quantitative analysis showed that Nd content increased from 0.17 (0.05) to 2.9 (0.1) at% when chitosan was suspended in 0.5 ppm and 50 ppm Nd^{3+} solutions, respectively and in agreement with the stoichiometry assuming that Nd^{3+} is coordinated by three amino groups. This investigation demonstrates that XPS can be successfully applied to the investigation of Nd-chitosan sorption providing evidence of the amount of Nd removed from the solutions. In addition, chitosan appears to be a suited alternative for the effective removal of Nd and other REEs.

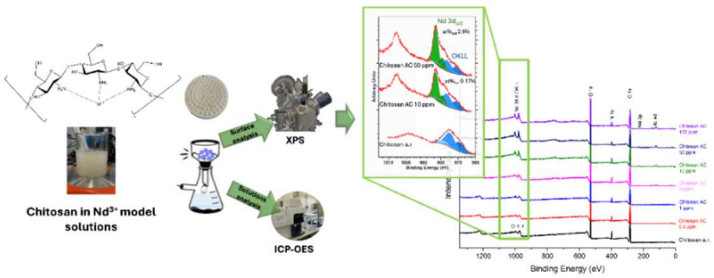

Figure 3: Nd^{3+} sorption by chitosan: Survey spectra of chitosan before contact (black curve) and after contact (AC) with Nd^{3+} model solution with different concentration ranging from 0.5 ppm to 100 ppm and high-resolution Nd 3d spectra.

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Acknowledgments: We acknowledge the financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 published on 14.9.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU– Project Title Recover and Separation of Rare Earth Elements (REE) by economically and environmentally sustainable methods – CUP F53D23008820001- Grant Assignment Decree No. 1186 adopted on 27.7.2023 by the Italian Ministry of Ministry of University and Research (MUR).

Unravelling Metabolic Alterations in Parental and Drug-Resistant Human Non Small Lung Cancer: from spectroscopic screening to high-resolution transcriptomics

Emilia Bramanti[a], *Giorgia Maroni*[b], *Eva Cabrera San Millan*[b], *Ettore Mosca*[b], *Alice Chiodi*[b], *Beatrice Campanella*[a], *Massimo Onor*[a], *Elena Levantini*[b]

[a] *CNR-Consiglio Nazionale delle Ricerche, Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), SS di Pisa, Area della Ricerca di Pisa, Italy;* [b] *CNR-Consiglio Nazionale delle Ricerche, Istituto di Tecnologie Biomediche (ITB-CNR), SS di Pisa, Area della Ricerca di Pisa.*
emilia.bramanti@pi.iccom.cnr.it.

Non-Small Cell Lung Cancer (NSCLC) is the most common type of lung cancer. Most NSCLC patients harbor epidermal growth factor receptor (EGFR) mutations like T790M/L858R (EGFR-TL), L858R (EGFR-LR), and exon 19 deletion (EGFR-D19). Although Osimertinib (Osi) is the standard treatment for EGFR-mutant NSCLC patients, resistance to the drug inevitably develops, leading to therapeutic failure. In this study we characterize the FTIR spectroscopic pattern and the metabolite composition of Osi-resistant (OR) cells compared to their parental (P) counterparts, integrating with metabolomics, trascriptomics and biological assays.
FTIR spectroscopy, in tandem with Principal Component Analysis (PCA) of P and OR cell spectra (N=5 technical replicates from n=3 biological samples), showed significant spectroscopic changes in the fingerprint region between 1800 and 900 cm^{-1}. PCA evidences the clusterization of P and OR cells (Figure 1). To gain insight into the mechanisms driving resistance, we analyzed the extracellular medium (ECM) of P and OR cells by HPLC-DAD, GC-MS, and LCMS to identify metabolites associated with Osi resistance. Metabolomic profiling, together with preliminary RNAseq analysis, highlighted resistance-associated metabolic pathways (Figure 2). These include functional alternative metabolic pathways such as glycolysis and the citric acid cycle, broader metabolic reprogramming, and evidence of mitochondrial dysfunction.

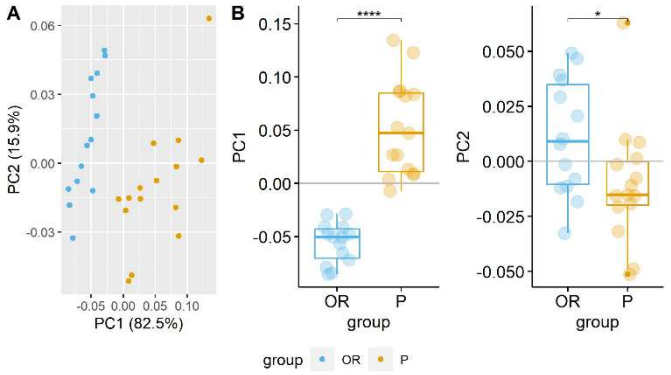

Figure 1

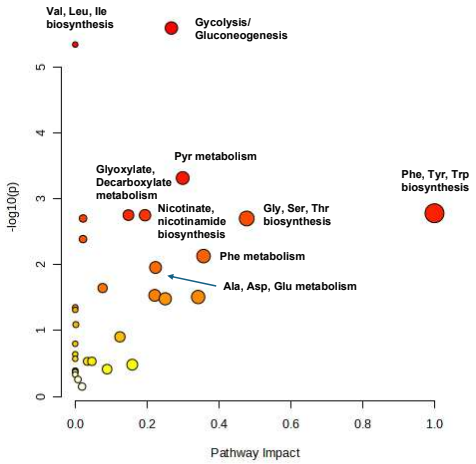

Figure 2

High throughput evanescent-wave biosensor for the early-stage detection of biomarkers in liquid biopsies

Caterina Dallari[a,b], *Laura Perego*[b], *Lucia Gardini*[a,b], *Caterina Credi*[a,b] *and Francesco Saverio Pavone*[a,b,c]

[a] *National Institute of Optics (INO), National Research Council (CNR), Sesto Fiorentino 50019, Italy*
[b] *European Laboratory for non-linear Spectroscopy (LENS), University of Florence, Florence, Italy*
[c] *Department of Physics, University of Florence, Sesto Fiorentino 50019, Italy*
dallari@lens.unifi.it

In recent years, liquid biopsy has emerged as a powerful non-invasive diagnostic alternative to traditional "gold-standard" assays, involving histological or genetic evaluation. Standard biopsies are invasive, risky, and often require long and expensive procedures. Consequently, there has been a significant push towards developing highly sensitive technologies for analyzing body fluids to reveal pathological biomarkers with improved sensitivity and specificity. Recurrent monitoring of these biomarkers can give real-time patient status updates, aiding in both early disease prevention and informed treatment decisions.
In this direction, Total internal reflection (TIR) spectroscopy has been exploited as a non-destructive, selective, and highly sensitive method for analyzing adsorption phenomena and biomolecular interactions within the nanometric evanescent wave (EW) region. The EW propagates a short distance (about 100-200 nanometers) inside the biological sample solution, which excites a limited sample portion while minimizing background noise, thus allowing single molecule detection. Additionally, gold nanoparticles (AuNPs) can be assembled on analytes in the EW region to significantly enhance the scattered optical signal. To improve specificity in detecting target analytes, the chemistry of NPs can be engineered using versatile surface chemistry approaches, inducing specific adsorption of the desired analytes, allowing for their selective recognition.
This work reports on the development of advanced EW-based biosensors for optical liquid biopsy screening and their miniaturization. These systems are designed to be highly portable, offering a promising direction for non-invasive, real-time diagnostic point-of-care applications. Our innovative design addresses the limitations of existing technologies by reducing costs, minimising overall size, and ensuring swift biofluid analysis with remarkable sensitivity. To validate its efficacy, we have tested this system with various analytes, demonstrating its potential in detecting lipopolysaccharides (LPS) for sepsis in blood and Alzheimer's biomarkers (beta-amyloid 40 and 42, tau protein) for early detection of Alzheimer's in blood and saliva. This multi-analyte testing showcases the system's versatility and robustness in addressing different pathological conditions, paving the way for broad clinical applications in disease detection and monitoring.

