Società Chimica Italiana

XXVII Congresso Divisione di Chimica Analitica

16-20 Settembre 2018, Bologna

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UNIVERSITÀ DI BOLOGNA

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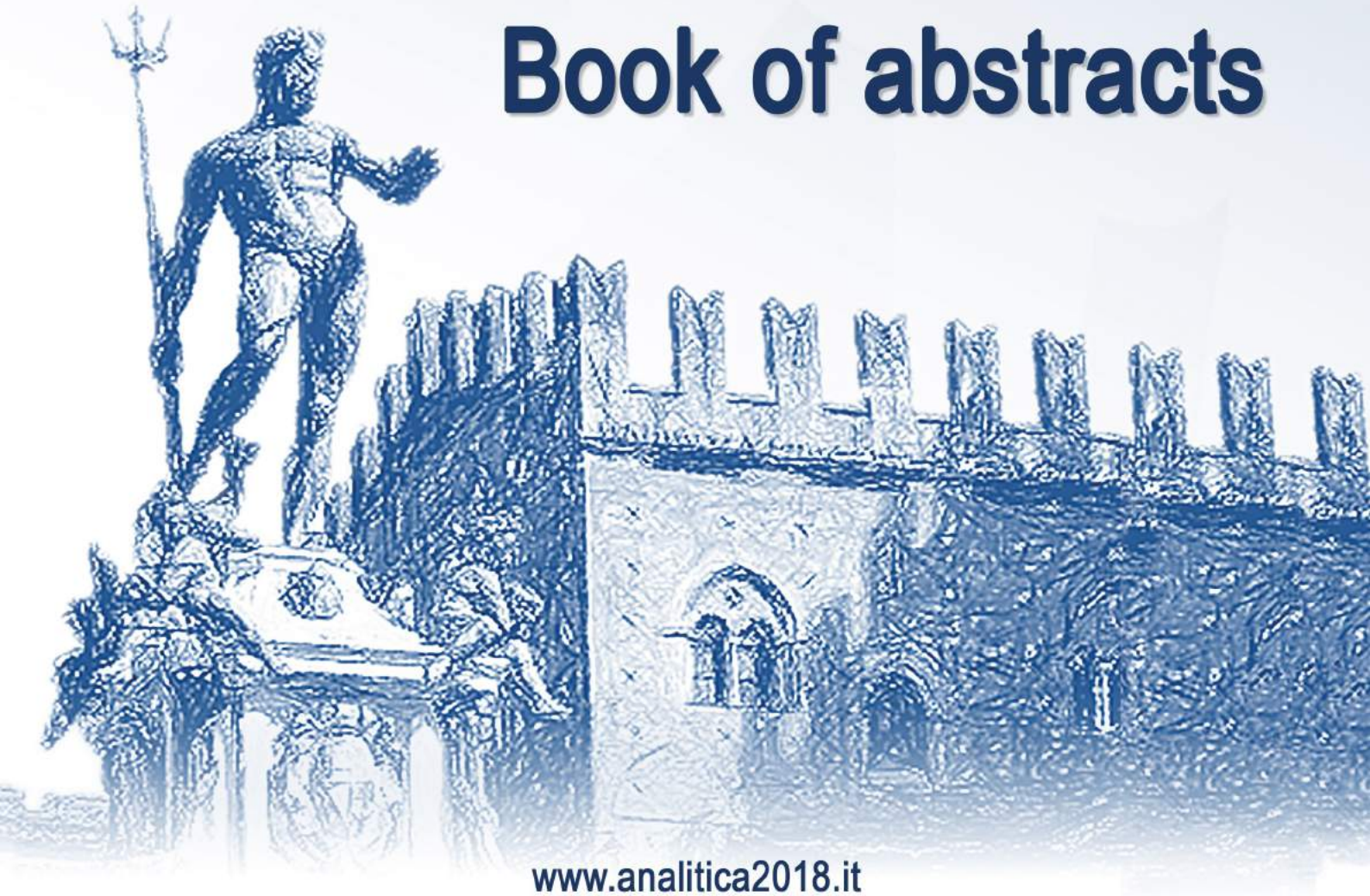

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XXVII Congresso Divisione di Chimica Analitica

16-20 Settembre 2018, Bologna

DAMSLab, Piazzetta P. P. Pasolini 5/b

www.analitica2018.it

ISBN 978-88-94952-04-9

Edited by Aldo Roda, Mara Mirasoli, Massimo Guardigli
Published online on 25 September 2018 at Bologna
by Alma Mater Studiorum – University of Bologna

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AIM OF THE CONGRESS

The Congress is organized yearly by the Analytical Chemistry Division of the Italian Chemical Society and it provides an opportunity for all researchers in the field to meet and debate key topics.

The different aspects of Analytical Chemistry are covered, from the traditional sectors to the most innovative ones. The main topics discussed have been:

- Analytical biotechnology
- Analytical spectroscopy
- Bioanalytics and "-omics"
- Chemometrics, "big data", data quality
- Electroanalytics, electrophotoanalytics
- Environment and cultural heritage
- Food and nutraceuticals
- Forensic analytical chemistry
- Green chemistry
- Mass spectrometry
- Sensors and biosensors, Lab-on-a-chip, POCT
- Separation sciences
- Solution equilibria and speciation
- Toxicology and human health

The Congress has been organized by the Analytical Chemistry groups of the Alma Mater Studiorum – University of Bologna (Department of Chemistry “Giacomo Ciamician” and Department of Industrial Chemistry “Toso Montanari”).

PROGRAM

Sunday, September 16

18:00-21:00 **Registration**
Hall

19:00-21:00 **Welcome cocktail**
Hall and Courtyard

Monday, September 17

8:00-9:00 **Registration**
Hall

9:00-9:30 **Opening**
Auditorium and (by streaming) Theater

Aldo Roda (President of the Local organizing and scientific committee of the XXVII Congress of the Analytical Chemistry Division)
Antonino Rotolo (Vice-Rector for Research, Alma Mater Studiorum - University of Bologna)
Angela Agostiano (President of the Italian Chemical Society)
Aldo Laganà (President of the Division of Analytical Chemistry, Italian Chemical Society)
Francesco Paolucci (Head of the Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna)
Fabrizio Cavani (Head of the Department of Industrial Chemistry "Toso Montanari", Alma Mater Studiorum - University of Bologna)

Plenary session

Auditorium and (by streaming) Theater
Chairman: Giuseppe Palleschi

9:30-10:10 **PL1** ANALYTICAL ASPECTS OF BIOSENSING SYSTEMS BASED ON ENZYME INHIBITION
A. Amine
Université Hassan II de Casablanca, Morocco

Lecture of the Young Researcher Award winner

10:10-10:30 **GR** INNOVATIVE ANALYTICAL APPROACHES BASED ON MASS SPECTROMETRY TECHNIQUES AND IMMUNOSENSING DEVICES FOR FOOD SAFETY CONTROL AND CLINICAL DIAGNOSIS
M. Mattarozzi
Department of Chemistry, Life Sciences and Environmental Sustainability - University of Parma, Parco Area delle Scienze, 17/A - 43124 Parma, Italy

10:30-11:00 **Coffee break**

Plenary session

Auditorium and (by streaming) Theater

Sensors and biosensors, Lab-on-a-chip, POCT (SB)

Separation sciences (SS)

Chairmen: Giovanna Marrazza, Luigi Mondello

11:00-11:20	**KN1** MOLECULARLY IMPRINTED NANOGEL PARTICLES: TAILOR-MADE PROTEIN AND PEPTIDE RECEPTORS FOR SENSING AND ASSAYS A. M. Bossi *Department of Biotechnology, University of Verona, Strada Le Grazie, 15 - 37134 Verona, Italy*
11:20-11:35	**O1 SB** SINGLE MOLECULE DETECTION OF MARKERS IN REAL BIO-FLUIDS WITH A LABEL-FREE ELECTRONIC SENSOR E. Macchia[1], K. Manoli[1], L. Torsi[1,2] *[1]Dipartimento di Chimica – Università degli Studi di Bari "A. Moro", Via Orabona, 4 - 70125, Bari, Italy* *[2]The Faculty of Science and Engineering - Åbo Akademi University – Finland*
11:35-11:50	**O2 SB** CHAMELEON PROBES FOR CHROMOGENIC SENSING OF VOLATILE SPOILAGE PRODUCTS OF CHICKEN MEAT L. R. Magnaghi, G. Alberti, R. Biesuz *Department of Chemistry, Università di Pavia, via Taramelli 12 - 27100 Pavia, Italy*
11:50-12:05	**O3 SB** A NEW CELL-BASED BIOLUMINESCENT ASSAY FOR REAL-TIME DETECTION OF ANDROGENIC ACTIVITY IN LIVING CELLS M. M Calabretta[1], E. Michelini[1,2], A. Lopreside[1], L. Montali[1], A. Roda[1,2] *[1]Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna, Via Selmi, 2 - 40126 Bologna, Italy* *[2]INBB, Istituto Nazionale di Biostrutture e Biosistemi, Viale Medaglie d'Oro 305, Roma, Italy*
12:05-12:25	**KN2** FIELD-FLOW FRACTIONATION FOR NANOANALYTICS: FROM GENESIS TO REVELATION B. Roda *Department of Chemistry "G. Ciamician, University of Bologna, via Selmi 2, 40126 Bologna, Italy*
12:25-12:40	**O1 SS** AN EFFICIENT STRATEGY FOR MOLECULARLY IMPRINTED SOLID PHASE EXTRACTION OF AILANTHONE FROM LEAVES OF AILANTHUS ALTISSIMA C. Giovannoli, G. Spano, S. Cavalera, F. Di Nardo, L. Anfossi, F. Trotta, C. Baggiani *Department of Chemistry, University of Torino, Via Giuria 7 – 10125 Torino, Italy*
12:40-12:55	**O2 SS** UNMATCHED KINETIC PERFORMANCE IN ENANTIOSELECTIVE SUPERCRITICAL FLUID CHROMATOGRAPHY BY COMBINING LATEST GENERATION WHELK-O1 CHIRAL STATIONARY PHASES WITH A LOW DISPERSION IN-HOUSE MODIFIED EQUIPMENT M. Catani[1], O. H. Ismail[2], F. Gasparrini[2], A. Cavazzini[1] *[1]Department of Chemistry and Pharmaceutical Sciences, University of Ferrara, via L. Borsari, 46 – 44121 Ferrara, Italy* *[2]Department of Drug Chemistry and Technology, "Sapienza" University of Rome, P.le Aldo Moro, 5 - 00185 Rome, Italy*

12:55-13:00 **F1 MS** HPLC-ES MS/MS METHOD FOR THE IDENTIFICATION AND QUANTIFICATION IN HUMAN FECES OF GUT MICROBIOTA PRODUCTS: OXO-BILE ACIDS

E. Porru[1], P. Franco[2], J. Fiori[1], A. Gioiello[4], B. Cerra[4], G. Roda[3], C. Caliceti[1,2], P. Simoni[5], A. Roda[1,2]

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[2]Centro Interdipartimentale di Ricerca Industriale Energia e Ambiente (CIRI EA), Alma Mater Studiorum - University of Bologna, Bologna, Italy

[3]IBD Center, Department of Gastroenterology, Humanitas Clinical and Research Institute, Rozzano, Milan, Italy

[4]Department of Pharmaceutical Sciences, University of Perugia, Via del Liceo 1, 06123 Perugia, Italy

[5]Department of Medical and Surgical Sciences, Alma Mater Studiorum – University of Bologna, Via Massarenti 9, 40138 Bologna, Italy

13:00-14:40 **Lunch**

13:00-14:40 **Poster session I**

Theater

Regular posters: P001 – P074

Flash communication posters: PF1 SB - PF4 SB, PF1 SS, PF1 FN, PF2 FN, PF1 AS, PF1 EC - PF3 EC, PF1 FO, PF1 MS

Parallel session

Auditorium

Sensors and biosensors, Lab-on-a-chip, POCT (SB)

Chairmen: Domenica Tonelli, Luisa Torsi

14:40-14:55 **O4 SB** SURFACE PLASMON RESONANCE TRANSDUCTION ON OPTICAL FIBER AS A LOW-COST ALTERNATIVE TO THE KRETSCHMANN CONFIGURATION

M. Pesavento[1], G. Alberti[1], N. Cennamo[2], L. Zeni[2], L. De Maria[3], S. Marchetti[1]

[1]Department of Chemistry - University of Pavia, Via Taramelli, 12 – 27100 PAVIA, Italy

[2]Department of Industrial and Information Engineering, University of Campania Luigi Vanvitelli, Via Roma 29, Aversa 81031, Italy

[3]Department of Transmission and Distribution Technologies, RSE Research on Energetic System S.p.A, Via Rubattino 54, Milano 20134, Italy

14:55-15:10 **O5 SB** DISSIPATIVE DNA-BASED NANOMACHINES

E. Del Grosso[1,‡], A. Amodio[1,‡], G. Ragazzon[2], L. Prins[2,*], F. Ricci[1,*]

[1]Department of Chemistry - University of Rome "Tor Vergata", Via della Ricerca Scientifica, 1 - 00133 Rome, Italy

[2]Department of Chemical Sciences - University of Padua, Via Marzolo 1 - 35131 Padua, Italy

15:10-15:25 **O6 SB** A SMARTPHONE-BASED THERMOCHEMILUMINESCENT IMMUNOSENSOR FOR VALPROIC ACID DETECTION

A. Roda[1], M. Zangheri[1], D. Calabria[1], M. Mirasoli[1], C. Caliceti[1], A. Quintavalla[1], M. Lombardo[1], C. Trombini[1], P. Simoni[2]

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[2]Department of Medical and Surgical Sciences, Alma Mater Studiorum – University of

Bologna, Via Massarenti 9, 40138 Bologna, Italy

15:25-15:40 **O7 SB** NEW ANTIFOULING PLATFORM FOR DNA DETECTION IN HUMAN PLASMA BASED ON MODIFIED POLY-L-LYSINE POLYMERS WITH ANIONIC PEPTIDE

N. Bellassai[1,2,3], A. Marti[3], J. Huskens[3], G. Spoto[2,4]

[1]*C.I.R.C.M.S.B. Consortium, c/o Department of Chemical Sciences, University of Catania, Catania, Italy*

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[3]*Molecular NanoFabrication Group, University of Twente, MESA+ Institute for Nanotechnology, P.O. Box 217 - 7500 AE Enschede, The Netherlands*

[4]*I.N.B.B. Consortium, c/o Department of Chemical Sciences, University of Catania, Catania, Italy*