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Co-registered Hyperspectral Imaging System with Multiblock Data Processing for Stratigraphic Investigation of Paintings

Zelan Li[a], Emilio Catelli[a], Enmanuel Cruz Muñoz[b], Michele Occhipinti[c], Silvia Prati[a], Alessandro Tocchio[c], Paolo Plebani[d], Davide Ballabio[b], Paolo Oliveri[e], Giorgia Sciutto[a]

[a] Department of Chemistry "G. Ciamician", University of Bologna, Ravenna Campus, Via Guaccimanni, 42, Ravenna, 48121, Italy; [b] Milano Chemometrics and QSAR Research Group, Department of Earth and Environmental Sciences, University of Milano-Bicocca, P.za della Scienza 1-20126, Milano, Italy; [c] Bruker Nano Analytics, via Conte Rosso 23, 20134, Milano, Italy; [d] Accademia Carrara, Piazza Giacomo Carrara, 82, 2412, Bergamo, Italy; [e] Department of Pharmacy (DIFAR), University of Genova, Viale Cembrano, 4, Genova, 16148, Italy;
zelan.li2@unibo.it

Cultural heritage investigation requires for non-invasive methods capable of extracting stratigraphic information from multilayered artworks. This demand has driven the rapid development of hyperspectral spectroscopy combined with chemometrics, an approach that has demonstrated both powerful capabilities and strong potential [1]. Nonetheless, a major challenge persists in capturing the in-depth distribution of organic and inorganic materials within multilayered structures [2]. Addressing this challenge, a new analytical set-up, able to co-register VNIR, SWIR, and XRF spectral data, was exploited in combination with a multivariate and multiblock data processing strategy for the analysis of multilayered paintings.

The IRIS hyperspectral imaging system simultaneously acquires co-registered X-ray fluorescence (XRF, 0.5–40 keV), visible & near-infrared (VNIR, 380–1100 nm), and short-wave infrared (SWIR, 1100–2500 nm) reflectance spectra, obtaining complementary elemental and molecular information from superficial to subsurface layers across the investigated area. This approach offers high spatial coherence across all three spectral blocks, each characterized by different penetration depths. The subsequent chemometric strategy, leveraging principal component analysis (PCA), multivariate curve resolution–alternating least squares (MCR-ALS), correlation diagrams and maps (within and between blocks), enables the extraction of meaningful insights from large datasets. Low-level data fusion further enhances the interpretation by integrating spectral details across multiple ranges.

The analytical approach was applied to Il San Sebastiano (1502) by Raffaello Sanzio (1483–1520), currently exhibited at the Accademia Carrara (Bergamo, Italy). Particular attention was given to areas that underwent recent restoration, such as the sky and the forest background. Analysis of these areas revealed the painting's stratigraphic structure by outlining pigment distribution, providing insights into the layering scheme, and highlighting spectral differences related to recent restoration. These findings underscore the synergy between non-destructive spectroscopy and advanced chemometrics in delivering data-driven support for cultural heritage restoration and diagnostic processes.

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Integrated analytical approach for the characterisation of dyed wool fibers in the oldest Moroccan carpet

El Jeddaoui Bensalem[a], Fikri Imane[a], Oubelkacem Yacine[a], El Bakkali Abdelmajid[a], Lamhasni Taibi[b], Amechrouq Ali[c], Haddad Mustapha[a], Tomasin Patrizia[d], Nodari Luca[d], Campanella Beatrice[e], Legnaioli Stefano[e], Lorenzetti Giulia[e], Poggialini Francesco[e], Bicchieri Marina[f], Ait Lyazidi Saadia[a]

[a]*Laboratory of Spectrometry, Materials and Archaeomaterials, (LASMAR, URL-CNRST, N°7), University of Moulay Ismail, Faculty of Sciences, Zitoune BP 11201, 50000 Meknes, Morocco.*
[b]*National Institute of Archaeology and Heritage Sciences (INSAP), BP 6828, Madinat al Irfane, avenue of Allal El Fassi, Rabat, Morocco.*
[c]*Laboratory of Molecular Chemistry and Natural Substances (CMSN), University of Moulay Ismail, Faculty of Sciences, Zitoune BP 11201, 50000 Meknes, Morocco.*
[d]*Institute of Condensed Matter Chemistry and Technologies for Energy, National Research Council, (ICMATE-CNR), Corso Stati Uniti 4, 35127, Padua, Italy*
[e]*Institute for the Chemistry of Organo Metallic Compounds, National Research Council, (ICCOM-CNR), Via Moruzzi 1, 56124, Pisa, Italy*
[f]*Independent researcher*
stefano.legnaioli@cnr.it

This work consists in a scientific documentation of the 18th century carpet of *Chiadma*, currently exhibited at the Dar Si Said museum of Marrakech in Morocco. It is one of the most ancient carpet known in Morocco, a beautiful example of the Moroccan tangible cultural Heritage commonly known as "Zarbia". The study highlights the mastery of natural dye processing, and, at the same time, provides relevant data to support any restoration of this prestigious carpet which had suffered from ancient non-controlled indoor conditions. The investigation crossed SEM-EDS measurements, optical reflectance, 3D fluorescence, SERS and confocal μ-Raman spectroscopies. Since the few studies carried out to date on the ancient Moroccan carpet have focused exclusively on the artistic aspect, the present work aims to develop an integrated and non-invasive analytical approach for the characterization of the dyes and the identification of the dyeing protocols used to produce them. All dyeing matters have been characterized. Hence carminic acid from cochineal extract has been identified in pink-red, flavonoids from weld in yellow shades and indigo from *Indigofera tinctoria* in blue colors. Mixtures of weld with either madder or indigo have been respectively highlighted in orange-yellow and green shades. The wool fibers, analyzed by electronic microscopy, evidenced a certain extent of degradation/tear and the presence of some contaminants, while EDS allowed to recognize the presence of mordants in red, dark-orange and bright yellow fibers.

From field to data: real-time protein and moisture analysis in wheat using portable spectroscopic sensors and chemometrics

Manuel Monti[a], Marina Cocchi[b], Alessandro D'Alessandro[c], Caterina Durante[b], Mattia Pietropaolo[b], Lorenzo Strani[b], Barbara Giussani[a]

[a]Department of Science and High Technology, University of Insubria, Via Valleggio, 9, 22100 Como, Italy.
[b]Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Via Campi 103, 41125 Modena, Italy.
[c]Barilla G. e R. Fratelli, Via Mantova 166, 43122 Parma, Italy.
mmonti2@uninsubria.it

Portable spectroscopic sensors working in the Near-Infrared range (NIR) are becoming increasingly popular thanks to their affordability, user-friendliness, and the growing availability of compact devices. Unlike traditional lab-based instruments, these portable tools can be used directly in the field, allowing quick and efficient testing without the need for complex lab setups. New developments in technology have made these instruments even more capable, opening up possibilities for use across many industries. However, portable NIR devices also have some drawbacks. Their smaller size usually means they cover a narrower range of wavelengths and offer fewer options for adjusting settings. They can also be more sensitive to changes in the environment or how they're handled. Therefore, it is essential to recognize that these instruments are not merely scaled-down versions of laboratory-based systems but represent a distinct class of analytical tools with their own specific capabilities and limitations.

This study explored how well portable NIR devices can measure the protein and moisture levels in wheat. A total of 103 wheat samples, sourced from various regions across Italy, were analysed using two different portable NIR devices: one operating within the 900–1700 nm spectral range and the other within the 1250–2500 nm range. Samples were scanned without any preparation, and different operating conditions were tested to see how they affected the results. The collected data was processed to remove noise and identify unusual findings. Then, models were created to link the NIR data to actual protein and moisture values using multivariate statistical techniques.

The findings highlight the increasing relevance of using portable spectroscopic sensors in the agri-food sector, particularly thanks to their ability to analyse samples in their native state and perform measurements directly on-site. This study further confirms that the combination of spectroscopy and chemometric analysis remains a highly effective strategy for rapid and reliable quality assessment.

The gardener of the Grand Duke: history and analysis of Ms. 462 Hortus Pisanus, Icones variarum plantarum

Giulia Lorenzetti[a], *Claudia Giostrella*[b], *Vincenzo Palleschi*[a], *Luca Nodari*[c], *Patrizia Tomasin*[c], *Stefano Legnaioli*[a]

[a] *ICCOM-CNR, Italy;* [b]*Ministry of Culture SABAP Pisa-Livorno, Italy;* [c] *ICMATE-CNR, Italy;*
giulia.lorenzetti@cnr.it

Since antiquity, the herbal has served as an essential tool for the collection and transmission of botanical and pharmacological knowledge. These works, whether manuscript or printed, describe the properties of plants and provide information about their natural habitat. Over time, this literary form underwent a significant evolution: alongside traditional herbals, the illustrated herbals—or *horti picti*—emerged between the Middle Ages and the Renaissance, where visual representation became central to the depiction and classification of plant species. These works differ markedly from the collections of dried specimens known as *horti sicci*, which represent a later development toward a more scientific systematization of botany [1,2].

Codex 462, held in the University Library of Pisa as part of the *Hortus Pisanus* collection, is an illustrated herbal dating back to the late 16th century, titled *Icones variarum plantarum*. The work includes 35 tempera plates painted by Georg Dyckman, a German soldier and self-taught artist, who accompanied the Flemish botanist Joseph Goedenhuize (Italianized as Giuseppe Casabona) on a scientific expedition to the island of Crete between 1590 and 1591. As prefect of the Giardino dei Semplici in Florence and a member of the Medici court, Casabona was tasked with identifying new wild plant species to enrich Tuscany's scientific and medicinal heritage [3].