15:40-15:55 **O8 SB** ALL-IN-PAPER (BLUE): SYNTHESIS, MATRIX PURIFICATION, REAGENT-FREE DETECTION. BLOOD GLUCOSE AS CASE OF STUDY

S. Cinti, F. Arduini, D. Moscone, G. Palleschi

Department of Chemical Science and Technologies, University of Rome "Tor Vergata", Via della Ricerca Scientifica, 1 – 00133 Rome, Italy

15:55-16:00 **F1 SB** LIFE MARKER DETECTION IN PLANETARY EXPLORATION: A NOVEL BIOSENSOR FOR ATP DETECTION BASED ON CHEMILUMINESCENT DNA SWITCH INTEGRATED WITH AMORPHOUS SILICON PHOTODIODES

E. Marchegiani[a], M. Mirasoli[a], M. Zangheri[a], M. Guardigli[a], C. Caliceti[a], A. Porchetta[b], D. Caputo[c], A. Nascetti[d], A. Roda[a]

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[c]*Department of Information, Electronics and Communication Engineering, Sapienza University of Rome, Via Eudossiana 18, 00184 Rome, Italy*

[d]*Aerospace Engineering School, Sapienza University of Rome, Via Salaria 851/881, 00138 Rome, Italy*

16:00-16:05 **F2 SB** A COMPETITIVE APTAMER ASSAY FOR GLUTEN DETECTION IN DEEP EUTECTIC SOLVENT

R. Svigelj[1], N. Dossi[1], R. Toniolo[1], R. Miranda-Castro[2], N. de-los-Santos-Álvarez[2], M. J. Lobo-Castañón[2]

[1]*Department of Agrifood, Environmental and Animal Sciences, University of Udine, via Cotonificio 108, Udine, Italy*

[2]*Department of Química Física y Analítica, Universidad de Oviedo, Av. Julián Clavería 8, 33006, Oviedo, Spain*

16:05-16:10 **F3 SB** RATIONAL CONTROL OF THE ACTIVITY OF A CU^{2+}-DEPENDENT DNAZYME BY RE-ENGINEERING PURELY ENTROPIC DISORDERED DOMAINS

S. Ranallo, D. Sorrentino, F. Ricci

Department of Chemistry, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy

16:10-16:15 **F4 SB** DNA-BASED QUARTZ CRYSTAL MICROBALANCE ARRAY FOR THE IDENTIFICATION OF AROMA PATTERNS IN FOODSS

S. Gaggiotti, F. Della Pelle, M. Mascini, V. Masciulli, D. Compagnone

Faculty of Bioscience and Technology for Food, Agriculture, and Environment - University of Teramo, Via Renato Balzarini, 1 - 64100 Teramo, Italy

16:15-16:30 **O9 SB** SIMULTANEOUS DETERMINATION OF GLUCOSE AND FRUCTOSE IN SYNTHETIC MUSTS BY SONOGEL-CARBON AMPEROMETRIC SENSORS

J. R. Crespo Rosa,[1] G. Foca,[2] A. Ulrici,[2] F. Terzi,[3] J. M. Palacios Santander[1], L. M. Cubillana Aguilera[1], L. Pigani[3], C. Zanardi[3]

[1]Institute of Research on Electron Microscopy and Materials (IMEYMAT), Department of Analytical Chemistry, Faculty of Sciences, Campus de Excelencia Internacional del Mar (CEIMAR), University of Cadiz, Campus Universitario de Puerto Real, Polígono del Río San Pedro, S/N. 11510 Puerto Real, Cadiz-Spain.

[2]Department of Life Sciences, University of Modena and Reggio Emilia, Padiglione Besta, Via Amendola 2, 42122 Reggio Emilia, Italy

[3]Department of Chemical and Geological Sciences, University of Modena e Reggio Emilia, Via Campi 183 - 41125 Modena, Italy

16:30-16:45 **O10 SB** DEVELOPMENT AND CHARACTERIZATION OF A NEW BETAINE / PT ELECTROCHEMICAL SENSOR FOR DETECTION OF B GROUP VITAMINS

D. Coviello, M. Contursi, M. A. Palmieri, I. G. Casella

Department of Science, University of Basilicata, Via dell'Ateneo Lucano, 10 - 85100 Potenza, Italy

Parallel session

Theater

Separation sciences (SS)

Food and nutraceuticals (FN)

Chairmen: Paolo Pastore, Pierluigi Reschiglian

14:40-14:55 **O3 SS** DISPERSIVE MAGNETIC SOLID-PHASE EXTRACTION USING GRAFENE@Fe_3O_4 NANOCOMPOSITE FOR THE UHPLC-PDA ANALYSIS OF THE NEW ORAL ANTICOAGULANT DRUGS (NAOCs) IN HUMAN PLASMA

V. Ferrone[1], G. Carlucci[1], P. Palumbo[5], M. Carlucci[4], E. Milanetti[2,3]

[1]Department of Pharmacy, [4]Department of Medical, Oral and Biotechnological Sciences - University "G. d'Annunzio" Chieti-Pescara, Via dei Vestini, 31 -66100 Chieti, Italy

[2]Department of Physics - University "La Sapienza" Rome

[3]Center for Life Science@Sapienza, Italian Institute of Technology - Viale Regina Elena- Rome, Italy

[5]Department of Life, Health and Environmental Sciences - University of L'Aquila - via Vetoio - 67100 L'Aquila, Italy

14:55-15:10 **O4 SS** THE "RACEMIC APPROACH" IN PHARMACEUTICAL ANALYSIS: A SELECTION OF LABORATORY STUDIES

F. Ianni, L. Pucciarini, R. Sardella, B. Natalini

Department of Pharmaceutical Sciences - University of Perugia, Via Fabretti, 48 – 06123 Perugia, Italy

15:10-15:25 **O5 SS** THERMALLY CONDENSED HUMIC ACIDS ONTO SILICA AS SPE FOR MULTI-CLASS PRECONCENTRATION OF STEROID HORMONES FROM ENVIRONMENTAL WATERS FOLLOWED BY HPLC-ESI-MS/MS

F. Merlo, A. Speltini, F. Maraschi, M. Sturini, A. Profumo

Department of Chemistry, University of Pavia, via Taramelli 12, 27100 Pavia, Italy

15:25-15:40 **O6 SS** DEVELOPMENT OF A FAST AND SIMPLE METHOD FOR THE ASSAY OF URINARY PHTHALATE MONOESTERS BY SOLID-PHASE MICROEXTRACTION-

	GAS CHROMATOGRAPHY-TRIPLE QUADRUPOLE MASS SPECTROMETRY R. Elliani[1], A. Naccarato[2], A. Tagarelli[1] *[1]Department of Chemistry and Chemical Technologies - University of Calabria, Via P. Bucci Cubo 12/C, I-87030 Arcavacata di Rende, CS, Italy* *[2]CNR- Institute of Atmospheric Pollution Research, Division of Rende, c/o UNICAL-Polifunzionale, I-87036 Arcavacata di Rende, CS, Italy*
15:40-15:55	**O7 SS** QuEChERS EXTRACTION FOLLOWED BY LIQUID CHROMATOGRAPHY COUPLED WITH TANDEM MASS SPECTROMETRY FOR PERFLUOROALKYL ACID DETERMINATION IN STRAWBERRIES IRRIGATED WITH TREATED WASTEWATER C. Scordo[1], M.C. Bruzzoniti[2], E. Giordani[3], S. Orlandini[1], S. Furlanetto[1], M. Del Bubba[1] *[1]Department of Chemistry "Ugo Schiff", University of Florence, via della Lastruccia 3 - 50019 Sesto Fiorentino, Italy.* *[2]Department of Chemistry - University of Turin, via Pietro Giuria 5 - 10125 Turin, Italy.* *[3]Department of Agri-Food and Environmental Science, University of Florence, viale delle Idee 30, 50019 Sesto Fiorentino, Italy*
15:55-16:00	**F1 SS** INVESTIGATION, ISOLATION AND CHARACTERISATION OF NEW PRIONOID PROTEIN AGGREGATES THROUGH HOLLOW FIBER FLOW FIELD FLOW FRACTIONATION AND MULTI ANGLE LIGHT SCATTERING: A TOOL TO FACILITATE THE COMPREHENSION OF INFECTIOUS PROCESSES V. Marassi[1], B. Roda[1], F. Beretti[2], A. Zattoni[1], M. Portolani[2], P. Reschiglian[1] *[1]Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna, Via Selmi, 2 - 40126 Bologna, Italy* *[2]Department of Laboratory Activities, and Morbid Anatomy, University of Modena and Reggio Emilia, 41125 Modena, Italy*
16:00-16:05	**F1 FN** EXTRACTION, ANALYSIS AND ANTIOXIDANT ACTIVITY EVALUATION OF PHENOLIC COMPOUNDS IN DIFFERENT ITALIAN EXTRA-VIRGIN OLIVE OILS C. Fanali[1], S. Della Posta[1], A. Vilmercati[1], L. Dugo[1], M. Russo[1], T. Petitti[1], L. Mondello[1,2,3], L. De Gara[1] *[1]Unit of Food Science and Nutrition, Department of Medicine, Università Campus Bio-Medico di Roma, via Álvaro del Portillo 21, 00128 Rome, Italy* *[2]Dipartimento di "Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali", University of Messina - Polo Annunziata, Viale Annunziata, 98168 Messina, Italy* *[3]Chromaleont S.r.L., Viale Boccetta 70, 98122 Messina, Italy*
16:05-16:10	**F2 FN** MULTIVARIATE OPTIMIZATION OF A QUECHERS PROCEDURE FOR THE LC-MS/MS ANALYSIS OF PHYTOESTROGENS IN SOY BURGERS B. Benedetti, M. Di Carro, E. Magi *Department of Chemistry and Industrial Chemistry, University of Genova, Via Dodecaneso, 31 - 16146 Genova, Italy*
16:10-16:25	**O1 FN** DEVELOPMENT OF A REFLECTANCE SMARTPHONE PAPER-BASED CHEMOSENSOR FOR THE QUANTIFICATION OF TOTAL POLYPHENOL CONTENT IN EXTRA VIRGIN OLIVE OIL C. Caliceti, D. Calabria, M. Zangheri, E. Porru, M. Guardigli, P. Simoni, M. Mirasoli, A. Roda *Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna, Via Selmi, 2 - 40126 Bologna, Italy*
16:25-16:40	**O2 FN** DETAILED PROFILING OF EXTRA-VIRGIN OLIVE OILS BY USING

COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY WITH DUAL QUADRUPOLE MASS SPECTROMETRY AND FLAME IONIZATION DETECTION

P. Q. Tranchida[1], I. Aloisi[1], B. Giocastro[1], M. Zoccali[1], P. Dugo[1,2,3], L. Mondello[1,2,3]

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[3]Unit of Food Science and Nutrition, Department of Medicine, University Campus Bio-Medico of Rome, via Alvaro del Portillo 21, 00128, Rome, Italy

16:40-17:10 **Coffee break**

Parallel session

Auditorium

Environment and cultural heritage (EC)

Chairmen: Luigia Sabbatini, Carlo Barbante, Cosimino Malitesta

17:10-17:30 **KN3** ADVANCED DIAGNOSTIC INVESTIGATIONS FOR THE STUDY OF ALTERED GILDINGS: NEW INSIGHTS INTO CIMABUE'S PAINTING TECHNIQUE

S. Prati[1], G. Sciutto[1], E. Catelli[1], R. Mazzeo[1], L. Monico[2,3], A. Romani[2], S. De Meyer[3], G. Nuyts[3], K. Janssens[3]

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[3]Department of Chemistry, University of Antwerp, Groenenborgerlaan, 171 - 2020 Antwerp, Belgium

17:30-17:45 **O1 EC** INVESTIGATING SYNTHETIC POLYMERS IN HERITAGE OBJECTS: A MULTI-ANALYTICAL APPROACH FOR THE STUDY OF POLYURETHANE FOAMS IN 1960S SCULPTURES

J. La Nasa, F. Sabatini, G. Biale, I. Degano, F. Modugno

Department of Chemistry and Industrial Chemistry, University of Pisa (Italy)

17:45-18:00 **O11 SB** HIERARCHICAL NANOSTRUCTURES COMPOSED BY Ag NANOSTARS ON Au/Cu NANOWIRES AS SERS SENSORS FOR PAINTING MATERIALS

M. S. Zalaffi[1], M. Longoni[1], A.M. Stortini[1], L.M. Moretto[1], L. Litti[2], M. Meneghetti[2], P. Ugo[1]

[1]Department of Molecular Sciences and Nanosystems, University Ca' Foscari Venice, Via Torino 155, 30172, Venezia Mestre, Italy

[2]Department of Chemical Sciences, University of Padova, Via Marzolo 1, 35131, Padova, Italy

18:00-18:05 **F1 EC** INVESTIGATING PAINT MATERIALS IN STREET ART MURAL PAINTINGS BY ANALYTICAL PYROLYSIS BASED TECHNIQUES

J. La Nasa, S. di Carlo, I. Degano, M. P. Colombini, F. Modugno

Department of Chemistry and Industrial Chemistry, University of Pisa, via Moruzzi 13, 56124 Pisa, Italy

18:05-18:10 **F2 EC** POTENTIALLY HARMFUL ELEMENT (PHE) OCCURRENCE AND PHASE

	PARTITIONING IN THE RIVER MOUTHS OF THE GULF OF TRIESTE (NORTHERN ADRIATIC SEA) E. Pavoni[1,2], M. Crosera[1], E. Petranich[2], K. Klun[3], J. Faganeli[3], S. Covelli[2], G. Adami[1] *[1]Department of Chemical & Pharmaceutical Sciences, University of Trieste, Via L. Giorgieri 1, 34127 Trieste, Italy* *[2]Department of Mathematics & Geosciences, University of Trieste, Via E. Weiss 2, 34128 Trieste, Italy* *[3]Marine Biological Station, National Institute of Biology, Fornace 41, 6330 Piran, Slovenia*
18:10-18:15	**F3 EC** USE OF NANO-STRUCTURAL MATERIALS FOR ABATEMENT OF NITRATES IN NATURAL AND WASTE WATER C. Cecone, G. Costamagna, M. Ginepro, S. Mariotti, J. A. Tafur Marinos, F. Trotta *Department of Chemistry University of Turin, Via Pietro Giuria 7, Torino - 10125, Italy*
18:15-18:30	**O2 EC** EMISSIONS FROM PELLETS COMBUSTION: A STUDY ON STOVES TO EVALUATE THE IMPACT ON ATMOSPHERIC AEROSOL P. Fermo[1], S. Gilardoni[2], V. Comite[1], S. Bertagna[3], G. Migliavacca[3], C. Morreale[3] *[1]Department of Chemistry, University of Milan, Milan, Via Golgi, 19 - 20133 Milano, Italy* *[2]ISAC-CNR, Via Piero Gobetti, 101- 40129 Bologna, Italy* *[3]Innovhub Stazioni Sperimentali per l'Industria area Combustibili, via Galilei,1 – 20097 San Donato Milanese (MI), Italy*

Parallel session

Theater

Analytical spectroscopy (AS)

Forensic analytical chemistry (FO)

Chairmen: Marco Vincenti, Maria Pesavento

17:10-17:25	**O1 AS** MORPHOLOGICAL AND COMPOSITIONAL ANALYZES OF SURFACES M. Innocenti[1,2], M. Passaponti[1], E. Salvietti[1], A. Giaccherini[3], W. Giurlani[1], A. De Luca[1], R. Felici[4], A. Lavacchi[2], F. Di Benedetto[3] *[1] University of Florence, Department of Chemistry, Via della Lastruccia 3, Sesto Fiorentino (FI) Italy and INSTM Consortium* *[2] Institute of Chemistry of Organo-Metallic Compounds, ICCOM-CNR and INSTM Consortium, 50019 Sesto F.no, (FI), Italy* *[3] University of Florence, Department of Earth Science, Via la Pira 4, 50121 Firenze, Italy* *[4] SPIN-CNR, Rome, Italy*
17:25-17:30	**F1 AS** INSIGHTS INTO THE INHIBITION OF *P. FLUORESCENS* BIOFILM FORMATION VIA AFM AND ATR-IR CHARACTERIZATIONS M. C. Sportelli[1], R. Quarto[1], R. A. Picca[1], C. Kranz[2], B. Mizaikoff[2], E. Tütüncü[2] A. Valentini[3], N. Cioffi[1] *[1]Dipartimento di Chimica, Università degli Studi di Bari "Aldo Moro", V. Orabona, 4, 70126, Bari, Italy;* *[2]Institute of Analytical and Bioanalytical Chemistry, Ulm University, Albert Einstein Allee, 11, 89081, Ulm, Germany;* *[3]Dipartimento di Fisica, Università degli Studi di Bari "Aldo Moro", V. Orabona, 4, 70126, Bari, Italy*

17:30-17:45 **O2 AS** THE UNCOMMON ELECTROCHEMISTRY OF COPPER NITROPRUSSIDE DISCLOSED BY SPECTROSCOPIC AND DIFFRACTION TECHNIQUES

A. Mullaliu[1], E. Musella[1], R. Denecke[2], M. Giorgetti[1]

[1]*Department of Industrial Chemistry "Toso Montanari", Alma Mater Studiorum - University of Bologna, Viale del Risorgimento, 4 - 40136 Bologna, Italy*

[2]*Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie Linnéstraße 2, D-04103 Leipzig, Germany*

17:45-18:00 **O3 AS** SURFACE CHARACTERIZATION OF NON-NOBLE METALS EMBEDDED IN N-DOPED CARBON CATALYSTS: THE IMPORTANCE OF HYDROPHILICITY ON OXYGEN REDUCTION REACTION ACTIVITY

M. Longhi[1], C. Cova[1], E. Pargoletti[1], M. Coduri[2], S. Santangelo[3], S. Patanè[4], N. Ditaranto[5], N. Cioffi[5], A. Facibeni[6], M. Scavini[1]

[1]*Università degli Studi di Milano, Dipartimento di Chimica, Via Golgi 19, 20133 Milano, Italy*

[2]*ESRF - The European Synchrotron, 71, Avenue des Martyrs, 38043 Grenoble, France*

[3]*Università "Mediterranea", Dipartimento di Ingegneria Civile, dell'Energia, dell'Ambiente e dei Materiali (DICEAM), Via Graziella, Loc. Feo di Vito, 89122 Reggio Calabria, Italy*

[4]*Università di Messina, Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra (MIFT), Viale Stagno d'Alcontres 31, 98166 Messina, Italy*

[5]*Università degli Studi di Bari "Aldo Moro", Dipartimento di Chimica, Via Orabona 4, 70125 Bari, Italy*

[6]*Politecnico di Milano, Dipartimento di Energia and NEMAS - Centre for NanoEngineered MAterials and Surfaces, Via Ponzio 34/3, 20133, Milano, Italy*

18:00-18:15 **O1 FO** MULTIVARIATE DATA ANALYSIS STRATEGIES FOR FIRE DEBRIS INVESTIGATION

E. Alladio[1,2], M. Pazzi[1], F. D'Aloise[3], F. Malaspina[3], Marco Vincenti[1,2]

[1]*Dipartimento di Chimica, Università degli Studi di Torino, Via P. Giuria, 7 - 10125 Torino, Italy*

[2]*Centro Regionale Antidoping e di Tossicologia "A. Bertinaria", Regione Gonzole, 10/1 - 10043 Orbassano (Torino), Italy*

[3]*Corpo Nazionale Vigili del Fuoco - Comando di Torino, Unità di Intervento Nucleare Biologico Chimico Radiologico, Corso Regina Margherita, 330 - 10143 Torino, Italy*

18:15-18:20 **F1 FO** DETERMINATION OF ETHYL-GLUCURONIDE IN HAIR BY MEANS PLE-SPE EXTRACTION AND HPLC-MS/MS ANALYSIS

F. Vincenti[1], R. Di Mambro[1], R. Curini[1], M. Sergi[2], D. Compagnone[2]

[1]*Department of Chemistry – Sapienza – University of Rome, Piazzale Aldo Moro, 5 – 00185 Rome, Italy*

[2]*Faculty of Bioscience and Technology for Food, Agriculture and Environment - University of Teramo, Via Balzarini, 1 - 64100 Teramo, Italy*

18:30-20:00 **"Assemblea Divisionale" and Awards and Medals of the Analytical Chemistry Division**

Auditorium

Tuesday, September 18

Plenary session

Auditorium and (by streaming) Theater

Bioanalytics and "-omics" (BO)

Chairmen: Maria Careri, Dario Compagnone

9:00-9:40	**PL2** IMPRINTED POLYMERS IN BIOANALYSIS, BIOMARKER DISCOVERY AND IMAGING B. Sellergren *Malmö University, Sweden*
9:40-10:00	**KN4** SEPARATION AND ENRICHMENT OF PEPTIDES AND AMINO ACIDS: A PIECE IN THE PUZZLE OF THE BIOACTIVITY OF PROTEIN DERIVATIVES S. Piovesana *Department of Chemistry, Sapienza Università di Roma – Piazzale Aldo Moro, 5 - 00185 Rome, Italy*
10:00-10:15	**O1 BO** IDENTIFICATION OF AUTISM SPECTRUM DISORDER BIOMARKERS BY LIQUID CHROMATOGRAPHY COUPLED WITH MASS SPECTROMETRY G. Ventura[1], C. D. Calvano[1,2], V. Porcelli[3], L. Palmieri[3,4], Y. Xu[5], R. Goodacre[5], F. Palmisano[1,2], T.R.I. Cataldi[1,2] *[1]Department of Chemistry, and* *[2]Interdepartmental Research Center SMART University of Bari Aldo Moro, via Orabona 4, 70126, Bari, Italy* *[3]Department of Biosciences, Biotechnologies and Biopharmaceutics, University of Bari Aldo Moro, via Orabona 4, 70126, Bari, Italy* *[4]Institute of Biomembranes and Bioenergetics, CNR, via Amendola 165/A, Bari Italy* *[5]The Manchester Institute of Biotechnology, School of Chemistry, University of Manchester, 131 Princess Street, Manchester, M1 7DN, UK*
10:15-10:30	**O2 BO** HYDROGEL EXTRACTION SURFACE ANALYSIS (HESA): AN OPTION FOR SHOTGUN QUANTITATIVE PROTEOMICS FROM CARDIAC MYXOMA FFPE BIOPSY D. Taverna, M. Gaspari *Research Center for Advanced Biochemistry and Molecular Biology, Department of Experimental and Clinical Medicine - Magna Graecia University of Catanzaro Campus "S. Venuta", Viale Europa, Loc. Germaneto - 88100 Catanzaro, Italy*
10:30-10:45	**O3 BO** URINARY STEROIDAL PROFILE AS INNOVATIVE TOOL FOR THE SCREENING OF PROSTATE DISEASES E. Amante[1,2], F. Marini[3], E. Alladio[1], S. Pruner[1], G. Guzzetti[1], G. Alleva[4], S. De Luca[4], A. Salomone[2], F. Porpiglia[4], M. Vincenti[1,2] *[1]Department of Chemistry, University of Torino, Via P. Giuria, 7 – 10125 Torino, Italy* *[2]Centro Regionale Antidoping "A. Bertinaria", Regione Gonzole, 10/1 – 10043 Orbassano (To), Italy.* *[3]Department. of Chemistry, University of Rome "La Sapienza", P.le Aldo Moro, 5 – 00185 Roma, Italy.*

[4]*Department of Clinical and biological Sciences, University of Torino, S. Luigi Hospital Regione Gonzole, 10/1 – 10043 Orbassano (To), Italy*

10:45-11:15 **Coffee break**

Plenary session

Auditorium and (by streaming) Theater

Analytical spectroscopy (AS)

Mass spectrometry (MS)

Chairmen: Gianpiero Adami, Achille Cappiello

11:15-11:30 **O4 AS** XPS CHARACTERIZATION OF POLYDOPAMINE LAYERS FOR IMPROVING SURFACE BIOMOLECULE IMMOBILIZATION

E. Mazzotta[1], S. Rella[1], A. Caroli[1], M. De Luca[2], C. Bucci[2], C. Malitesta[1]

[1]*Laboratorio di Chimica Analitica, Dipartimento di Scienze e Tecnologie Biologiche ed Ambientali, Università del Salento, Via Monteroni – 73100 Lecce, Italy*

[2]*Laboratorio di Biologia Cellulare, Dipartimento di Scienze e Tecnologie Biologiche ed Ambientali, Università del Salento, Via Monteroni – 73100 Lecce, Italy*

11:30-11:45 **O5 AS** STREPTAVIDIN-COATED GOLD NANOPARTICLES: CRITICAL ROLE OF OLIGONUCLEOTIDES ON STABILITY AND LINEAR AGGREGATION

R. D'Agata[1], P. Palladino[2], G. Spoto[1,2]

[1]*Department of Chemical Sciences, University of Catania, Viale Andrea Doria 6, 95125, Italy*

[2]*I.N.B.B. c/o Department of Chemical Sciences, University of Catania, Viale Andrea Doria 6, 95125, Catania, Italy*

11:45-12:00 **O1 MS** FAST DILUTE-AND-SHOOT APPLICATIONS USING AN LEI LC-MS INTERFACE

M. Piergiovanni, V. Termopoli, G. Famiglini, P. Palma and A. Cappiello

Department of Pure and Applied Sciences "DiSPeA", University of Urbino "Carlo Bo" Piazza Rinascimento 6 - 61029 Urbino, Italy

12:00-12:15 **O2 MS** LIPIDOMIC ANALYSIS OF TISSUE FROM HIGH FAT AND HIGH FRUCTOSE DIET TREATED MICE

F. Dal Bello[1], M. Zorzi[1], R. Aigotti[1], R. Mastrocola[2], C. Medana[1]

[1]*Department of Molecular Biotechnology and Health Sciences - University of Turin, Via Pietro Giuria, 5 - 10125 Torino, Italy.*

[2]*Department of Clinical and Biological Sciences - University of Turin, Corso Raffaello, 30 – 10125 Torino, Italy*

12:15-12:30 **O1 SP** BIO/NANO TECHNOLOGIES: HOW TO CHARACTERIZE SIZE AND NUMBER CONCENTRATION IN LIQUID MATRICES

R. Santoliquido

Alfatest Srl, Via Giulio Pittarelli, 97 - 00166 Rome, Italy

12:30-12:45 **O2 SP** HIGH PURITY WATER FOR ADVANCED ANALYTICAL TECHNIQUES

E. Pirovano

Merck S.p.A., Via Monte Rosa 93, 20149 milano, Italy

12:45-13:45 **Lunch**

13:45-14:45 **Assembly GI Sensors**
Auditorium
Assembly GI Separation sciences
Theater
Assembly GD Chemometry
Seminar room

14:45-15:45 **Assembly GD Analytical spectroscopy**
Auditorium
Assembly GD Forensic analytical chemistry
Seminar room

16:00 **Departure for social events (FICO, Ducati Museum, Bologna experience)**

Wednesday, September 19

Plenary session

Auditorium and (by streaming) Theater

Chemometrics, "big data", data quality (CB)

Green chemistry (GC)

Chairmen: Federico Marini, Marina Cocchi

9:00-9:40	**PL3** ENVIRONMENTAL CHEMOMETRICS R. Tauler *Spanish Council of Scientific Research*
9:40-9:55	**O1 CB** SO-COVSEL: A NOVEL METHOD FOR VARIABLE SELECTION IN MULTIBLOCK DATA A. Biancolillo[1,2], F. Marini[1], J-M. Roger[2] *[1]University of Rome La Sapienza, Piazzale Aldo Moro 5, I-00185, Rome, Italy* *[2] ITAP, Irstea, Montpellier SupAgro, Univ Montpellier, Montpellier, France*
9:55-10:10	**O2 CB** CHEMICAL MODIFICATIONS OF RICE GERM DURING STORAGE: FOCUSING ON WATER BY THE AQUAPHOTOMICS APPROACH C. Malegori[1], P. Oliveri[1], R. Tsenkova[2], C. Cappa[3], M. Lucisano[3] *[1]DIFAR Department of Pharmacy, University of Genova – Genova – Italy* *[2]Bio Measurement Technology Lab, Kobe University – Kobe – Japan* *[3]DeFENS Department of Food, Environmental and Nutritional Sciences, Università degli Studi di Milano – Milano – Italy*
10:10-10:25	**O3 CB** MULTIVARIATE CLASSIFICATION OF CHIANTI RED WINES BASED ON MASSIVE SAMPLING AND ICP-MS ELEMENT COMPOSITION D. Ballabio[1], B. Bronzi[2], C. Brilli[2], G.M. Beone[3], M.C. Fontanella[3], R. Todeschini[1], V. Consonni[1] *[1]Department of Earth and Environmental Sciences, University of Milano - Bicocca, P.zza della Scienza 1, 20126 Milano, Italy* *[2]Ruffino, P.le Ruffino 1, 50065 Pontassieve, Italy* *[3]Facoltà di Scienze Agrarie, Alimentari e Ambientali, Università Cattolica del Sacro Cuore, Via Emilia Parmense 84, 29122 Piacenza, Italy*
10:25-10:40	**O1 GC** PHOTOCATALYTIC HYDROGEN EVOLUTION FROM (WASTE) AQUEOUS BIOMASS UNDER SIMULATED SOLAR LIGHT: TITANIUM DIOXIDE VS. GRAPHITIC CARBON NITRIDE A. Speltini, F. Gualco, F. Maraschi, M. Sturini, D. Dondi, L. Malavasi, A. Profumo *Department of Chemistry, University of Pavia, Via Taramelli, 12 – 27100 Pavia, Italy*
10:40-10:45	**F1 GC** CADMIUM UPTAKE AND DIFFUSION IN BIVALVE MOLLUSK SHELLS FROM AQUEOUS MATRICES – AN LA-ICP-MS LINE SCAN AND ELEMENT IMAGING STUDY T. Chenet[1], G. Schwarz[2], M. Burger[2], B. Hattendorf[2], D. Günther[2], C.