The illustrations in the manuscript document a significant shift in botanical representation: the images, drawn from direct observation, anticipate the standards of scientific accuracy in botanical illustration that would become established in the centuries to follow. Notable among the depicted species are *Paeonia peregrina*, *Euphorbia spinosa*, and *Ranunculus asiaticus*, the latter introduced into Italy only after the manuscript's creation.

During a recent conservation project, the manuscript underwent a non-invasive diagnostic campaign that included digital microscopy, multispectral imaging, and Raman, FTIR, and XRF spectroscopy. The data obtained enabled a deeper understanding of the materials and painting techniques used, providing key insights for the conservation process and opening up new perspectives for interdisciplinary research in the fields of the history of science, botany, and art history.

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Qualitative Study of Apatite and Clays Using IR Spectroscopy: The Case Study of Riparo Gaban

Alessia Santiglia[a], *Anna Laura Tassi, Martina Sciortino*[b], *Annaluisa Pedrotti*[b], *Laura Santagostini*[a], *Vittoria Guglielmi*[a]

[a] *Department of Chemistry, Università degli Studi di Milano, Via Golgi 19, Milano, Italy;* [b] *Labaaf, Università di Trento, Via Tommaso Gar 14, Trento, Italy*
alessia.santiglia@unimi.it

Bones are composite materials consisting of approximately equal volumetric fractions of apatite and collagen. Their infrared spectroscopic characteristics reflect this specific composition [1].
According to recent studies, burned bones found in archaeological sites undergo varying degrees of calcination depending on the temperature and duration of exposure to fire. Infrared spectroscopy (IR) has proven to be a valuable tool for distinguishing cremated bones subjected to different burning conditions. However, archaeological samples may have undergone post-burial alterations, including the adsorption or incorporation of carbonates from the surrounding soil. To mitigate these potential alterations, samples are pretreated with sodium hypochlorite and acetic acid before analysis [2].
Given the promising results obtained through Fourier-transform infrared spectroscopy in attenuated total reflectance (FT-IR/ATR), the same pretreatment protocol was then applied to 11 loose sediment samples from neolithic ash rich layers of Riparo Gaban, a Neolithic archaeological site located near Trento. Furthermore, an additional treatment using 1M hydrochloric acid was tested, following methodologies previously reported in the literature to remove calcite from sediment samples for phytolith extraction [3].
As an initial approach, reference standards of calcite, hydroxyapatite, and quartz, along with mixtures of these components, were subjected to the pretreatment to assess the effectiveness of the technique and to verify that hydroxyapatite, a key constituent of bones, remained unaltered. The treated standards were subsequently analyzed using infrared spectroscopy in the form of KBr pellets after one hour of exposure to both acids. Encouraged by the promising results, the protocol was extended to the 11 loose sediment samples. The treatment was performed twice, and IR spectroscopic analyses were conducted after each step to ensure the complete removal of calcite.
Given the encouraging outcomes of this study, future research will focus on the quantitative analysis of hydroxyapatite using infrared spectroscopy, incorporating artificial intelligence to enhance data interpretation and improve analytical precision.

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Degradation of Silk under the Influence of Dyes and Different Aging Conditions

Cecilia Campi[a], *Emilia Bramanti*[b], *Ilaria Bonaduce*[a], *Ilaria Degano*[a]

[a] *Department of Chemistry and Industrial Chemistry, Università di Pisa, Pisa, Italy;* [b]*Institute of Chemistry of Organometallic Compounds, CNR, Pisa, Italy;*
cecilia.campi@phd.unipi.it

In the field of cultural heritage, organic materials are extremely fragile and present significant challenges for conservation. Among them, textiles are particularly vulnerable, as they tend to degrade over time, accumulate dirt, and suffer from dye fading. These issues make them difficult to clean using traditional methods. Silk, in particular, is considered one of the most delicate and sensitive materials among both natural and synthetic fibers [1].
The work presented here is part of the MOXY project, which aims to develop a novel, non-contact cleaning method based on the generation of a cold plasma of Atomic Oxygen (AO). AO is a highly reactive species capable of oxidizing carbon-based contaminants and removing them without mechanical contact, thereby minimizing damage to the underlying surface.
Before evaluating the effect of AO on silk, it is necessary to clearly understand the degradation mechanisms that occur in silk during aging. Our work focuses on the effects of different aging factors on silk, and on the contribution of dyes and mordants.
ATR-FTIR is widely used to investigate the secondary structure of proteinaceous materials, as modifications in the geometry of polypeptide chains are reflected in the amide I, II, and III bands [2-3]. Deconvolution of these signals and peak-fitting algorithms can be applied to gain deeper insights into changes in the secondary structure. In this work, ATR-FTIR and spectral deconvolution were applied to mock-up silk samples unaged and aged under different conditions. These data were further supported by thermoanalytical techniques such as pyrolysis–gas chromatography–mass spectrometry (Py-GC-MS) and evolved gas analysis–gas chromatography–mass spectrometry (EGA-MS).
Three different types of samples were created. Silk was dyed with a direct dye (Rhodamine B) and a mordant-requiring dye (carminic acid, using alum as the mordant). The silk samples underwent different aging conditions: exposure to heat only, UV light only, and a combination of light, heat, and humidity.
Changes in the secondary structure and thermoanalytical properties of aged silk were assessed and found to depend not only on environmental conditions (thermal and photo-aging showed different outcomes) but also on the dyes and mordants used. Interestingly, some combinations exhibited a protective effect, significantly slowing down the aging process of silk.

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Natural materials Development from Collagen-based Wastes – ArtDECOW: treatment and solubilization methods

Eleonora Micheli[a], Elena Pulidori[b], Chiara Pelosi[b], Brunella Cipollina[c], Celia Duce[b], Erika Ribechini[b], Leila Birolo[c], Iacopo Corsi[d], Emilia Bramanti[a], Ilaria Bonaduce[b]

[a] National Research Council (CNR), Pisa, Italy; [b] Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy; [c] Department of Chemical Science, University of Naples Federico II, Napoli, Italy; [d] Conceria Zabri S.p.A., Fucecchio, Italy
eleonora.micheli@pi.iccom.cnr.it

The leather industry poses a significant environmental challenge due to the substantial waste it generates. Implementing a sustainable approach to repurpose this waste can facilitate the sustainable recovery of proteins, transforming them into valuable bioresources.[1] The ARTDECOW project aims to develop eco-friendly methods for collagen treatment and solubilization, promoting the sustainable recovery of proteins from leather waste. This approach facilitates the utilization of collagen to produce versatile, high-performance collagen-based biomaterials (CBBM). In the first part of the study, vegetable-tanned leather was treated with a green solvent system composed of choline chloride and lactic acid (molar ratio 1:1), successfully producing a biomaterial suitable for use as glue. In the second part, the same solvent system was applied to fully solubilize the leather and isolate collagen gelatin. The yields obtained were promising, particularly when compared to the yields reported in the literature for untanned leather waste. [2] The vegetable tanned leather and the samples obtained from the developed methods were analysed by Fourier transform infrared spectroscopy (FTIR-ATR) to analyse the secondary structure of proteins[3], differential scanning calorimetry (DSC) to investigate the thermal behaviour of samples in greater detail, and thermogravimetric analysis (TGA) to assess their thermal degradation.

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Advancing Liquid Biopsy: Direct Capture of Circulating Tumor DNA from Plasma with Superparamagnetic Beads

Alessandro Del Grosso[a], *Daria Paladych*[b], *Roberta D'Agata*[a,b], *Giuseppe Spoto* [a,b]

[a] *Dipartimento di Scienze Chimiche, Università di Catania, Viale Andrea Doria 6, 95122, Catania, Italia;* [b] *INBB, Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna 19, 00165, Roma, Italia;*
alessandro.delgrosso@unict.it

Liquid biopsy is a powerful emerging diagnostic tool for early diagnosis and prognosis of tumors, while supporting personalized oncological treatments. Compared to tissue biopsy, liquid biopsy is minimally invasive and provides several benefits, such as ease of collection, and the capacity to monitor the disease progression in real time. Liquid biopsy utilizes various biomarkers present in bodily fluids, including circulating tumor DNA (ctDNA), circulating tumor cells (CTCs), and exosomes.
The analysis of ctDNA in bodily fluids, such as plasma and serum, typically begins with the isolation of circulating free DNA (cfDNA). However, such process can be labor-intensive, costly, and time-consuming, often leading to the loss of cfDNA. To overcome these issues, we propose capturing and isolating ctDNA directly from plasma using paramagnetic beads. A challenge in using beads directly in plasma is protein coagulation caused by thermal treatment. To mitigate this, ionic and anionic surfactants were employed, allowing the capture and isolation of ctDNA with magnetic beads.
To validate this approach, a fluorescent DNA sandwich assay was utilized. Peptide nucleic acid (PNA) served as the capture probe due to its superior binding affinity and specificity for complementary DNA, forming highly stable duplexes that outperform DNA/DNA hybrids. For detection, DNA labeled with the Cy5 fluorophore was used as the detection probe. The study evaluated various magnetic beads for their efficiency in target capture and different experimental conditions.