Stevanin[1], A. Cavazzini[1], L. Pasti[1]
[1]*Department of Chemistry and Pharmaceutical Sciences, University of Ferrara, Via Borsari, 46 - 44121 Ferrara, Italy*
[2]*Laboratory of Inorganic Chemistry, ETH Zürich, Vladimir-Prelog-Weg, 1 - 8093 Zürich, Switzerland*

10:45-11:15 **Coffee break**

Plenary session

Auditorium and (by streaming) Theater

Solution equilibria and speciation (EQ)
Environment and cultural heritage (EC)

Chairmen: Giuseppe Arena, Concetta De Stefano, Piergiuseppe Daniele

11:15-11:35 **KN5** USE OF GANTREZ™ COPOLYMERS AS POTENTIAL CHELATING AGENTS FOR THE SELECTIVE SEQUESTRATION OF METAL IONS
F. Crea
Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, Università degli Studi di Messina. Viale F. Stagno. D'Alcontres, 31 – 98166 Messina, Italy

11:35-11:50 **O1 EQ** CURCUMIN AS POTENTIAL CHELATING AGENT TOWARDS Al(III) AND Fe(III)
E. Furia, A. Beneduci, L. Di Donna
Department of Chemistry and Chemical Technologies, University of Calabria, Via P. Bucci, 12/D - 87036 Rende (CS), Italy

11:50-12:05 **O2 EQ** INORGANIC ARSENIC SPECIATION IN WATER SAMPLES: AN ULTRAFAST METHOD BASED ON FRONTAL CHROMATOGRAPHY/ICP-MS
D. Spanu, M. Pinna, C. Dossi, S. Recchia
Department of Science and High Technology, University of Insubria, Via Valleggio, 11 - 22100 Como, Italy

12:05-12:20 **O3 EQ** EXPLORING VARIOUS LIGAND CLASSES FOR THE EFFICIENT SEQUESTRATION OF STANNOUS CATIONS IN THE ENVIRONMENT
C. Bretti, P. Cardiano, R. M. Cigala, C. De Stefano, A. Irto, G. Lando, S. Sammartano
Department of Chemical, Biolofical, Pharmaceutical and Environmental Science. University of Messina, Viale Ferdinando Stagno d'Alcontres, 31 - 98166 Messina, Italy

12:20-12:25 **F1 EQ** CALIXARENE-BASED SUPRAMPHIPHILES IN NEUTRAL BUFFERED SOLUTION: DETERMINATION OF CMC AND ΔH_{mic} BY A SINGLE EXPERIMENT
R. Migliore, C. Sgarlata, G. Arena
Department of Chemical Sciences, University of Catania, Viale Andrea Doria 6, 95125 Catania, Italy

12:25-12:30 **F2 EQ** SPECIATION STUDY OF A BIS-(3-HYDROXY-4-PYRIDINONE) TOWARDS M^{2+}
P. Cardiano[1], K. Chand[2], R. M. Cigala[1], F. Crea[1], C. De Stefano[1], G. Gattuso[1], A. Irto[1], S. Sammartano[1], M. A. Santos[2]
[1]*Department of Chemical, Biological, Pharmaceutical and Environmental Sciences – University of Messina, Viale F. Stagno d'Alcontres, 31 – 98166 Messina, Italy*
[2]*Centro de Química Estrutural, Instituto Superior Técnico, University of Lisbon, Av. Rovisco*

Pais 1, 1049-001 Lisbon, Portugal

12:30-12:50 **KN6** CHEMICAL COMPOSITION OF ATMOSPHERIC AEROSOL AND SURFACE SNOW AT DOME C (EAST ANTARCTIC ICE SHEET): AN OVERVIEW FROM 10-YR LONG RECORDS

R. Traversi[1], S. Becagli[1], L. Caiazzo[1], M. Busetto[2], F. Calzolari[2], P. Cristofanelli[2], B. Petkov[2], M. Severi[1]

[1]*Chemistry Dept. "Ugo Schiff", University of Florence, Sesto F.no, Florence (Italy)*

[2]*ISAC-CNR (Institute of Atmospheric Sciences and Climate – National Research Council of Italy), Bologna (Italy)*

12.50-13:05 **O3 EC** UNVEILING RISKS CONCEALED IN TEXTILES

C. Crescenzi[1], P. Russo[1], G. Luongo[2], F. Iadaresta[3], J. Holmbäck[3], C. Östman[3]

[1]*Department of Pharmacy - University of Salerno, Via Giovanni Paolo II, 132 - 84084 Fisciano (SA), Italy*

[2]*Unidad de Hepatología Exparimental, Instituto de Investigación Sanitaria Fundación Hospital La Fe, Avinguda de Fernando Abril Martorell, 106 - 46026 València, Spain*

[3]*Department of Environmental Science and Analytical Chemistry – Stockholm University, Svante Arrhenius väg 8, SE-11418 Stockholm, Sweden*

13:05-13:20 **O4 EC** SELECTIVE EXTRACTION OF WATER-SOLUBLE THALLIUM FRACTION FROM CONTAMINATED DRINKING-WATER DISTRIBUTION NETWORKS: OPTIMIZATION OF THE PROCEDURE AND EXTRACTS SPECIATION

E. Veschetti[1], M. Le Donne[1,2], C. Sette[1,2], L. Lucentini[1], G. Favero[2]

[1]*Department of Environment and Health, Istituto Superiore di Sanità, Viale Regina Elena, 299, 00161, Rome, Italy*

[2]*Department of Chemistry and Drug Technologies, SAPIENZA University of Rome, P.le A. Moro 5, 00185, Rome, Italy*

13:20-13:35 **O3 SP** PYROLYSIS GC-MS FOR IDENTIFICATION AND CHARACTERIZATION OF UNKNOWN POLYMERIC MATERIAL USED FOR BIODEGRADABLE PACKAGING AND MEMBRANE (DIAPHRAGM) PUMPS

M. Soll[1], I. Watanabe[1], T. Ramus[2], I. Iwai[2]

[1]*Frontier Laboratories LTD, Koriyama, Fukushima 963-8862, Japan*

[2]*Diablo Analytical, Inc., 5141 Lone Tree Way, Antioch, CA 94531, USA*

13:35-15:00 **Lunch**

13:35-15:00 **Poster session II**

Theater

Regular posters: P075 – P149

Flash communication posters: PF1 GC, PF1 EQ, PF2 EQ, PF1 CB, PF5 – PF7 SB, PF1 EL, PF2 EL, PF1 AB

Parallel session

Auditorium

Chemometrics, "big data", data quality (CB)
Environment and cultural heritage (EC)

Chairmen: Patrizia Romana Mussini, Paolo Ugo

15:00-15:15 **O4 CB** SMARTPHONE-BASED DETERMINATION OF GRAPE PHENOLIC

	MATURITY R. Calvini, G. Orlandi, G. Foca, G. Montevecchi, F. Masino, A. Antonelli, A. Ulrici *Department of Life Sciences and Interdepartmental Research Centre BIOGEST-SITEIA, University of Modena and Reggio Emilia, Pad. Besta Via Amendola, 2 – 42122 Reggio Emilia, Italy*
15:15-15:20	**F1 CB** NEAR-INFRARED BASED DETECTION OF INSECTS INFESTATION IN RICE SAMPLES A. Biancolillo, P. Firmani, R. Bucci, A. Magrì, F. Marini *Department of Chemistry "Stanislao Cannizzaro", La Sapienza - University of Rome, P.le Aldo Moro, 5 – 00185 Rome, Italy*
15:20-15:35	**O5 CB** PREDICTION OF ODOUR CONCENTRATION BY USE OF SUPERVISED KOHONEN NETWORKS ON ELECTRONIC NOSE SIGNAL RECORDS OF ODORANT SAMPLES AND REAL ENVIRONMENT AIR SAMPLES S. Licen[1], S. Cozzutto[2], G. Barbieri[2], P. Barbieri[1] *[1]Department of Chemical and Pharmaceutical Sciences, University of Trieste, Via L. Giorgieri 1, 34127 Trieste, Italy* *[2] ARCO SolutionS s.r.l., spin-off company of the Dept. of Chemical and Pharmaceutical Sciences, University of Trieste, Via L. Giorgieri 1, 34127 Trieste, Italy*
15:35-15:50	**O5 EC** MICROPLASTIC POLLUTION IN ICE, SNOW AND SEDIMENTS FROM VESIJÄRVI AND PIKKU VESIJÄRVI LAKES, FINLAND C. Scopetani[1,3], A. Cincinelli[1,2], D. Chelazzi[2], M. Esterhuizen-Londt[3], T. Martellini[1], S. Pflugmacher[3,4] *[1]Department of Chemistry "Ugo Schiff", University of Florence, 50019 Sesto Fiorentino (Florence), Italy.* *[2]Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), 50019 Sesto Fiorentino (Florence), Italy.* *[3]Faculty of Biological and Environmental Sciences Ecosystems and Environment Research programme Niemenkatu 73, Lahti FI-15140, University of Helsinki Finland.* *[4]Korean Institute of Science & Technology (KIST Europe) Environmental Safety Group Joint Laboratory of Applied Ecotoxicology Campus E 7.1 66123 Saarbrücken, Germany*
15:50-16:05	**O6 EC** ISOTOPIC ANALYSIS OF ANTARCTIC SNOW BY QUADRUPOLE INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY USING A TOTAL-CONSUMPTION SAMPLE INTRODUCTION SYSTEM F. Ardini, M. Grotti *Department of Chemistry and Industrial Chemistry, University of Genoa, Via Dodecaneso, 31 - 16146 Genoa, Italy*
16:05-16:20	**O7 EC** MINIATURIZED BIOSENSORS TO PRESERVE AND MONITOR CULTURAL HERITAGE: FROM MEDICAL TO CONSERVATION DIAGNOSIS G. Sciutto[1], M. Zangheri[1], L. Anfossi[2], M. Guardigli[1], S. Prati[1], M. Mirasoli[1], F. Di Nardo[2], C. Baggiani[2], R. Mazzeo[1], A. Roda[1] *[1]Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna, Via Selmi, 2 - 40126 Bologna, Italy* *[2]Department of Chemistry, University of Torino, Via P. Giuria 7- 10125 Torino, Italy*
16:20-16:35	**O8 EC** CHARACTERIZATION AND TEMPORAL EVOLUTION OF THE ELEMENTAL COM-POSITION OF PM_{10} COLLECTED AT NY-ÅLESUND (THE ARCTIC)

E. Conca[1], O. Abollino[1], A. Giacomino[2], S. Buoso[1], A. Ruo Redda[2], R. Traversi[3], S. Becagli[3], M. Grotti[4], M. Malandrino[1]
[1]*Department of Chemistry, University of Turin, Via P. Giuria 5 - 10125 Turin, Italy*
[2]*Department of Drug Science and Technology, University of Turin, Via P. Giuria 5 - 10125 Turin, Italy*
[3]*Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia, 3-13 - 50019 Sesto Fiorentino, Italy*
[4]*Department of Chemistry and Industrial Chemistry, University of Genoa, Via Dodecaneso 31 - 16146 Genoa, Italy*

Parallel session

Theater

Sensors and biosensors, Lab-on-a-chip, POCT (SB)

Chairmen: Maria Minunni, Francesco Ricci

15:00-15.20 **KN7** CONTINUOUS, REAL-TIME MEASUREMENT OF A CANCER CHEMOTHERAPEUTIC IN A LIVING BODY USING ELECTROCHEMICAL APTAMER-BASED SENSORS AND A NOVEL DRIFT CORRECTION APPROACH

A. Idili,[1,2] N. Arroyo-Currás,[1,2] K. L. Ploense,[1,2] A. T. Csordas,[1,2] K. Plaxco[1,2]
[1]*Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106*
[2]*Center for Bioengineering, University of California, Santa Barbara, CA 93106*

15:20-15:35 **O12 SB** MICRONEEDLE-BASED BIOSENSOR FOR MINIMALLY-INVASIVE LACTATE DETECTION

R. Antiochia[1], S. Sharma[2], A.E.G. Cass[3], P. Bollella[1]
[1]*Department of Chemistry and Drug Technologies - Sapienza University of Rome, Rome, Italy*
[2]*College of Engineering - Swansea University, Swansea, Wales*
[3]*Department of Chemistry & Institute of Biomedical Engineering - Imperial College, London, UK*

15:35-15:50 **O13 SB** DISPOSABLE pH BIOSENSOR FOR UREA MEASUREMENT

A. Bonini[1], E. Herrera[1], F. Vivaldi[1], B. Melai[1], N. Poma[1], P. Salvo[2], A. Kirchhain[1], F. Di Francesco[1]
[1]*Department of Chemistry and Industrial Chemistry, University of Pisa, Via Moruzzi, 13 - 56124 Pisa, Italy*
[2]*Institute of Clinical Physiology, National Research Council, Via Moruzzi, 3 - 56124 Pisa, Italy*

15:50-16:05 **O14 SB** PROXIMITY-BASED OPTICAL AND ELECTROCHEMICAL PLATFORMS FOR THE RAPID, SINGLE-STEP DETECTION OF ANTIBODIES IN BODILY FLUIDS

A. Porchetta[1], M. Rossetti[1], R. Ippodrino[2], B. Marini[2], G. Palleschi[1], F. Ricci[1]
[1]*Department of Chemistry, University of Rome "Tor Vergata", Via della Ricerca Scientifica, 1 - 00133 Rome, Italy*
[2]*Ulisse BioMed S.r.l., Area Science Park, 34149 Trieste, Italy*

16:05-16:10 **F5 SB** DEVELOPMENT OF A REFLECTANCE SMARTPHONE PAPER-BASED CHEMOSENSOR FOR THE EVALUATION OF ANTIOXIDANT ACTIVITY BY IN SITU GOLD-NANOPARTICLES SYNTHESIS