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Elenco Posters

P1	**IC-HRMS for the Determination of Fosetyl and Phosphonic Acid in the Official Control of Organic Agricultural Products** *Leonardo Sabatino, Monica Scordino, Alberto Spada, Giovanni Morabito, Ornella Morana, Pasqualino Traulo and Stefania Carpino* *Ministry of Agriculture, Food Sovereignty and Forests (MASAF) Department of the Central Inspectorate for the Protection of Quality and the Repression of Fraud of Agri-food Products (ICQRF) - Catania Laboratory*
P2	**Exploring Poly-Serotonin (PSE) as a Next-Generation Biomimetic Receptor: Growth, Imprinting, and Kinetic Insights for Biosensing Applications** *Davide Sestaioni[a], Gianmaria Boldrini[a], Pasquale Palladino[a], Simona Scarano [a]* *[a] Dipartimento di Chimica "Ugo Schiff", Università degli studi di Firenze, Sesto Fiorentino (FI)*
P3	**Chitosan-based self-standing films for biodegradable food packaging** *Michele Amoia[a], Andrea Brattelli[a], Margherita Izzi[a,b,c], Luigi Gentile[a,b], Nicola Cioffi[a,b], Rosaria Anna Picca[a,b,c], Maria Chiara Sportelli[a,b,c]* *[a]Dipartimento di Chimica,, Università degli Studi di Bari Aldo Moro* *[b]Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Bari* *[c]CNR-Istituto di Fotonica e Nanotecnologie, Unità di Bari*
P4	**Banana peel extract as a green source for the synthesis of Ag- and Ce-based nanoantimicrobials** *Salvatore Mastromarino[a], Valerio De Marzo[a], Nicoletta Ditaranto[a,b]* *[a]Dipartimento di Chimica, Università degli Studi di Bari, Bari, Italy;* *[b]CSGI – Bari Unit, Dipartimento di Chimica, Università degli Studi di Bari, Italy*
P5	**Magnetically Induced Strand Displacement Monitored by SPRi: An Innovative Approach for Biosensor Development** *Daria Paladych[a], Alessandro Del Grosso[b], Noemi Bellassai[a,b], Roberta D'Agata[a,b], Giuseppe Spoto[a,b]* *[a]INBB, Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna 19, 00136, Roma, Italy;* *[b]Department of Chemical Sciences, University of Catania, Viale Andrea Doria, 6, 95125, Catania, Italy.*
P6	**A novel microfluidic strategy for magnetic beads-based capture and plasmonic detection of mutated genomic DNA from circulating tumor cells** *Chiara Pastura[a], Giuseppa Ida Grasso[a], Noemi Bellassai[a,b], Roberta D'Agata[a,b], Giuseppe Spoto[a,b]* *[a] Department of Chemical Sciences, University of Catania, Viale Andrea Doria 6, 95122, Catania, Italy;* *[b] INBB, Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna, 19, 00165 Roma, Italy*

P7	**Integrated microfluidic cell lysis and plasmonic assay for detecting circulating tumor genetic biomarkers in liquid biopsies** *Giuseppa Ida Grasso[a], Chiara Pastura[a], Noemi Bellassai[a,b], Federica Di Padua, Alessia Finotti [c], Rberto Gambari [c], Roberta D'Agata[a,b], Giuseppe Spoto[a,b]* *[a] Dipartimento di Scienze Chimiche, Università degli Studi di Catania, Viale Andrea Doria 6, 95125, Catania, Italia; [b]Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna 19, 00165, Roma, Italia; [c]Dipartimento di Scienze della Vita e Biotecnologie, Università di Ferrara, Via Luigi Borsari 46, 44121, Ferrara, Italia.*
P8	**XPS study of highly dispersed Ni/Ce catalysts over clay bentonite support. Correlation between surface chemistry and catalytic activity** *Francesco Nocito[a,b] , Nicoletta Ditaranto[a,c], Angela Dibenedetto[a,b]* *[a] Dipartimento di Chimica, Università degli Studi Bari Aldo Moro, via E. Orabona 4, 70126 Bari, Italy; [b] CIRCC - Consorzio Interuniversitario per la Reattività Chimica e la Catalisi, Unità di Bari, c/o Villa La Rocca, via C. Ulpiani 27, 70126, Bari, Italy; [c] CSGI – Consorzio Interuniversitario per lo sviluppo dei Sistemi a Grande Interfase, Unità di Bari, c/o Dipartimento di Chimica, Università degli Studi Bari Aldo Moro, via E. Orabona 4, 70126, Bari, Italy*
P9	**ATR-FTIR characterization of zinc/copper basic carbonates as catalyst precursors for CO_2 hydrogenation** *G. Fedele[a], D. Calia[a], M.F. Sforza[a], A.L. Aloia[a], M. Izzi[a,b,c], N. Cioffi[a,b], A. Monopoli[a], M.C. Sportelli[a,b,c], R.A. Picca[a,b,c]* *[a] Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Via E. Orabona 4, 70126 Bari, Italy; [b] CSGI (Center for Colloid and Surface Science), Unità di Bari, via E. Orabona 4, 70126, Bari, Italy; [c] CNR-IFN di Bari, Via G. Amendola, 173, 70126 – Bari*
P10	**Neodymium and Gadolinium recovery by chitosan: a spectroscopic investigation** *M. Fantauzzi[a], G. Casula[a], N. Aramu[a], D. Biggio[a], B. Elsener[a], A. Rossi[a]* *[a] Università di Cagliari, Dipartimento di Scienze Chimiche e Geologiche, ss 554 bivio per Sestu – 09042, Monserrato, CA, Italy*
P11	**Identifying Fakes in Early 20th-Century Paintings through Spectroscopic and Microscopic Methods** *Paola Fermo[a], Andrea Bergomi[a], Mattia Borelli[a], G. Galli[a], G. Carabelli[a], Chiara Lombardi[a,b], Valeria Comite[a]* *[a]Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, Milano, Italy* *[b]Dipartimento di Scienze dell'Antichità, Sapienza Università di Roma, Piazzale A. Moro 5, Roma, Italy*

IC-HRMS for the Determination of Fosetyl and Phosphonic Acid in the Official Control of Organic Agricultural Products

Leonardo Sabatino, Monica Scordino, Alberto Spada, Giovanni Morabito, Ornella Morana, Pasqualino Traulo and Stefania Carpino

Ministry of Agriculture, Food Sovereignty and Forests (MASAF) Department of the Central Inspectorate for the Protection of Quality and the Repression of Fraud of Agri-food Products (ICQRF) - Catania Laboratory
l.sabatino@masaf.gov.it

The use of high-resolution mass spectrometry (HRMS) coupled with ion chromatography (IC) has proven to be an effective analytical technique for the determination of fosetyl and phosphonic acid in organic agricultural products, particularly wines. This approach ensures compliance with the regulatory limits established by European and Italian legislation for organic production. The present study discusses the application of IC-HRMS in official control programs, focusing on its sensitivity, specificity, and reliability in detecting and quantifying these substances.
This study highlights the advantages of IC-HRMS, including its high analytical precision and ability to detect and quantify traces of fosetyl and phosphonic acid, which is crucial for accurate risk assessment and regulatory compliance [1]. The implementation of this method in official monitoring programs strengthens the integrity of organic agricultural products, ensuring consumer safety and adherence to legal standards [2-5]. Throughout 2024, various organic agricultural matrices were analyzed (almonds, hazelnuts, must, vinegar, wine) to assess the presence of phosphonic acid and fosetyl residues. Notably, must samples have shown phosphonic acid levels exceeding the threshold for organic products, with no fosetyl residues detected. Vinegar samples, especially balsamic varieties, had significant variations in phosphonic acid levels, indicating potential contamination, and no fosetyl residues were found. Almonds showed high phosphonic acid levels, likely due to post-harvest treatments or soil uptake, with no fosetyl residues detected. A single hazelnut sample showed phosphonic acid levels surpassing the action limit. Remarkably, wine samples presented a wide range of phosphonic acid residues levels, with some values below the limit of quantification (0.010 mg/kg) and a maximum concentration up to 48 mg/kg. Fosetyl residues were detected in several wine samples, raising concerns about unauthorized plant protection products use, and thus requiring verification of grape origin and vineyard practices. Furthermore, some wine samples exceeded the regulatory limit (0.010 mg/kg) [4,5], indicating a widespread issue. In conclusion, wine and almonds emerged as the most critical matrices, due to their high maximum residue levels. Moreover, the extensive presence of phosphonic acid across different matrices suggests possible environmental contamination or indirect use of non-compliant substances. Further investigations and monitoring are required to determine organic farming residues origin and ensure organic production compliance with law regulations.

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Exploring Poly-Serotonin (PSE) as a Next-Generation Biomimetic Receptor: Growth, Imprinting, and Kinetic Insights for Biosensing Applications

Davide Sestaioni[a], *Gianmaria Boldrini*[a], *Pasquale Palladino*[a], *Simona Scarano*[a]

[a] *Dipartimento di Chimica "Ugo Schiff", Università degli studi di Firenze, Sesto Fiorentino (FI)*
davide.sestaioni@unifi.it

Within the biosensing field, applied to bioanalytical chemistry, diagnostics, and immune-based therapeutics, the replacement of traditional biological receptors with mimetic entities represents an important goal for the scientific community and for ethical reasons, as indicated by Directive 2010/63/EU on the *protection of animals used for scientific purposes* [1].
On this purpose, Molecularly Imprinted Poly-Serotonin (PSE) constitutes one of the latest advances in the field of soft molecular imprinting [2]. Thanks to its ability to form thinner films, with respect to other previously-exploited polymers (Poly-Dopamine, PDA and Poly-Norepinephrine, PNE), it is particularly indicated for optical-based detection platforms such as SPR and LPFGs. Moreover, PSE displays a marked reduction (-35%) of the unspecific surface interaction with plasma proteins under biological conditions compared to PDA, due to lower surface adhesion [3], lower critical surface tension, but higher hydrophilicity [4].
In this presentation, we report the first results of a rationale investigation into the features of PSE to exploit this emerging biopolymer in bioanalytics. Specifically, we explored different conditions for PSE growth and imprinting, employing the epitope approach. Building on previous results obtained for PNE, we leveraged a multiplexed and colorimetric/plasmonic method, combining experimental techniques with a machine learning approach. The recognition capabilities of PSE-based imprinted biopolymers, specifically targeting their epitope, were thoroughly assessed using a well-established kinetic assay known as "Single Cycle Kinetics" (SCK) on SPR platform. This advanced analytical technique allowed for a detailed evaluation of the binding interactions between the imprinted biopolymers and their epitope targets. By employing SCK, it was possible to systematically monitor the binding events in real-time, providing valuable insights into the affinity of the molecular recognition process and allowing the extraction of kinetic parameters such as the equilibrium dissociation constant (K_D) and the maximum binding capacity (R_{max})
This work not only aims to optimize the efficacy of PSE imprinted biopolymers but also lays the groundwork for their potential applications in biosensing, diagnostics, and targeted drug delivery systems.

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Chitosan-based self-standing films for biodegradable food packaging

Michele Amoia[a], Andrea Brattelli[a], Margherita Izzi[a,b,c], Luigi Gentile[a,b], Nicola Cioffi[a,b], Rosaria Anna Picca[a,b,c], Maria Chiara Sportelli [a,b,c]

[a]Dipartimento di Chimica,, Università degli Studi di Bari Aldo Moro. Via E. Orabona 4 – 70125 Bari (Italy)
[b]Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Unità di Bari, Via E. Orabona 4 – 70125 Bari (Italy)
[c]CNR-Istituto di Fotonica e Nanotecnologie, Unità di Bari, Via Amendola 173– 70126 Bari (Italy)
maria.sportelli@uniba.it

The objective of this work was to develop a green and non-toxic composite material for potential application in the field of food packaging. The study specifically focused on the use of a polymeric chitosan (CS) matrix, with citric acid (or sodium citrate) and glycerol as additives [1-2]. Two different preparation methods were used: dipping of bare CS films in a sodium citrate solution, or curing of multicomponent CS/citric acid/glycerol films at high temperatures. This work also contains a comparison of two different types of chitosan (commercial and organic) and the determination of their respective degree of de-acetylation.
In this context, the role of each additive was evaluated in order to improve the functional properties of the final material. Citric acid (or its sodium salt) functioned as a green cross-linking agent, enhancing the structural cohesion of the polymer network through potential esterification reactions with the amine groups of the biopolymer. Conversely, glycerol functioned as a plasticizer, enhancing the flexibility and processability of the resulting films. The objective of incorporating copper-based antimicrobial additives, namely Cu@PVP particles (copper particles stabilized by polyvinylpyrrolidone) [3] and $CuCl_2$ salt, was to enhance bioactivity in the composites. A broad spectrum of characterization techniques was employed. Attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) was used to analyze molecular interactions and verify film homogeneity; transmission electron microscopy (TEM) and UV-Vis spectroscopy were used to characterize Cu@PVP particles. The polymer deacetylation degree was determined by a potentiometric titration method [4], after a purification step to improve the reproducibility and performance of the material.
Furthermore, the influence of antimicrobial additives such as Cu@PVP particles and $CuCl_2$ on the mechanical properties and stability in contact with moisture, was evaluated. Specifically, water uptake measurements and dynamic mechanical analysis (DMA) were performed to assess the interactions between the additives and the polymer matrix. The outcome of the aforementioned characterizations demonstrated the importance of a preliminary purification step for CS, which improves the mechanical and moisture resistance properties of the prepared composite films; it was also possible to discriminate the influence of the antimicrobial additives on the overall material properties.

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Banana peel extract as a green source for the synthesis of Ag- and Ce-based nanoantimicrobials

Salvatore Mastromarino[a], *Valerio De Marzo*[a], *Nicoletta Ditaranto*[a,b]

[a] *Dipartimento di Chimica, Università degli Studi di Bari, via E. Orabona 4, 70125 Bari, Italy;* [b] *CSGI – Bari Unit, Dipartimento di Chimica, Università degli Studi di Bari, via E. Orabona 4, 70125 Bari, Italy*
salvatoremastromarino@hotmail.it

This work is part of the PON PNR 2015-2020 One Health-One Welfare-One World (Innovations in Dairy and Meat Supply Chains for Health Welfare and Environment) research project, aiming at the use of green methods for the preparation of metal and metal-oxide antimicrobials. In this study, silver and cerium-based nanoantimicrobials systems were prepared in presence of banana peel extract (BPE) in an aqueous solution [1-2], in place of 2-propanol [3]. Given BPE composition, it acts both as an antioxidant agent with a good reducing power towards metal cations, and as a capping agent. BPE was obtained according to the procedure reported by Ibrahim et al. [1]. Then, Ag-based NPs were prepared by dissolving $AgNO_3$ in BPE, at basic conditions, allowing the formation of capped Ag_2O clusters [4], on which metallic Ag, resulting from the reduction of silver cations by BPE, is deposited. The formation of Ag-AgONPs was confirmed by X-ray photoelectron spectroscopy (XPS) analysis. BPE was also employed to prepare CeONPs, taking advantage of the possibility of using BPE as a capping agent. The procedure was performed in the presence of oxygen to guarantee the transition of Ce from Ce^{3+} to CeO_2 nanoparticles [5]. Both Ag- and Ce-based nanoparticles were characterized by UV-Vis Diffuse Reflection Spectroscopy (UV-Vis DRS), Fourier Transformed Infrared Spectroscopy in Attenuated Total Reflectance mode (FTIR-ATR), and X-ray photoelectron spectroscopy (XPS). In perspective, the synthesized nanoantimicrobials will be embedded in food-grade polymer films and will be tested in antimicrobial analyses. The role of BPE as a capping agent was crucial in the preparation process; also, its presence will be investigated as an additional factor for a synergic antimicrobial action.