D. Calabria, C. Caliceti, M. Zangheri, E. Porru, M. Mirasoli, M. Guardigli, P.

	Simoni, A. Roda *Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna, Via Selmi 2 - 40126 Bologna, Italy*
16:10-16:15	**F6 SB** ENVIRONMENTAL AND OPERATIONAL STABILITY OF ORGANIC FIELD EFFECT TRANSISTORS FOR BIOSENSING APPLICATIONS R.A. Picca[1], E. Macchia[1], K. Manoli[1], C. Di Franco[2], G. Palazzo[1], N. Cioffi[1], G. Scamarcio[2,3], L. Torsi[1] *[1]Dipartimento di Chimica - Università degli Studi di Bari "Aldo Moro", Via E. Orabona, 4 - 70126 Bari, Italy* *[2]CNR-IFN U.O.S. Bari, via Amendola 173 - 70126 Bari, Italy* *[3]Dipartimento Interateneo di Fisica "M. Merlin" - Università degli Studi di Bari "Aldo Moro", via Amendola 173 - 70126 Bari, Italy*
16:15-16:20	**F7 SB** POLYDOPAMINE: MOLECULAR IMPRINTING, PLASMONS AND CATALYSIS P. Palladino**,** A. Brittoli, E. Pascale, S. Scarano, M. Minunni *Department of Chemistry "Ugo Schiff"- University of Florence, Via della Lastruccia, 3-13 - 50019 Sesto Fiorentino (FI), Italy*
16:20-16:35	**O15 SB** AN INTEGRATED IOT-WIFI BOARD CONNECTED WITH AN INNOVATIVE IMMUNOSENSOR FOR REMOTE DATA ACQUISITION. CASE OF STUDY: DIAGNOSIS OF CELIAC DISEASE M. Giannetto[1], V. Bianchi[2], S. Gentili[1], S. Fortunati[1], I. De Munari[2], M. Careri[1] *[1]Department of Chemistry, Life Sciences and Environmental Sustainability - University of Parma, Parco Area delle Scienze 17/A - 43124 Parma, Italy* *[2]Department of Engineering and Architecture - University of Parma, Parco Area delle Scienze 181/A – 40124 Parma, Italy*

16:35-17:05 **Coffee break**

Parallel session

Auditorium

Environment and cultural heritage (EN)
Electroanalytics, electrophotoanalytics (EL)

Chairmen: Claudio Minero, Carlo Dossi

17:05-17:20	**O9 EC** REMOVAL OF HEAVY METALS FROM CONTAMINATED ZEOLITIC TUFF WITH (S,S) ETHYLENEDIAMINE-N,N'-DISUCCINIC ACID G. De Tommaso[1], R. Andreozzi[2], F. Di Duca[1], M. Iuliano[1], R. Marotta[2] *[1]Department of Chemical Sciences, University of Naples "Federico II" Via Cupa Nuova Cintia, 21 - 80126 Naples (Italy)* *[2]Department of Chemical Engineering, Materials and Industrial Production, University of Naples "Federico II" P.le V. Tecchio 80 80125 Naples (Italy)*
17:20-17:35	**O10 EC** IDENTIFICATION AND QUANTIFICATION OF SYSTEMIC INSECTICIDES AND THEIR METABOLITES BY UHPLC-HRMS A. Lentola[1,2], S. Bogialli[1], A. Tapparo[1] *[1]Department of Chemical Sciences, University of Padova, via Marzolo 1 - 35131 Padova, Italy* *[2]Laimburg Research Centre, Laimburg 6 - 39040 Auer, Bozen, Italy*
17:35-17:50	**O1 EL** DETERMINATION OF ULTRATRACE IRON IN SEAWATER: NEW

	DEVELOPMENTS OF A CATALYTIC ADSORPTIVE STRIPPING VOLTAMMETRY METHOD F. Sanvito, L. Pacileo, D. Monticelli *Dipartimento di Scienza e Alta Tecnologia -Università degli Studi dell'Insubria, Via Valleggio, 11 - 22100 Como, Italy*
17:50-18:05	**O2 EL** WIDE-SCOPE ENANTIOSELECTIVE VOLTAMMETRY: TESTING INHERENTLY CHIRAL SELECTORS WITH CHIRAL PROBES REPRESENTATIVE OF DIFFERENT STEREOGENIC ELEMENTS P. R. Mussini[1], S. Arnaboldi[1], S. Grecchi[1] M. Magni[1], G. Tomboni[1], F. Sannicolò[1], T. Benincori[2], S. Rizzo[3], R. Cirilli[4], H. Lang[5], M. Korb[5] *[1]Università degli Studi di Milano, Dipartimento di Chimica, Via Golgi 19,20133 Milano* *[2]Univ. degli Studi dell'Insubria, Dip. Scienza e Alta Tecnologia, Via Valleggio 11, 22100 Como* *[3]CNR ISTM, Via Golgi 19, 20133 Milano* *[4]Ist. Superiore di Sanità, Dipartimento del Farmaco Viale Regina Elena 299, 00161 Roma* *[5]Technische Universität Chemnitz, Straße der Nationen 62, 09111 Chemnitz, Germany*
18:05-18:10	**F1 EL** SINGLE CELL ELECTROCHEMILUMINESCENCE IMAGING: FROM THE PROOF-OF-CONCEPT TO DISPOSABLE DEVICE-BASED ANALYSIS G. Valenti[1], S. Voci[2], A. Zanut[1], M. Zangheri[1], S. Scarabino[2], B. Goudeau[2], A. Lesch[3], M. Jović[3], M. Mirasoli[1], S. Rapino[1], S. Arbault[2], A. Roda[1], N. Sojic[2], F. Paolucci [1] *[1]Department of Chemistry "Giacomo Ciamician", Alma Mater Studiorum - University of Bologna, Via Selmi, 2 - 40126 Bologna, Italy* *[2]University of Bordeaux, Bordeaux INP, ISM, UMR CNRS 5255, 33607 Pessac, France.* *[3]Laboratory of Physical and Analytical Electrochemistry, EPFL Valais Wallis, CH-1951 Sion, Switzerland*
18:10-18:15	**F2 EL** OPTIMIZING THE ELECTRODEPOSITION PROTOCOL OF ENANTIOSELECTIVE INHERENTLY CHIRAL ELECTRODE SURFACES: A MULTI-TECHNIQUE INVESTIGATION S. Arnaboldi[1], M. Magni[1], P. Mussini[1], T. Benincori[2], S. Cauteruccio[1] *[1]Università degli Studi di Milano, Dipartimento di Chimica, Via Golgi 19, 20133, Milano, Italy* *[2]Università degli Studi dell'Insubria, Dipartimento di Chimica, Via Valleggio 11, 22100, Como, Italy*

Parallel session

Theater

Analytical biotechnology (AB)

Bioanalytics and "-omics" (BO)

Chairmen: Mara Mirasoli, Claudio Baggiani

17:05-17:20	**O1 AB** DYNAMIC DNA AND RNA NANOTECHNOLOGY FOR BINDING-RESPONSIVE BIOMOLECULAR SENSING A. Bertucci[1,2], A. Porchetta[1], J. Guo[2], N. Oppmann[2], F. Caruso[2], F. Cavalieri[1,2], F. Ricci[1] *[1]Department of Chemical Sciences and Technologies, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy* *[2]Department of Chemical and Biomolecular Engineering, The University of Melbourne, Parkville, Victoria 3010, Australia*
17:20-17:35	**O2 AB** A GC/MS APPROACH FOR THE SCREENING OF BIOACTIVE SECONDARY

	METABOLITES PRODUCED BY FUNGAL STRAINS M.M. Salvatore[1], M. Ciaravolo[1], R. Nicoletti[2,3], M. DellaGreca[1], M. Gallo[4], F. Salvatore[1], D. Naviglio[1], A. Andolfi[1] *[1]Department of Chemical Sciences, University of Naples 'Federico II', Naples 80126, Italy;* *[2]Council for Agricultural Research and Agricultural Economy Analysis, Rome 00184, Italy;* *[3]Department of Agriculture, University of Naples 'Federico II', Portici 80055, Italy;* *[4]Department of Molecular Medicine and Medical Biotechnology, University of Naples "Federico II", 80131 Naples, Italy*
17:35-17:40	**F1 AB** AN ANALYTICAL STUDY OF THE INFLUENCE OF CHITOSAN FEATURES ON THE CHEMICAL, PHYSICAL AND MECHANICAL AND IN-VITRO PROPERTIES OF 3D PRINTED SCAFFOLDS C. Intini, C. Bergonzi, A. Bianchera, R. Bettini, L. Elviri *Department of Food and Drug Science, University of Parma, Parco Area delle Scienze 27/A, 43124, Parma, Italy*
17:40-17:55	**O4 BO** MICRO EXTRACTION BY PACKED SORBENT COUPLED TO LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY FOR THE ANALYSIS OF PROSTANOIDS AND ISOPROSTANOIDS IN DRIED BLOOD SPOTS D. Biagini[1], S. Antoni[1], T. Lomonaco[1], S. Ghimenti[1], F. G. Bellagambi[1], A. Cuttano[2], R. T. Scaramuzzo[2], M. Ciantelli[2], F. Di Francesco[1], R. Fuoco[1] *[1]Department of Chemistry and Industrial Chemistry, University of Pisa, Via Moruzzi, 13 - 56124 Pisa, Italy* *[2]Division of Neonatology, Santa Chiara Hospital, University of Pisa, Via Roma, 67 – 56124 Pisa, Italy*
17:55-18:10	**O5 BO** IMPROVING LC-MS DETECTION OF PHOSPHOLIPIDS BY MOLECULARLY DESIGNED CLASS SELECTIVE SPE SORBENTS G. Grasso[1,2], S. Shinde[3], C. Crescenzi[1], B. Sellergren[3] *[1]Department of Pharmacy, University of Salerno, Via Giovanni Paolo II, 132 - 84084 Fisciano (SA), Italy* *[2]PhD Program in "Drug Discovery and Development", University of Salerno, Via Giovanni Paolo II, 132 - 84084 Fisciano (SA), Italy* *[3]Biofilm Research Centre, Department of Biomedical Sciences, Malmö University, Per Albin Hanssons väg, 35 - SE 20506 Malmö, Sweden*

20:00 **Social Dinner and awarding of the Best Posters and Best Flash Communications**

Palazzo Isolani – Piazza delle Sette Chiese

Thursday, September 20

Plenary session

Auditorium and (by streaming) Theater

Mass spectrometry (MS)

Electroanalytics, electrophotoanalytics (EL)

Chairmen: Danila Moscone, Tommaso Cataldi

9:30-10:10	**PL4** UN NUOVO MODELLO PER L'AGGIORNAMENTO E LA RAZIONALIZZAZIONE DELLA CLASSIFICAZIONE DEI SAPERI ACCADEMICI E DEL SISTEMA DELLE CLASSI DI CORSO DI STUDIO M. R. Tinè *Department of Chemistry, University of Pisa, via Risorgimento 35, 56126 Pisa, Italy*
10:10-10:30	**KN8** STRUCTURAL CHARACTERIZATION OF GLYCOSPHINGOLIPIDS BY MULTIPLESTAGE LINEAR ION TRAP MASS SPECTROMETRY C. D. Calvano[1,2], A. M. Sardanelli[3], M. Glaciale[1], G. Ventura[1], V. Addabbo[1], F. Palmisano[1,2], T.R.I. Cataldi[1,2] [1]*Dipartimento di Chimica and* [2]*Centro Interdipartimentale di Ricerca SMART, Università di Bari Aldo Moro, via Orabona 4, 70126, Bari, Italy* [3]*Dipartimento di Scienze mediche di base, neuroscienze e organi di senso, Università di Bari Aldo Moro, Piazza G. Cesare 11, 70120 Bari*
10:30-10:45	**O3 MS** LC-MS BASED STRATEGIES FOR THE COMPREHENSIVE ANALYSIS OF MARINE TOXINS IN ENVIRONMENTAL AND FOOD MATRICES C. Dell'Aversano, L. Tartaglione *Department of Pharmacy, School of Medicine and Surgery, University of Napoli Federico II, Via D. Montesano 49, 80131, Napoli, Italy*
10:45-11:00	**O4 MS** HIDDEN SOURCES OF BISPHENOL A FROM FOOD CONTACT MATERIALS A. Cavazza, C. Bignardi, P. Salvadeo, C. Corradini *Department of Chemistry, Life Sciences, and Environmental Sustainability - University of Parma, Parco Area delle Scienze 17/A - 43124 Parma, Italy*
11.00-11:15	**O3 EL** MULTIPLE PAPER-BASED ELECTROCHEMICAL BIOSENSORS FOR PESTICIDE DETECTION F. Arduini[1], V. Caratelli[1], S. Cinti[1], L. Amendola[2], G. Palleschi[1], D. Moscone[1] [1]*Department of Chemical Science and Technologies, University of Rome "Tor Vergata", Via della Ricerca Scientifica, 00173 Rome, Italy* [2] *ArpaLazio, Via Giuseppe Saredo 52, 00173, Rome, Italy*
11:15-11:30	**O4 EL** NANOSTRUCTURED TIO2 ELECTRODES FOR PHOTO-ELECTROCHEMICAL BIOSENSING OF NUCLEIC ACIDS F. Bettazzi[1], V. Pifferi[2], L. Falciola[2], C. Ingrosso[3], L. Curri[3], I. Palchetti[1] [1]*Department of Chemistry "Ugo Schiff", Via della Lastruccia 3, 50019 Sesto Fiorentino (Fi), Italy;*

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11.30-11:45	**O5 EL** PREPARATION AND CHARACTERIZATION OF NOVEL SONOGEL-CARBON ELECTRODES CONTAINING CARBON BLACK: APPLICATION AS AMPEROMETRIC SENSORS FOR DETERMINATION OF POLYPHENOLIC COMPOUNDS L. Pigani[1], C. Rioli[1], D. López Iglesias[2], J. García Guzmán[2], L. Cubillana Aguilera[2], J. Palacios Santander[2], F. Terzi[1], C. Zanardi[1] [1]*Department of Chemical and Geological Sciences, Unveristy of Modena and Reggio Emilia, Via G. Campi, 103 – 41125 Modena, Italy* [2]*Institute of Research on Electron Microscopy and Materials, University of Cadiz, Campus Universitario de Puerto Real, Polígono del Río San Pedro, S/N, 11510 Puerto Real, Cadiz, Spain*
11.45-12:00	**O6 EL** LAYERED DOUBLE HYDROXIDES AS ELECTRODE MODIFIERS FOR (BIO)SENSING APPLICATIONS D. Tonelli, E. Scavetta, I. Gualandi, M. Giorgetti, E. Musella, F. Mariani Department of Industrial Chemistry "Toso Montanari", Alma Mater *Studiorum - University of Bologna, Viale del Risorgimento, 4 - 40136 Bologna, Italy*