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Magnetically Induced Strand Separation Monitored by SPRi: An Innovative Approach for Biosensor Development

Daria Paladych[a], Alessandro Del Grosso[b], Noemi Bellassai[a b], Roberta D'Agata[a,b], Giuseppe Spoto[a b]

[a]INBB, Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna n. 19, 00136, Roma, Italy;
[b]Department of Chemical Sciences, University of Catania, Viale Andrea Doria, 6, 95125, Catania, Italy
paladich1994@gmail.com

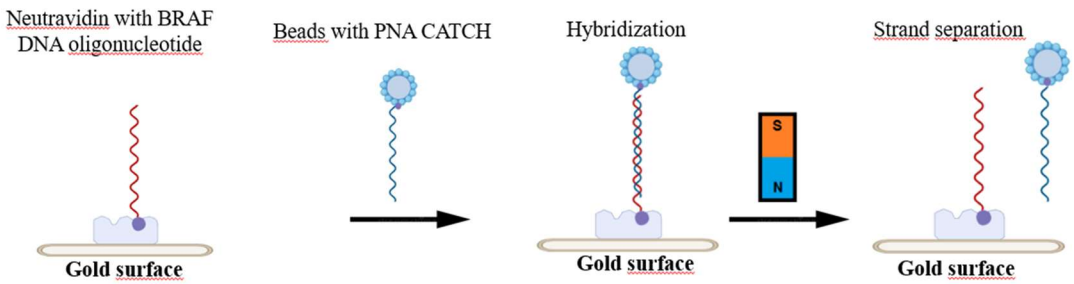
The BRAF V600E is one of the most prevalent mutation in solid tumors, including melanoma, colorectal, and thyroid cancers[1]. It results from a single nucleotide substitution (T>A at position 1799) [2], this single-base alteration causes constitutive activation of the MAPK/ERK signaling pathway, driving uncontrolled cell growth and survival[3]. Given the minimal difference from the wild-type sequence, the ability to detect BRAF V600E with high specificity is critical for accurate molecular diagnostics, and the selection of targeted therapies in precision oncology.

In this study, we investigated the effect of an external magnetic field on the strand separation between tumor-specific BRAF V600E DNA and a complementary peptide nucleic acid (PNA CATCH), using superparamagnetic beads and monitoring the process in real time via Surface Plasmon Resonance imaging (SPRi). The PNA probe, due to its high binding affinity and backbone neutrality, forms highly stable duplexes with complementary DNA. This enhanced thermodynamic stability, combined with its sensitivity to even a single-base mismatches makes the PNA a better probe for mutation detection compared to the conventional DNA oligonucleotide probes.

Two different types of paramagnetic beads were tested in this study: Dynabeads M270 Streptavidin (diameter 2.8 µm) and MonoMag 450 (diameter 4.5 µm). These beads differ in diameter and magnetic content, which directly affects the amount of mechanical force they can exert on the DNA/PNA duplex when exposed to an external magnetic field.

In our experimental setup, BRAF V600E DNA, biotinylated at the 5' end, was immobilized on a gold surface coated with neutravidin, enabling a stable and specific anchoring of the capture strand. The complementary PNA CATCH probe, also biotinylated at the 5' end, was conjugated to the paramagnetic beads via streptavidin–biotin interaction. To achieve the interaction between the two complementary strands, the functionalized beads suspension was flowed through a microfluidic device, allowing controlled and localized hybridization to occur on the SPRi detection surface.

Application of an external magnetic field at controlled distances (2–5 cm) from the sensor surface generated a localized mechanical force on the beads functionalized with the PNA. This force was transmitted to the duplex, and—when sufficient—induced strand separation, which was detected in real time as a decrease in plasmonic signal on the SPRi sensor.



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A novel microfluidic strategy for magnetic beads-based capture and plasmonic detection of mutated genomic DNA from circulating tumor cells

Chiara Pastura[a], *Giuseppa Ida Grasso*[a], *Noemi Bellassai*[a,b], *Roberta D'Agata*[a,b], *Giuseppe Spoto*[a,b]

[a] *Department of Chemical Sciences, University of Catania, Viale Andrea Doria 6, 95122, Catania, Italy;*
[b] *INBB, Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna, 19, 00165 Roma, Italy*
chiara.pastura@phd.unict.it

Cancer is one of the leading causes of death in the world, demanding innovative approaches for early diagnosis and timely treatment. In this context, liquid biopsy has emerged as a minimally invasive procedure for diagnosis and monitoring, enabling the detection and analysis of tumor-derived biomarkers directly from bodily fluids. However, the low abundance of tumor-specific biomarkers, particularly in early-stage cancer patients, necessitates the development of highly sensitive and reliable detection methods [1].
To this aim, this work is focused on developing innovative integrated microfluidic and plasmonic platform for liquid biopsy [2], leveraging the peculiar capabilities of surface plasmon resonance imaging (SPRI) when combined with functionalized beads to enhance detection sensitivity [3].
A microfluidic device was designed and tested to perform the pre-analytical steps required to isolate DNA from tumor cells, minimizing sample volume and handling. The DNA is then transferred to the SPR imaging fluidic system for highly sensitive, amplification-free detection.
Various devices were designed and tested to capture the target DNA using superparamagnetic beads functionalized with peptide nucleic acid (PNA) probes. A magnetic field is incorporated into the microfluidic device to immobilize the beads, facilitating efficient washing and the removal of impurities from liquid biopsy samples. Preliminary fluorescence-based evaluations confirmed the interaction between labelled target DNAs and the functionalized beads.
Pilot SPRI experiments were conducted based on previous research [4]. These experiments aimed to detect G13D KRAS-mutated genomic DNA extracted from LoVo cells, which were derived from the tissues of patients with colorectal adenocarcinoma. PNA probes were used for SPRI detection due to their unique properties, allowing for the design of specific and highly sensitive assays [5].
By minimizing sample volumes and providing high sensitivity, this method has significant potential for application in early diagnosis based on circulating tumor cells. Detecting these cells is particularly challenging due to their low abundance in early-stage patients.

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Integrated microfluidic cell lysis and plasmonic assay for detecting circulating tumor genetic biomarkers in liquid biopsies

Giuseppa Ida Grasso[a], *Chiara Pastura*[a], *Noemi Bellassai*[a,b], *Federica Di Padua*[c], *Alessia Finotti*[c], *Roberto Gambari*[c], *Roberta D'Agata*[a,b], *Giuseppe Spoto*[a,b]

[a]*Dipartimento di Scienze Chimiche, Università degli Studi di Catania, Viale Andrea Doria 6, 95125, Catania, Italia;*
[b]*Istituto Nazionale di Biostrutture e Biosistemi, Via dei Carpegna 19, 00165, Roma, Italia;*
[c]*Dipartimento di Scienze della Vita e Biotecnologie, Università di Ferrara, Via Luigi Borsari 46, 44121, Ferrara, Italia.*
gigrasso@unict.it

Liquid biopsy represents a transformative advancement in cancer diagnostics, offering a non-invasive alternative to traditional tissue biopsies. Liquid biopsies can be performed with minimal discomfort, allowing for repeated testing without significant risk to patients, and have shown promise in identifying cancers at earlier stages, significantly improving treatment outcomes. [1,2]
This innovative approach utilizes body fluids to detect cancer-related biomarkers, facilitating early diagnosis and ongoing monitoring of disease progression. The technology primarily focuses on circulating tumor cells (CTCs), circulating tumor DNA (ctDNA), and other genetic materials, which provide insights into tumor heterogeneity and treatment responses. [3]
Current technologies for analyzing liquid biopsy samples often involve complex procedures, such as pre-analytical treatment and target isolation. These processes typically require a polymerase chain reaction to amplify sequences for genomic DNA analysis.
Liquid biopsy leverages microfluidics to simplify these procedures. Microfluidics enhance the analysis of circulating tumor cells (CTCs) and tumor-derived nucleic acids and facilitate the efficient separation and enrichment of these biomarkers from blood, enabling comprehensive insights into tumor biology and patient-specific treatment responses. The integration of microfluidics with advanced imaging and sequencing technologies has significantly improved the accuracy and utility of liquid biopsies. [4]
With this aim, we developed a microfluidic device for the management of liquid biopsy samples, improving the handling of circulating tumor cells. The device integrates cellular lysis using two inlet channels for the liquid biopsy sample and for the lysis reagent. It is provided for a serpentine zone, for the starting homogenization of the samples, and a long channel for the lysis completion. The width and depth of the channel, 500 µm and 80 µm respectively, allow handling of a few tens of microliters of sample.
The lysis was optimized using human wild type (All-RAS WT) HT-29 and mutated (KRAS p. G13D) LoVo cell lines isolated from tissues of colorectal adenocarcinoma patients and expressing a mutation on the exon2 of the K-RAS oncogene. Genomic DNA from HT-29 and LoVo cells was analyzed through optical fluorescence microscopy using dsDNA-specific intercalating dyes. gDNA detection was carried out by plasmonic assay based on surface plasmon resonance imaging. [5,6]

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XPS study of highly dispersed Ni/Ce catalysts over clay bentonite support. Correlation between surface chemistry and catalytic activity

Francesco Nocito,[a,b] Nicoletta Ditaranto,[a,c] Angela Dibenedetto,[a,b]

[a] Dipartimento di Chimica, Università degli Studi Bari Aldo Moro, via E. Orabona 4, 70126 Bari, Italy; [b] CIRCC - Consorzio Interuniversitario per la Reattività Chimica e la Catalisi, Unità di Bari, c/o Villa La Rocca, via C. Ulpiani 27, 70126, Bari, Italy; [c] CSGI – Consorzio Interuniversitario per lo sviluppo dei Sistemi a Grande Interfase, Unità di Bari, c/o Dipartimento di Chimica, Università degli Studi Bari Aldo Moro, via E. Orabona 4, 70126, Bari, Italy
nicoletta.ditaranto@uniba.it