12:00-13:00 **Lunch**

Plenary session

Auditorium and (by streaming) Theater

Environment and cultural heritage (EC)

Sensors and biosensors, Lab-on-a-chip, POCT (SB)

Chairmen: Elisa Michelini

13:00-13:15	**O11 EC** EXPERIMENTAL METHODOLOGY TO MEASURE THE REACTION RATE CONSTANTS OF PROCESSES SENSITIZED BY THE TRIPLET STATE OF 4-CARBOXYBENZOPHENONE AS PROXY OF THE TRIPLET STATES OF CHROMOPHORIC DISSOLVED ORGANIC MATTER M. Minella[1], L. Rapa[1], L. Carena[1], M. Pazzi[1], V. Maurino[1], C. Minero[1], M. Brigante[2], D. Vione[1] [1]*Department of Chemistry, University of Torino, Via P. Giuria, 5 - 10125 Torino, Italy* [2]*Université Clermont Auvergne, CNRS, Sigma Clermont, Institut de Chimie de Clermont-Ferrand, F-63000 Clermont-Ferrand, France*
13:15-13:30	**O12 EC** FRAGRANCES AS NEW ENVIRONMENTAL CONTAMINANTS M. Vecchiato[1], E. Barbaro[2], E. Gregoris[1], A. Spolaor[2], C. Turetta[2], C. Barbante[1,2], R. Piazza[1,2], A. Gambaro[1,2] [1]*Department of Environmental Sciences, Informatics and Statistics (DAIS), Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia-Mestre, Venice, Italy* [2]*Institute for the Dynamics of Environmental Processes (IDPA-CNR), Via Torino 155, 30172 Venezia-Mestre, Venice, Italy*
13:30-13:45	**O13 EC** CHEMICAL COMPOSITION OF ATMOSPHERIC AEROSOL IN ANTARCTICA S. Illuminati**,** A. Annibaldi, C. Truzzi, G. Scarponi

	Department of Life and Environmental Sciences, Università Politecnica delle Marche, Ancona, Via Brecce Bianche, 60131 Ancona, Italy
13:45-14:00	**O16 SB** NON-SPHERICAL GOLD NANOPARTICLES: A VERSATILE COLORIMETRIC PROBE FOR AGGREGATION-BASED ASSAY AND POINT-OF-NEED TEST L. Anfossi, F. Di Nardo, S. Cavalera, C. Giovannoli, G. Spano, C. Baggiani *Department of Chemistry, University of Turin, Via P. Giuria, 5 – 10125 Torino, Italy*
14:00-14:15	**O17 SB** CARBON BLACK-MoS_2 NANOCOMPOSITE AS NOVEL SCREEN-PRINTED ELECTRODES MODIFIER D. Rojas[1,2], F. Della Pelle[1], M. Del Carlo[1], D. Compagnone[1] [1]*Faculty of Bioscience and Technology for Food, Agriculture and Environment, University of Teramo, 64100, Teramo, Italy* [2]*Department of Analytical Chemistry, Physical Chemistry and Chemical Engineering, Faculty of Biology, Environmental Sciences and Chemistry, University of Alcalá, E-28871 Alcalá de Henares, Madrid, Spain*

14:15 **Closing Remarks**
Auditorium

Poster Session I

Monday, September 17

Theater

Regular posters

P001 – P003, P005 – P030, P033 – P074, P130

P001 GOLD NANOPARTICLES@POLYDOPAMINE FILMS AS INNOVATIVE NANOMATERIALS FOR p-NITROPHENOL DETERMINATION IN URINE

A. Brittoli, E. Pascale, P. Palladino, S. Scarano*, and M. Minunni*

Department of Chemistry "Ugo Schiff", Alma Mater Studiorum - University of Florence, Via della Lastruccia, 3-13 - 50019 Sesto Fiorentino (FI), Italy

P002 SPUTTERING-ENABLED INTRACELLULAR X-RAY PHOTOELECTRON SPECTROSCOPY (SEI-XPS): A VERSATILE METHOD TO ANALYZE THE BIOLOGICAL FATE OF METAL NANOPARTICLES. INVESTIGATION OF AG AND PT CASES

Antonio Turco[1], S. Rella[1], M. Moglianetti[2], S. Corvaglia[2], T. Catelani[3], R. Marotta[3], P. P. Pompa[4] and C. Malitesta[1]

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[2]*Istituto Italiano di Tecnologia, Nanobiointeractions&Nanodiagnostics, Center for Bio-Molecular Nanotechnologies, Via Barsanti – 73010 Arnesano (Lecce), Italy*

[3]*Istituto Italiano di Tecnologia, Electron microscopy laboratory, Nanochemistry department, Via Morego 30 – 16163 Genova, Italy*

[4]*Istituto Italiano di Tecnologia, Nanobiointeractions&Nanodiagnostics, Via Morego 30 – 16163 Genova, Italy*

P003 GG-MH HNT HYBRID MULTIFUNCTIONAL MATERIALS FOR CARTILAGE REPAIR: DEVELOPMENT AND ANALYTICAL CHARACTERIZATION

M.A. Bonifacio[1], S. Cometa[2], A. Cochis[3], P. Gentile[4], A.M. Ferreira[4], B. Azzimonti[3], E.Ceci[5], L. Rimondini[3], E. De Giglio[1]

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[5]*Department of Veterinary Medicine, University of Bari "Aldo Moro", S.P. per Casamassima - 70010 Valenzano, Italy*

P005 ELECTRODEPOSITION OF METAL ALLOYS OF TECHNOLOGICAL AND INDUSTRIAL INTEREST

Massimo Innocenti[1,2], Maurizio Passaponti[1], Emanuele Salvietti[1], Riccardo Chelli[1], Antonio De Luca[1], Ferdinando Capolupo[1], Silvano Bellandi[1], Annalisa Guerri[1], Giorgio Federico Signorini[1], Marco Fontani[1], Luca Capaccioli[3], Andrea Capaccioli[3], Paolo Giusti[4] and Andrea Caneschi[5]

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[2] *Institute of Chemistry of Organo-Metallic Compounds, ICCOM-CNR and INSTM Consortium, 50019 Sesto F.no, (FI), Italy*

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[5] *Dipartimento di Ingegneria Industriale, Via Santa Marta 3, 50139 (FI), Italy and INSTM Consortium, 50019 Sesto F.no, (FI), Italy*

P006 SPECTROSCOPIC CHARACTERIZATION OF EXCEPTIONALLY STABLE SILVER NANOPARTICLES SYNTHESIZED BY LASER ABLATION IN ISOPROPYL ALCOHOL

M. C. Sportelli[1], M. Clemente[1], M. Izzi[1], A. Volpe[2], A. Ancona[2], G. Palazzo[1], N. Cioffi[1]
[1]*Dipartimento di Chimica, Università degli Studi di Bari "Aldo Moro", V. Orabona, 4, 70126, Bari, Italy*
[2]*IFN-CNR, Physics Department "M. Merlin", Bari, Italy, via Amendola 173 – 70126 Bari, Italy*

P007 ELONA-BASED APPROACHES FOR THE ANTIBODY-FREE DETECTION OF TROPONIN T, THE KEY BIOMARKER OF ACUTE MYOCARDIAL INFARCTION

F. Torrini, A. Brittoli, P. Palladino, M. Minunni, S. Scarano*
Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia, 3-13, 50019 Sesto Fiorentino (FI), Italy

P008 EDX THICKNESS ANALYSIS OF METAL COATINGS USING MONTE CARLO STANDARDS

W. Giurlani[1], A. De Luca[1], F. Capolupo[1], A. Lavacchi[2], M. Innocenti[1,2]
[1]*Dipartimento di Chimica, Università degli Studi di Firenze, via della Lastruccia 3, 50019 Sesto Fiorentino (FI), Italy*
[2]*Consiglio Nazionale delle Ricerche - Istituto di Chimica dei Composti OrganoMetallici (CNR-ICCOM), via Madonna del Piano 10, 50019 Sesto Fiorentino (FI), Italy*

P009 PM EFFECTS ON METALLIC SURFACES: DEVELOPMENT OF A NEW ACCELERATED AGEING METHODOLOGY

I. Vettori[1], I. Vassura[1], E. Venturini[1], C. Chiavari[2], C. Martini[3], F. Passarini[1], E. Bernardi[1]
[1]*Department of Industrial Chemistry "Toso Montanari", Alma Mater Studiorum - University of Bologna, Viale del Risorgimento, 4 - 40136 Bologna, Italy*
[2]*Department of Cultural Heritage, Alma Mater Studiorum - University of Bologna, Via degli Ariani, 1 - 48121 Ravenna, Italy*
[3]*Department of Industrial Engineering, Alma Mater Studiorum - University of Bologna, Viale del Risorgimento, 4 - 40136 Bologna, Italy*

P010 NIR SPECTROSCOPY, THERMOGRAVIMETRY AND CHEMOMETRICS TO DIFFERENTIATE BURNED AND UNBURNED ANCIENT HUMAN BONES

A. Biancolillo[1], S. Izzo[1], R. Bucci[1], F. Candilio[2], F. Marini[1], M. Tomassetti[1]
[1]*Chemistry Department, University of Rome La Sapienza, P.zzale Aldo Moro 5, I-00185, Rome, Italy*
[2]*Environmetal Biology Department, University of Rome La Sapienza, P.zzale Aldo Moro 5, I-00185, Rome, Italy*

P011 Z POTENTIAL FOR THE EVALUATION OF THE WATER SENSITIVITY IN MODERN OIL PAINTINGS

F. Modugno, J. La Nasa, I. Bonaduce, S. Bianchi, V. Castelvetro
Department of Chemistry and Industrial Chemistry, University of Pisa (Italy)

P012 CHARACTERIZATION OF MATERIALS IN HISTORIC STRINGED MUSICAL INSTRUMENTS BY ANALYTICAL PYROLYSIS GC-MS WITH ON FIBER SILYLATION

L. Kasprzok[1], D. Fabbri[1], A. G. Rombolà[1], M. Malagodi[2], T. Rovetta[2]
[1]*Department of Chemistry "Giacomo Ciamician", University of Bologna, Campus of Ravenna, Via S. Alberto 163, 48100 Ravenna, Italy*
[2]*Laboratorio Arvedi di analisi diagnostiche non invasive, Università degli Studi di Pavia, Museo del Violino, via Bell'Aspa 3, 26100 Cremona, Italy*

P013 DEVELOPMENT OF BIOACTIVE NANOCOMPOSITES FOR THE CONSERVATION OF MURAL PAINTINGS

I.D. van der Werf[1,2], D. Scardigno[1], L. Sabbatini[1,2]

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P014 CHARACTERIZATION OF ARABIC/CHRISTIAN MANUSCRIPTS USING A NON-INVASIVE APPROACH

M. Titubante[1], F. Giannini[1], L. Micheli[1], C. Mazzuca[1], M. Marinelli [2], A. Pasqualucci[2], M. Romani[2], G. Verona-Rinati[2], A. de Fouchier[3], E. Proverbio[3], A. Nuñez Gaitan[3]

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P015 CHASING THE FUGITIVE – THE RED-COLOURED TEXTILES OF PHARAONIC EGYPT

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P016 TARGETED FORENSIC SCREENING AND SEMI-QUANTITATION OF DRUGS IN PLASMA USING HIGH-RESOLUTION ACCURATE-MASS DETECTION AND ONLINE SAMPLE PREPARATION

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P017 PROPOSAL OF A COLOURIMETRIC TOOL FOR PROVIDING ACRYLAMIDE CONTENT IN FOOD PRODUCTS

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P018 TETRADESMUS OBLIQUUS MICROALGAE AS A SOURCE OF BIOACTIVE PEPTIDES: PURIFICATION AND IDENTIFICATION BY MULTIDIMENSIONAL LIQUID CHROMATOGRAPHY - MASS SPECTROMETRY

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P019 TOWARDS A MISPE FOR ROXARSONE: MOLECULARLY IMPRINTED POLYMERS BASED ON TAILOR-MADE MONOMERS FOR THE RECOGNITION OF ORGANO-ARSENIC COMPOUNDS

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P020 SYNTHESIS AND CHARACTERIZATION OF AN IRON (II) CITRATE NEUTRAL COMPLEX TO EVALUATE ITS USE AS A FOOD SUPPLEMENT TO OFFSET IRON DEFICIENCIES

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P021 DISCRIMINATION OF OLIVE TREE VARIETIES INFECTED BY *XYLELLA FASTIDIOSA* USING VOLATILES BY HS-SPME-GC-MS COMBINED WITH MULTIVARIATE STATISTICAL ANALYSIS

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P022 SIMULTANEOUS DETERMINATION OF 12 RED DYES IN MEAT PRODUCTS BY A SIMPLE EXTRACTION FOLLOWED BY HPLC-UV-DIODE ARRAY DETECTION

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P023 STUDY OF LANTHANIDES DISTRIBUTION PATTERN IN DIFFERENT SOIL MIXTURE

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P024 RARE EARTH ELEMENTS ANALYSIS FOR GARLIC ASSESSMENT: THE CASE STUDY OF RED VARIETY CULTIVATED IN ITALY

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P025 BIOACTIVE MOLECULES FROM TOMATO FRUITS AND BY-PRODUCTS

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P026 RELEASE OF HYDROCARBONS FROM FRESH CHEESE PACKAGING

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P027 BIOGENIC AMINES IN TYPICAL ITALIAN CHEESES AND CORRELATION OF THEIR CONTENT TO THE MAIN PROCESSING AND NUTRITIONAL CHARACTERISTICS

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P028 ANALYSIS OF MILK AND NONDAIRY BEVERAGES: METHOD VALIDATION FOR DETERMINATION OF MERCURY BY HYDRIDE GENERATION ATOMIC FLUORESCENCE SPECTROSCOPY AND OF MAJOR AND TRACE ELEMENT BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY

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P029 CORE-SHELL COLUMNS IN THE HPLC DETERMINATION OF ANTIBACTERIAL DRUGS IN FOOD AND FEED

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P030 A NEW RAPID AND GREENER METHOD FOR EXTRACTION OF CANNABINOIDS FROM FLOWERS OF *CANNABIS SATIVA:* COMPARISON BETWEEN THREE VARIETIES OF HEMP