In this study, we report on the surface analytical characterization of different supported Ni/Ce catalysts and the correlation between the surface properties and their catalytic activity. Various alumina-, silica- and alumino/silicate- systems were investigated as supports, with and without Ce species as promoters. X-ray photoelectron spectroscopy (XPS) analyses performed on all the catalysts were able to detect the overall nickel loading on the surface, as well as the nickel speciation, and interaction with the different supports. NiO-like and Ni-Aluminate or Ni-Silicate like species were detected, in agreement with what was previously reported about Ni interaction with silica- and alumina-supported catalysts [1-4], and their diverse relative abundance was correlated with reducibility and catalytic activity. In particular, we found that Ni interacts with aluminate- and silicate-containing support in a different way, resulting in nickel species occupying different sites, especially on the base of the Ni loading [1]. On the base of $Ni2p_{3/2}$ signal curve fitting and BE values we found the presence of different abundances of nickel species weakly interacting with aluminate and silicate; those species are thought to be located in octahedral sites and are easier to reduce than Ni located in tetrahedral sites [1].
Also, the effect of cerium species as a promoter was elucidated from the surface chemistry point of view: when Ce is deposited, the location of nickel on the surface of the catalysts is affected. All these experimental evidences were used to explain the different behaviour of the catalytic materials, in terms of activity, recoverability, and reusability.

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ATR-FTIR characterization of zinc/copper basic carbonates as catalyst precursors for CO_2 hydrogenation

G. Fedele[a], D. Calia[a], M.F. Sforza[a], A.L. Aloia[a], Margherita Izzi[a,b,c], N. Cioffi[a,b], A. Monopoli[a], M. C. Sportelli[a,b,c], R.A.Picca[a,b,c]

[a]Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Via E. Orabona 4, 70126 Bari, Italy;
[b]CSGI (Center for Colloid and Surface Science), Unità di Bari, via E. Orabona 4, 70126, Bari, Italy;
[c]CNR-IFN di Bari, Via G. Amendola, 173, 70126 – Bari
rosaria.picca@uniba.it

CO_2 thermal hydrogenation to formic acid or other value-added chemicals is of great importance, but it requires suitable catalysts for CO_2 conversion and selectivity [1]. Zinc-Copper mixed oxides are interesting materials to be used as catalysts for this reaction and can be prepared by co-precipitation of zinc/copper basic carbonates followed by calcination [2]. In this contribution, we present the synthesis of several carbonates starting from different Cu/Zn molar ratios by a titrimetric method [2] and a batch co-precipitation route [3]. All the produced materials were successfully characterized by ATR-FTIR spectroscopy [4] and TEM analysis suggesting that the titration approach allows a fine tuning of the final product. Moreover, depending on the conditions, different compounds were synthesized. In particular, titration gives products with a more controlled composition and defined morphology. Calcination above 350°C was also performed at different temperatures to prepare oxides. Preliminary data on their catalytic role in CO_2 hydrogenation are also provided.

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Neodymium and Gadolinium recovery by chitosan: a spectroscopic investigation

M. Fantauzzi[a], G. Casula[a], N. Aramu[a], D. Biggio[a], B. Elsener[a], A. Rossi[a]

[a] *Università di Cagliari, Dipartimento di Scienze Chimiche e Geologiche, ss 554 bivio per Sestu – 09042, Monserrato, CA, Italy*
marzia.fantauzzi@unica.it

Rare earth elements (REEs) are feedstocks of critical importance for many industrial sectors, such as automotive, electronics, machinery, and chemical. [1] The supply chain of REEs in Europe is currently vulnerable, and diversification of REE production is urgently required. [2] In the framework of a project aiming at developing innovative, cost-effective, and environmentally sustainable methods for extracting REE from the leachate and/or wastewater produced during the processing of raw ore, chitosan is investigated as sorbent for REEs. Chitosan is derived from the deacetylation of chitin from a waste biomass. Thus, its exploitation is in line with the principles of the "circular economy".
A commercial chitosan powder with a deacetylation degree equal to 93 (2)%, experimentally determined by different titrimetric methods, was suspended in $Nd(NO_3)_3$ and $Gd(NO_3)_3$ solutions with different concentrations ranging between 0.5 ppm and 100 ppm for three hours under stirring. After filtration, Nd and Gd concentrations in the solutions were determined by inductively coupled plasma-optical emission spectroscopy (ICP-OES). The detection limit (LoD) was 0.003 ppm for Nd at 430 nm, and 0.002 ppm for Gd at 342 nm. After 3 hours of contact with chitosan, the concentration of Nd^{3+} and Gd^{3+} in the solutions decreased: the percentage of ion removal is about 100 % when the initial concentration of the ion is lower than 10 ppm. At concentrations higher than 10 ppm it decreases, probably due to the more acidic pH of the nitrate solutions at the highest concentrations that might lead to a partial protonation of $-NH_2$ groups of chitosan. The removal seems to be more efficient for Gd than for Nd (Figure 1, left); the recovery capacity, defined as the mass of recovered ions (mg) by the mass of the chitosan (g), ranged between 0.05 and 3.35 mg/g and from 0.05 to 4.63 mg/g for Nd and Gd, respectively (Figure 1, right).

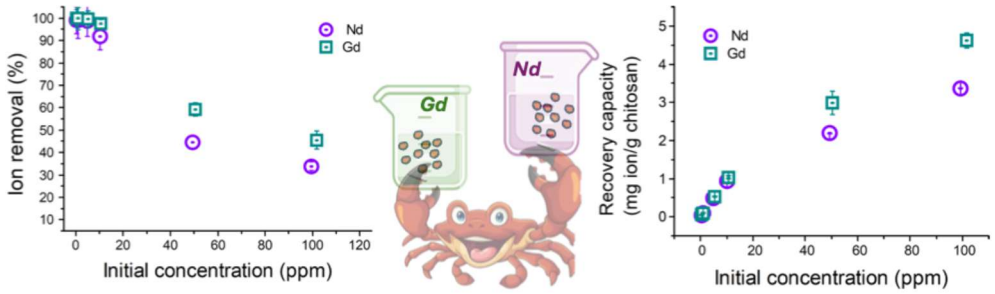

Figure 1. Percentage of recovered Nd^{3+} and Gd^{3+} and recovery capacity of chitosan towards Nd^{3+} and Gd^{3+} ions

The effect of contact time and of the suspensions' initial pH will also be discussed, and preliminary results on the simultaneous recovery of gadolinium and neodymium from model solutions will be presented. The surface characterization of the solid phase is presented in this conference by G. Casula.

Acknowledgments
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Identifying Fakes in Early 20th-Century Paintings through Spectroscopic and Microscopic Methods

Paola Fermo[a], *Andrea Bergomi*[a], *Mattia Borelli*[a], *G. Galli*[a], *G. Carabelli*[a], *Chiara Lombardi*[a,b], *Valeria Comite*[a]

[a] *Dipartimento di Chimica, Università degli Studi di Milano, Via Golgi 19, Milano, Italy*
[b] *Dipartimento di Scienze dell'Antichità, Sapienza Università di Roma, Piazzale A. Moro 5, Roma, Italy*
paola.fermo@unimi.it

Authenticating paintings from the early 20th century is a significant challenge, especially due to the increasing number of fakes entering the art market. During this period, artists began using innovative materials and new techniques, driven by scientists' discoveries and synthesis of new molecules [1]. This study illustrates the application of both non-destructive and micro-destructive analytical techniques, such as Raman spectroscopy and reflectance spectroscopy, for molecular identification, as well as Scanning Electron Microscopy combined with Energy-Dispersive X-ray Spectroscopy (SEM-EDX) for elemental composition analysis. Using these techniques provides a scientific basis for detecting fakes by identifying materials specific to that historical period.
Several artworks from the early 20th century, coming from private collections, were analyzed to verify whether the materials used were consistent with those documented at the time. A key finding was the detection, primarily through Raman spectroscopy, of phthalocyanine-based pigments [2], used as green and blue pigments in some of the analyzed works. Their presence was confirmed through colorimetric measurements, comparing the spectra with those obtained from standard samples. It's important to note that these synthetic pigments were commercially introduced only after the 1930s, making their use in authentic early 20th-century paintings unlikely. SEM-EDX further supported this conclusion by highlighting the absence of chromophores and elements typical of inorganic pigments commonly associated with that period. Conversely, some of the analyzed works displayed pigments consistent with the first decades of the 20th century, suggesting they could be authentic.
In conclusion, this study highlights the importance of combining various analytical techniques to address issues related to the identification of fake artworks, a problem that is widespread even in modern and contemporary art.