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P033 NUTRACEUTICAL PROPERTIES OF EXTRAVIRGIN OLIVE OIL: OLEOCANTHAL CHARACTERIZATION BY LIQUID CHROMATOGRAPHY-ELECTROSPRAY IONIZATION FOURIER-TRANSFORM MASS SPECTROMETRY

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P034 ANALYSIS OF VOLATILE ORGANIC COMPOUNDS OF HONEY PRODUCED IN TRIESTE KARST AREA BY HS-SPME-GC-MS, EVALUATION OF AN ELECTRONIC NOSE DISCRIMINATION POTENTIAL AND CORRELATION WITH VOCs PRODUCED BY LOCAL BEE HOST PLANTS

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P035 MULTIDIMENSIONAL LIQUID-GAS CHROMATOGRAPHY COUPLED TO A SIMULTANEOUS ISOTOPE RATIO AND QUADRUPOLE MASS SPECTROMETRY FOR OLIVE OIL TRIGLYCERIDES ANALYSIS

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P036 AUTHENTICATION OF TRUFFLES AND PRODUCTS CONTAINING TRUFFLE BY MEANS OF MDGC-C-IRMS / qMS WITH A LOW-BLEED IONIC LIQUID SECONDARY COLUMN

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P037 AN ANALYTICAL STRATEGY FOR MALDI–MS-BASED UNTARGETED METABOLOMICS OF VITREOUS HUMOR TO ESTIMATE POST-MORTEM INTERVAL

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P038 AN USER-FRIENDLY R SHINY APP FOR THE INTERPRETATION OF CHRONIC ALCOHOL ABUSE BIOMARKERS

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P039 DEVELOPMENT OF A INNOVATIVE ANALYTICAL PROCEDURE FOR ORGANIC GUNSHOT RESIDUES (OGSR) INVESTIGATION

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P040 ELECTRODEPOSITED PRUSSIAN BLUE ON CARBON BLACK MODIFIED DISPOSABLE ELECTRODES FOR DIRECT ENZYME-FREEH2O2SENSING IN A PARKINSON'S DISEASE *IN VITRO*MODEL

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P041 EFFECT OF MOBILE IONS IN THE ELECTRON TRANSFER PROCESS IN ENZYME- BASED AMPEROMETRIC SENSORS

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P042 SENSING PLATFORM APPLIED TO OLIVE OILS ANALYSES: SCREEN PRINTED ELECTRODES MODIFIED WITH NANOMATERIALS AND GREEN IONIC LIQUIDS

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P043 ELECTROCHEMICAL PRINTED AND MINIATURISED SENSORS TO EVALUATE THE STATE OF CONSERVATION OF CONCRETE-BASED SAMPLES

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P044 ELECTROCHEMICAL SENSOR FOR NADH DETECTION BASED ON ELECTROCHEMICALLY EXFOLIATED GRAPHENE OXIDE

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P045 AMPEROMETRIC DETECTION OF HISTAMINE WITH A DIAMINE OXIDASE – POLY[(TAT)Ru(TpyCOOH)]$^{2+}$- BASED SENSOR

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P046 CHARACTERIZATION AND APPLICATION OF ELECTROCHEMICAL SENSORS BASED ON CONDUCTING POLYMER NANOCOMPOSITES

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P047 A VERSATILE AND SENSITIVE VERSATILE POINT-OF-CARE TEST FOR THE RAPID DIAGNOSIS OF VISCERAL LEISHMANIASIS

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P048 SCREEN PRINTED ELECTRODES MODIFIED WITH BIOCHAR: TOWARDS A NOVEL ELECTROCHEMICAL PLATFORM

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P049 DISPOSABLE PAPER-BASED SENSOR FOR RAPID FREE CHLORINE DETECTION

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P050 FLUORESCENT DNA-BASED IMMUNOASSAY FOR THE DETECTION OF SMALL MOLECULES

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P051 ANALYTICAL AND ENERGETIC APPLICATIONS USING A YEAST-DMFC DEVICE AND GLUCOSE AS FUEL

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P052 A COMPETITIVE AMPEROMETRIC MAGNETO-IMMUNOSENSING STRATEGY FOR HE4 OVARIAN CANCER BIOMARKER DETECTION

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P053 DEVELOPMENT OF AN ORIGAMI-LIKE REAGENT-FREE ELECTROCHEMICAL BIOSENSOR FOR ON-SITE DETECTION OF SULFUR MUSTARD

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P054 ALIZARINE RED S-BASE RECEPTOR FOR SIMULTANOUES DETERMINATION OF FE(III) AND AL(III)

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P055 ENVIROMENTAL SENSOR FOR HEAVY METAL BASED ON ION IMPRINTED POLYMER

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P056 STUDY OF PROCESS MARKERS DERIVING FROM DRYING TREATMENT OF PASTA USING A PEPTIDE BASED GAS SENSOR

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P057 A POCT FLUORESCENCE-BASED INTEGRATED PLATFORM AGAINST LIFE-THREATENING INFECTIONS

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P058 IMMOBILIZATION OF CARBONIC ANHYDRASE ON AuNPs DEPOSITED ONTO SILANIZED GLASS SUBSTRATE FOR HEAVY METALS DETECTION

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P059 A NOVEL EASY TO USE AND PORTABLE DETECTION TOOL: A LAB-ON-A-TIP DEVICE FOR COPPER DETECTION

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P060 NANOATRAZINE OPTICAL DETECTION FOR SMART AGRICULTURE

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P061 HUMIC ACIDS PYROLYZED ONTO SILICA MICROPARTICLES FOR SPE OF BENZOTRIAZOLES AND BENZOTHIAZOLES FROM ENVIRONMENTAL WATERS

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P062 CHARACTERIZATION AND CHEMICAL PROFILING OF GREEN TEA SAMPLES USING CAPILLARY ELECTROPHORESIS COMBINED WITH CHEMOMETRICS

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P063 STUDY OF THE ADSORPTION EQUILIBRIA OF A PHARMACEUTICAL RELEVANT PEPTIDE IN RP-LC THROUGH ADVANCED NUMERICAL MEANS

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P064 COMPUTER-ASSISTED DEVELOPMENT OF RP-HPLC METHODS FOR THE ANALYSIS OF PLANT BIOACTIVE COMPOUNDS

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P065 EXTRACTION AND CLEAN-UP OF STEROID HORMONES FROM AQUEOUS PROTEIC MATRICES: A PRELIMINARY STUDY

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P066 DEVELOPMENT AND VALIDATION OF A MULTI-RESIDUE EXTRACTION METHOD FOR THE DETERMINATION OF ORGANIC MICROPOLLUTANTS IN SURFACE WATER

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P067 OPTIMIZATION AND VALIDATION OF A SPE-HPLC-PDA METHOD USING QUANTITATIVE STRUCTURE-RETENTION RELATIONSHIP BASED ON MAPPING THE HYDROPATHY FOR SIMULTANEOUS DETERMINATION OF DRUGS

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P068 IOHEXOL A NON-RADIOLABELED CONTRAST MEDIUM IN HUMAN PLASMA MEASURED BY ULTRA HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY (UHPLC) WITH DAD DETECTION

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P069 SELECTIVITY OF SOLID PHASE MICROEXTRACTION FIBERS TOWARDS POLYCYCLIC AROMATIC HYDROCARBONS IN AIRBORNE PARTICULATE

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P070 NEW ASCORBIC ACID-BASED SPECTROPHOTOMETRIC METHOD FOR MEASUREMENT OF THE OXIDATIVE POTENTIAL OF ATMOSPHERIC AEROSOL

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P071 ZWITTERIONIC TEICOPLANIN CHIRAL STATIONARY PHASES ON 2.0 µM AND 2.7 µM SUPERFICIALLY POROUS PARTICLES: CHROMATOGRAPHIC EVALUATION AND COMPARISON WITH TEICOPLANIN ON 1.9 µM FULLY POROUS PARTICLES

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P072 DEVELOPMENT OF A MICROEXTRACTION BY PACKED SORBENT-PROGRAMMED TEMPERATURE VAPORIZATION-GAS CHROMATOGRAPHY-TRIPLE QUADRUPOLE MASS SPECTROMETRY METHOD FOR PHTHALATE MONOESTERS ASSAY IN HUMAN URINE

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P073 NON-mAb PROTEIN PURIFICATION BY MEANS OF SPLIT-INTEIN MEDIATED AFFINITY CHROMATOGRAPHY

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P074 ORTHOGONAL CHARACTERISATION OF NANOVESICLES THROUGH DIFFERENTIAL AND DENSITY GRADIENT CENTRIFUGATION HYPHENATED TO FLOW FIELD FLOW FRACTIONATION:

DIFFERENCES IN SIZE, COMPOSITION AND RELATIVE ABUNDANCE OF DIFFERENT SPECIES IN EXOSOMAL SUBPOPULATIONS

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P130 INSIGHT ON THE OCEAN-ATMOSPHERE INTERACTION IN POLAR SOUTHERN EMISPHERE BY LONG TERM AEROSOL MEASUREMENTS IN CENTRAL ANTARCTICA.

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Flash communication posters

PF1 SB - PF4 SB, PF1 SS, PF1 FN, PF2 FN, PF1 EC - PF3 EC, PF1 AS, PF1 FO, PF1 MS

PF1 SB LIFE MARKER DETECTION IN PLANETARY EXPLORATION: A NOVEL BIOSENSOR FOR ATP DETECTION BASED ON CHEMILUMINESCENT DNA SWITCH INTEGRATED WITH AMORPHOUS SILICON PHOTODIODES

E. Marchegiani[1], M. Mirasoli[1], M. Zangheri[1], M. Guardigli[1], C. Caliceti[1], A. Porchetta[2], D. Caputo[3], A. Nascetti[4], A. Roda[1]

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PF2 SB A COMPETITIVE APTAMER ASSAY FOR GLUTEN DETECTION IN DEEP EUTECTIC SOLVENT

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PF3 SB RATIONAL CONTROL OF THE ACTIVITY OF A CU^{2+}-DEPENDENT DNAZYME BY RE-ENGINEERING PURELY ENTROPIC DISORDERED DOMAINS

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PF4 SB DNA-BASED QUARTZ CRYSTAL MICROBALANCE ARRAY FOR THE IDENTIFICATION OF AROMA PATTERNS IN FOODSS

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PF1 SS INVESTIGATION, ISOLATION AND CHARACTERISATION OF NEW PRIONOID PROTEIN AGGREGATES THROUGH HOLLOW FIBER FLOW FIELD FLOW FRACTIONATION AND MULTI ANGLE LIGHT SCATTERING: A TOOL TO FACILITATE THE COMPREHENSION OF INFECTIOUS PROCESSES

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PF1 FN EXTRACTION, ANALYSIS AND ANTIOXIDANT ACTIVITY EVALUATION OF PHENOLIC COMPOUNDS IN DIFFERENT ITALIAN EXTRA-VIRGIN OLIVE OILS

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PF2 FN MULTIVARIATE OPTIMIZATION OF A QUECHERS PROCEDURE FOR THE LC-MS/MS ANALYSIS OF PHYTOESTROGENS IN SOY BURGERS

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PF1 EC INVESTIGATING PAINT MATERIALS IN STREET ART MURAL PAINTINGS BY ANALYTICAL PYROLYSIS BASED TECHNIQUES

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PF2 EC POTENTIALLY HARMFUL ELEMENT (PHE) OCCURRENCE AND PHASE PARTITIONING IN THE RIVER MOUTHS OF THE GULF OF TRIESTE (NORTHERN ADRIATIC SEA)

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PF3 EC USE OF NANO-STRUCTURAL MATERIALS FOR ABATEMENT OF NITRATES IN NATURAL AND WASTE WATER

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PF1 AS INSIGHTS INTO THE INHIBITION OF *P. FLUORESCENS* BIOFILM FORMATION VIA AFM AND ATR-IR CHARACTERIZATIONS

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PF1 FO DETERMINATION OF ETHYL-GLUCURONIDE IN HAIR BY MEANS PLE-SPE EXTRACTION AND HPLC-MS/MS ANALYSIS

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PF1 MS HPLC-ES MS/MS METHOD FOR THE IDENTIFICATION AND QUANTIFICATION IN HUMAN FECES OF GUT MICROBIOTA PRODUCTS: OXO-BILE ACIDS

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Poster session II

Wednesday, September 19

Theater

Regular posters

P004, P075 – P105, P107 – P109, P111 – P129, P131 – P149

P004 XPS STUDY OF REACTION CENTERS EMBEDDED IN POLYDOPAMINE THIN FILMS

M. R. Guascito[1], F. Milano[2], L. Giotta[1], M. Lo Presti[3], A. De Bartolomeo[4], S. Rella[1], D. Chirizzi[5], G. M. Farinola[3], M. Trotta[2]

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P075 PHENOLS BIOCONVERSION BY IMMOBILIZED LACCASE IN A FLOW REACTOR

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P076 MAKING ORDER OF DNA NANODEVICES THROUGH DISORDER

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P077 A COLORIMETRIC APPROACH TO EASILY MEASURE GOD ENZYME ACTIVITY

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P078 STRATEGIES TO IMPROVE THE SENSITIVITY OF AN ELIME ASSAY FOR THE DETECTION OF CAMPYLOBACTER

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P079 RULES TO PREPARE PEPTIDE-IMPRINTED NANOGELS WITH HIGH-AFFINITY BINDING SUITABLE FOR SENSING AND ASSAYS BY PRECIPITATION POLYMERIZATION

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P080 QUANTITATIVE ANALYSES OF PROTEIN PROFILING TO STUDY THE DUAL PROTECTIVE/DAMAGING EFFECT OF 4-HYDROXYNONENAL (HNE) ON THE INTESTINAL BARRIER

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P081 QUALITY BY DESIGN-DRIVEN OPTIMIZATION OF DRIED BLOOD SPOT EXTRACTION FOR A BIOANALYTICAL LC–MS METHOD

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P082 MULTI-OMICS PROFILING OF PANCREATIC CANCER STEM-LIKE CELLS

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P083 TIME MONITORING OF ENDURANCE ATHLETES' URINARY STEROIDAL PROFILE

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P084 SILVER NANOPARTICLES: A POSSIBLE VERSATILE COLORIMETRIC LABEL IN LATERAL FLOW IMMUNOASSAY

F. Di Nardo, L. Anfossi, S. Cavalera, C. Giovannoli, G. Spano, C. Baggiani
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P085 DETERMINATION OF PROSTAGLANDINE-LIKE MARKERS FOR OXIDATIVE STRESS IN HUMAN URINE BY SPE-UHPLC-MS/MS

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P086 NOVEL CARBON NITRIDE NANOPARTICLES AS CUSTOMIZABLE FLUORESCENT PROBES FOR IMMUNO-ANALYTICAL ASSAYS