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References
[1] F. Pozzi, A. van Loon, F. Casadio, A review of synthetic organic pigments in 20th-century art, Studies in Conservation (2019), 64(2), 61–78. https://doi.org/10.1080/00393630.2018.1509251.
[2] N.C. Scherrer, S. Zumbuehl, F. Delavy, A. Fritsch, R. Kuehnen, Synthetic organic pigments of the 20th and 21st century relevant to artist's, Spectrochimica Acta Part A (2009), 73, 505–552. https://doi.org/10.1016/j.saa.2008.11.029.

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Sponsors

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PROGRAMMA GIOVEDÌ 19/06/2025

Ore 8.30 Registrazione

Ore 9.15 Apertura dei lavori (Aula Coro di Notte, Monastero dei Benedettini)

Emilia Bramanti, Coordinatrice del gruppo di Spettroscopia Analitica (GSA), Roberta D'Agata

Ore 9.30-10.10 **Invited lecture**

JAKUB DOSTÁLEK: Single Molecule Detection with Plasmonically Enhanced Readout
FZU – Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

SESSIONE 1

Chair: Roberta D'Agata

Ore 10.10-10.30
SIMONA SCARANO Molecular Imprinting Meets Spectroscopy: A New Frontier in Bioanalytical Sensing
Department of Chemistry "Ugo Schiff", University of Florence

Ore 10.30-10.50
MARIA JOSÈ LO FARO Fractal Networks of Nanostructures for Imaging and Sensing
Dipartimento di Fisica ed Astronomia, Università di Catania

Ore 10.50-11.10
ELVIRA DE GIGLIO Analytical characterization by spectroscopic techniques of Gellan gum-based hydrogels for cartilage tissue regeneration
Department of Chemistry, University of Bari Aldo Moro

Ore 11.10-11.50 **Coffee Break**

SESSIONE 2

Chair: Marzia Fantauzzi

Ore 11.50-12.10
ADELE FERRETTI Raman spectroscopy for fingerprinting historical inks: a valuable tool for discriminating logwood recipes
Department of Chemistry and Industrial Chemistry, Università di Pisa

Ore 12.10-12.30
A. VALERIA MONTEFUSCO Spectroscopic characterization of novel cross-linked biopolymeric sodium alginate films with ZnO NSs for food packaging
Dipartimento di Chimica, Università degli Studi di Bari Aldo Moro, Dipartimento di Ingegneria Elettrica e dell'Informazione, Politecnico di Bari, CSGI (Center for Colloid and Surface Science)-Unità di Bari.

Ore 12.30-12.50
ANNA LAURA TASSI From Surface to Air: Leveraging Spectroscopy to Monitor Iso-Eugenol Release from Mesoporous Silica
Università degli Studi di Milano, Dipartimento di Chimica

Ore 12.50-13.10 SPONSOR (**Shimadzu**)
ANDREA D'ALESSANDRO Analysis of microplastics with IR technique coupled to Raman in a microscope
Shimadzu srl, Italy

13.10-15.10 **PRANZO (Chiostro di Levante)** e **SESSIONE POSTER**

SESSIONE 3

Chair: Rosaria Anna Picca

Ore 15.10-15.30
MARGHERITA IZZI Statistical analysis of bacterial motion as a new methodology to study bacteria/antimicrobial interactions
Chemistry Department, University of Bari; Consorzio per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), Sesto Fiorentino

Ore 15.30-15.50
TIZIANO DI GIULIO Decoding Plastic Behavior in Environment through Surface Characterization: an X-ray photoelectron spectroscopy (XPS) study
Laboratorio di Chimica Analitica, Dipartimento di Scienze e Tecnologie Biologiche e Ambientali

Ore 15.50-16.10
ENRICA TUVERI The optimization of a combined analytical approach for clarifying the cadmium removal mechanism by Sardinian limestone and Carrara marble
Dipartimento di Scienze Chimiche e Geologiche, Università di Cagliari

Ore 16.10-16.30
VALERIO DE MARZO Synthesis and characterization of silver-based nanoantimicrobials included in food-grade polypropylene
Dipartimento di Chimica, Università degli Studi di Bari

Ore 16.30-16.50
DEBORAH BIGGIO A multi-analytical approach for assessing the performance of hydrogen permeation barriers on iron
Department of Chemical and Geological Science, University of Cagliari, Cittadella Universitaria, Monserrato, Cagliari

Ore 16.50-17.10
EVA LUNA RAVAN Investigating sulfur crystal formation in arsenic sulfide pigments by using advanced mobile X-rays methods
ISPC-CNR, Catania; Sapienza University of Rome

Ore 17.10-17.30
GIULIO CASULA An XPS investigation on Neodymium – Chitosan interaction
University of Cagliari, Department of Chemical and Geological Science, Monserrato, Cagliari

Ore 17.30-18.00 **Riunione del Gruppo Spettroscopia Analitica**

Ore 20.30 **CENA SOCIALE**

PROGRAMMA VENERDÌ 20/06/2025

Chair: Giuseppe Spoto

Ore 9.20-10.00 **Invited lecture**
PATRIZIO GIACOMINI Circulating tumor DNA (ctDNA): clinical applications and outlook on optical biosensors
Fondazione Policlinico Universitario Agostino Gemelli IRCCS, Roma.

SESSIONE 4

Chair: Roberta D'Agata

Ore 10.00-10.20
EMILIA BRAMANTI Unravelling Metabolic Alterations in Parental and Drug-Resistant Human Non Small Lung Cancer: from spectroscopic screening to high-resolution transcriptomics
Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), Pisa

Ore 10.20-10.40
CATERINA DALLARI High throughput evanescent-wave biosensor for the early-stage detection of biomarkers in liquid biopsies
National Institute of Optics (INO), National Research Council (CNR), Sesto Fiorentino; European Laboratory for non-linear Spectroscopy (LENS), University of Florence

Chair: Emilia Bramanti

Ore 10.40-11.20 **Relazione su invito e Premiazione Vincitrice del premio "Ambrogio Mazzucotelli"**

NOEMI BELLASSAI Advances in analytical technologies for sensitive detection of circulating biomarkers in clinical and food samples
Department of Chemical Sciences, University of Catania
INBB, Istituto Nazionale di Biostrutture e Biosistemi, Roma

Ore 11.20-11.50 **Coffee Break**

SESSIONE 5

Chair: Paola Fermo

Ore 11.50-12.10
ZELAN LI Co-registered Hyperspectral Imaging System with Multiblock Data Processing for Stratigraphic Investigation of Paintings
Department of Chemistry "G. Ciamician", University of Bologna, Ravenna Campus

Ore 12.10- 12.30
STEFANO LEGNAIOLI Integrated analytical approach for the characterisation of dyed wool fibers in the oldest Moroccan carpet
Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), Pisa

Ore 12.30-12.50
MANUEL MONTI From field to data: real-time protein and moisture analysis in wheat using portable spectroscopic sensors and chemometrics
Department of Science and High Technology, University of Insubria

Ore 12.50-13.10 SPONSOR (**Renishaw**)
RICCARDO TAGLIAPIETRA Simultaneous and colocalised Raman and SEM imaging for correlated multimodal analysis
Renishaw SpA, Italy

Ore 13.10-14.10 **PRANZO (Chiostro di Levante)**

SESSIONE 6

Chair: Sandro Recchia

Ore 14.10-14.30
GIULIA LORENZETTI The gardener of the Grand Duke: history and analysis of Ms. 462 Hortus Pisanus, Icones variarum plantarum
Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), Pisa

Ore 14.30-14.50
ALESSIA SANTIGLIA Qualitative Study of Apatite and Clays Using IR Spectroscopy: The Case Study of Riparo Gaban
Department of Chemistry, Università degli Studi di Milano

Ore 14.50-15.10
CECILIA CAMPI Degradation of Silk under the Influence of Dyes and Different Aging Conditions
Department of Chemistry and Industrial Chemistry, Università di Pisa

Ore 15.10-15.30
ELEONORA MICHELI Natural materials Development from Collagen-based Wastes – ArtDECOW: treatment and solubilization methods
Istituto di Chimica dei Composti OrganoMetallici (ICCOM-CNR), Pisa

Ore 15.30-15.50
ALESSANDRO DEL GROSSO Advancing Liquid Biopsy: Direct Capture of Circulating Tumor DNA from Plasma with Superparamagnetic Beads
Dipartimento di Scienze Chimiche, Università di Catania

Ore 15.50-16.30 **Premio "Franco Cariati" e Chiusura dei Lavori**

Ore 16.30 **Visita guidata al Monastero dei Benedettini**