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P087 DEVELOPMENT OF AN ANALYTICAL STRATEGY FOR THE METAPROTEOMIC INVESTIGATION OF ATMOSPHERIC BIOAEROSOL

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P088 HIGH-THROUGHPUT SCREENING OF HEMOGLOBINOPATHIES

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P089 EVALUATION OF AN ELIME ASSAY TO REVEAL THE PRESENCE OF HEPATITITIS A IN DRINKING WATER

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P090 PHARMACOKINETICS OF GEMCITABINE HYDROCHLORIDE AND IRINOTECAN HYDROCHLORIDE ALONE AND IN COMBINATION IN RAT PLASMA BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-DIODE ARRAY DETECTOR

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P091 FPSE-HPLC-PDA METHOD FOR THE DETERMINATION OF INFLAMMATORY BOWEL DISEASE TREATMENT DRUGS IN WHOLE BLOOD, PLASMA AND URINE

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P092 FAST METHOD FOR THE DETERMINATION OF MAJOR AND TRACE ELEMENTS IN BREAST MILK: OPTIMIZATION AND VALIDATION

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P093 POLAR LIPID PROFILE OF SPIRULINA MICROALGA BY LIQUID CHROMATOGRAPHY COUPLED TO HIGH RESOLUTION MASS SPECTROMETRY

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P094 AUTHENTICATION OF "NOCCIOLA ROMANA" PDO HAZELNUT BY NIR COUPLED WITH CHEMOMETRICS

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P095 DIRECT QUANTIFICATION OF CHEMICAL SPECIES BY MULTIVARIATE STANDARD ADDITION AND NET ANALYTE SIGNAL METHOD

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P096 DETERMINATION OF PLANT-DERIVED CONTAMINANTS IN SAFFRON BY MEANS OF SPME-HS/GC-MS AROMA PROFILING COMBINED WITH CHEMOMETRICS

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P097 GEOGRAPHICAL CLASSIFICATION OF SAFFRON (CROCUS SATIVUS L.) BY MEANS OF MULTIVARIATE STATISTICAL ANALYSIS OF UHPLC DATA

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P098 DISCRIMINATION OF ARABICA AND ROBUSTA COFFEE SPECIES BY HS-SPME-GC-MS ANALYSIS OF VOLATILE ORGANIC COMPOUNDS OF GREEN BEANS AND A CHEMOMETRIC APPROACH

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P099 IMAGE TEXTURE ANALYSIS ON HYPERSPECTRAL DATACUBES: A COMPARATIVE STUDY

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P100 FROM CHEMOMETRIC MODELS TO CHEMICAL INTERPRETATION: TOOLS AND CAVEAT

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P101 A SURVEY OF DATA FUSION APPROACHES IN CHEMOMETRICS CONTEXT

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P102 EXPLOITING THE PERFORMANCE OF NEAR-INFRARED HYPERSPECTRAL IMAGING: TRANSFLECTANCE AND TRANSMISSION ANALYSES

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P103 ELECTROCHEMILUMINESCENT DNA SENSOR FOR THE DETECTION OF SPECIFIC DNA SEQUENCES

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P104 THALLIUM VOLTAMMETRIC DETERMINATION IN PRESENCE OF METAL INTERFERENCE IN FOOD AND BIO-MONITOR SPECIES:
APPLICATION TO MUSSELS, CLAMS AND OYSTERS

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P105 ELECTROCHEMICAL AND SPECTROSCOPIC INVESTIGATION ON THE STABILITY OF POLY ORTHO- AMINOPHENOL (PoAP), GROWN AS A VERY THIN MEMBRANE ON PLATINUM, UNDER PROLONGED IMMERSION IN WATER

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P107 3D FLOWER-LIKE PT NANOSTRUCTURES ON POLYPYRROLE NANOWIRE MATRIX FOR ENHANCED METHANOL OXIDATION

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P108 ELECTRODEPOSITION OF THIN FILMS FOR THE GALVANIC INDUSTRY

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P109 VOLTAMMETRY IN HYDROGEL FOR THE ANALYTICAL CHARACTERIZATION OF WATER SENSITIVE SURFACES

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P111 DETERMINATION OF PHARMACEUTICALS IN SURFACE WATERS BY AN ELECTRO-ACTIVATED GLASSY-CARBON ELECTRODE

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P112 DOPAMINE QUANTIFICATION IN RAT STRIATUM TISSUES TREATED WITH PERMETHRIN BY HLPC-ECD

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P113 CHARACTERIZATION OF DUSTY AND DUST FREE PM SAMPLES COLLECTED IN A SUBURBAN SITE IN SOUTHERN ITALY

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P114 DETERMINATION OF POLYSTYRENE ACCUMULATION IN MUSSELS (*Mytilus galloprovincialis*) BY PYROLYSIS AND GC-MS

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P115 ASSESSMENT OF PARTICULATE MATTER DIMENSIONAL PROFILES AT AN INDUSTRIAL SITE BY MEANS OF SELF ORGANIZING MAP ALGORITHM APPLIED TO OPTICAL PARTICLE COUNTER DATA

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P116 IDENTIFICATION OF POLICYCLIC AROMATIC HYDROCARBONS IN POLYHYDROXYALKANOATE BIOPOLYMERS OBTAINED FROM URBAN SOLID WASTE BY GAS CHROMATOGRAPHY/MASS SPECTROMETRY ANALYSIS

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P117 GAS AND AEROSOL COMPOSITION DURING THE AEROCLO-SA CAMPAIGN IN HENTIES BAY (NAMIBIA)

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P118 DETERMINATION OF CONTAMINANT SORPTION CAPABILITY OF BIOCHAR IN CULTIVATED SOILS: MODEL VS REAL SYSTEM APPROACH

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P119 THE HIDDEN MICROPLASTICS: SEPARATION AND CHARACTERIZATION OF MICROPLASTICS AND OF THEIR DEGRADATION BYPRODUCTS IN COASTAL SEDIMENTS

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P120 ADSORPTION OF FLUORIDE ONTO TUFF VARIETIES OF THE NEAPOLITAN AREA

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P121 USE OF ZEOLITES FOR THE ABATEMENT OF AMMONIUM INTO NATURAL WATER AND SAWAGE BREEDING

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P122 RELEASE AND SORPTION OF HEAVY METALS FROM BIOCHAR PRODUCED AT DIFFERENT TEMPERATURES

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P123 STRATIGRAPHIC DATING OF A 80 M DEEP FIRN CORE DRILLED IN COASTAL EAST ANTARCTIC ICE SHEET (EASTERN WILKES LAND)

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P124 PAHs AND PCPs IN THE LOWER ADIGE RIVER: AN UNDEREVALUATED MATTER

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P125 CHARACTERIZATION OF THE OXIDATIVE POTENTIAL OF WATER SOLUBLE FRACTION OF ATMOSPHERIC AEROSOL IN AN URBAN BACKGROUND SITE IN SOUTHERN ITALY

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P126 VARIATION OF LEVELS OF FATTY ACIDS COMPOSITION IN THE LIVER OF ANTARCTIC FISH TREMATOMUS BERNACCHII IN FUNCTION OF TIME AND TEMPERATURE: A MODELLING APPROACH

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P127 DETERMINATION OF KEY COMPOUNDS IN ANAEROBIC DIGESTION AND BIOMETHANE PRODUCTION: VOLATILE FATTY ACIDS AND METHYL SILOXANES

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P128 SYNCHRONIZATION OF FIVE ANTARCTIC ICE CORES ACROSS THE LAST ICE AGE

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P129 DETERMINATION BY GC-MS/MS AND GCXGC-TOFMS TECHNIQUES OF PERSISTENT ORGANIC POLLUTANTS IN BIOTA: DEVELOPMENT AND VALIDATION OF A MODIFIED QUECHERS EXTRACTION

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P131 THERMODYNAMIC PROPERTIES OF LEVULINIC ACID, A SUSTAINABLE PLATFORM MOLECULE

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P132 As(III) INTERACTION WITH NITRILOTRIACETIC ACID DERIVATIVE COMPOUNDS IN AQUEOUS SOLUTION

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P133 METAL-BINDING ABILITY OF CALCITERMIN, AN ANTIMICROBIAL PEPTIDE OF HUMAN AIRWAYS

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P134 STUDY ON THE INTERACTION OF Ca^{2+} WITH AMPICILLIN AND AMOXICILLIN IN AQUEOUS SOLUTION

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P135 ON METAL-LIGAND SYSTEMS AS CONTRAST AGENTS IN DIAGNOSTICS (MRI)

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P136 AUXINE: THERMODYNAMIC PROPERTIES, COMPLEXING ABILITY AND DOSAGE IN HUMAN SERUM

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P137 LIPID PROFILING OF LUPINUS LUTEUS BY HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY COUPLED TO ELECTROSPRAY IONIZATION AND MULTISTAGE MASS SPECTROMETRY (HILIC-ESI-MSn)

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P138 CHARACTERIZATION OF A SINGLE CYSTEIN-ENRICHED PHASEOLIN EXPRESSED IN TRANSPLASTOMIC TOBACCO PLANTS

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P139 DESI-HRMS DETERMINATION OF NEW PSYCHOACTIVE SUBSTANCES IN ORAL FLUIDS BY USING NOVEL SAMPLING SUBSTRATES

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P140 DETERMINATION OF POLYCHLORINATED DIBENZO-P-DIOXINS (PCDDS), POLYCHLORINATED DIBENZOFURANS (PCDFS) AND POLYCHLORINATED BIPHENYLS (PCBS) IN HENS EGGS

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P141 FIRST DETERMINATION OF CYLINDROSPERMOPSIN IN DRINKING WATER CHAIN OF VICO LAKE WITH SPE-LC-MS/MS

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P142 SURFACE MODIFICATION OF CHITOSAN FILMS WITH FIBRONECTIN-DNA APTAMER COMPLEX TO ENHANCE OSTEOBLASTIC CELL ACTIVITY: A MASS SPECTROMETRY APPROACH TO PROVIDE EVIDENCE ON PROTEIN BEHAVIOR

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P143 IMPLEMENTATION OF THE MODIFIED STANDARD ADDITIONS CALIBRATION METHOD FOR THE GC/MS QUANTIFICATION OF AMINO ACIDS

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P144 CONDENSED PHASE MEMBRANE INTRODUCTION MASS SPECTROMETRY COUPLED WITH LIQUID ELECTRON IONIZATION INTERFACE (CP-MIMS-LEI): A POWERFUL TOOL TO MONITOR ON-LINE CHEMICAL REACTIONS IN NON-ACQUEOUS SOLUTIONS

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P145 SPRINKLER IRRIGATION: A GOLDEN BULLET TO MINIMIZE THE BIOACCUMULATION IN RICE GRAIN OF THE MOST HEALTH-THREATENING ELEMENTS?

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P146 REAL-TIME MEASUREMENTS AND CHARACTERISATION OF ULTRAFINE AND SUBMICRON AIRBORNE PARTICLES NEAR AN INTEGRATED STEEL PLANT (TRIESTE-ITALY)

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P147 A RARE CASE OF DRINKING WATER CONTAMINATION BY THALLIUM: PIPE MONITORING ALONG DISTRIBUTION NETWORKS IN PIETRASANTA (LU)

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P148 PSEUDOMONAS REDUCTION IN DRINKING-WATER AND WASTEWATER DISTRIBUTION SYSTEMS BY CHLORINE DISINFECTION

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P149 STUDY ON DISCOLORATION OF POLYVINYLCHLORIDE SHEET BY EVOLVED GAS ANALYSIS AND HEART CUTTING EGA-GC/MS ANALYSIS

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Flash communication posters

PF1 GC, PF1 EQ, PF2 EQ, PF1 CB, PF5 SB – PF7 SB, PF1 EL, PF2 EL, PF1 AB

PF1 GC CADMIUM UPTAKE AND DIFFUSION IN BIVALVE MOLLUSK SHELLS FROM AQUEOUS MATRICES – AN LA-ICP-MS LINE SCAN AND ELEMENT IMAGING STUDY

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PF1 EQ CALIXARENE-BASED SUPRAMPHIPHILES IN NEUTRAL BUFFERED SOLUTION: DETERMINATION OF CMC AND ΔH_{mic} BY A SINGLE EXPERIMENT

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PF2 EQ SPECIATION STUDY OF A BIS-(3-HYDROXY-4-PYRIDINONE) TOWARDS M^{2+}

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PF1 CB NEAR-INFRARED BASED DETECTION OF INSECTS INFESTATION IN RICE SAMPLES

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PF5 SB DEVELOPMENT OF A REFLECTANCE SMARTPHONE PAPER-BASED CHEMOSENSOR FOR THE EVALUATION OF ANTIOXIDANT ACTIVITY BY IN SITU GOLD-NANOPARTICLES SYNTHESIS

D. Calabria, C. Caliceti, M. Zangheri, E. Porru, M. Mirasoli, M. Guardigli, P. Simoni, A. Roda
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PF6 SB ENVIRONMENTAL AND OPERATIONAL STABILITY OF ORGANIC FIELD EFFECT TRANSISTORS FOR BIOSENSING APPLICATIONS

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PF7 SB POLYDOPAMINE: MOLECULAR IMPRINTING, PLASMONS AND CATALYSIS

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PF1 EL SINGLE CELL ELECTROCHEMILUMINESCENCE IMAGING: FROM THE PROOF-OF-CONCEPT TO DISPOSABLE DEVICE-BASED ANALYSIS

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PF2 EL OPTIMIZING THE ELECTRODEPOSITION PROTOCOL OF ENANTIOSELECTIVE INHERENTLY CHIRAL ELECTRODE SURFACES: A MULTI-TECHNIQUE INVESTIGATION

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PF1 AB AN ANALYTICAL STUDY OF THE INFLUENCE OF CHITOSAN FEATURES ON THE CHEMICAL, PHYSICAL AND MECHANICAL AND IN-VITRO PROPERTIES OF 3D PRINTED SCAFFOLDS

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PLENARY LECTURES

PL1

ANALYTICAL ASPECTS OF BIOSENSING SYSTEMS BASED ON ENZYME INHIBITION

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There is a growing interest in the study of enzymes with the aim of identifying pollutants that act as enzyme inhibitors or inhibitory molecules that may serve as the starting points for drug discovery. Many drugs based on enzyme inhibition have been commercialized, demonstrating the importance of enzyme inhibitors. The pharmacological treatment of some diseases is currently based on enzyme inhibitors like cancer, diabetes type II and neurologic disorders.

Biosensing systems based on enzyme inhibition represent a cost-effective device for fast screening of inhibitors. They could be used as a complementary approach to traditional methods [1].

In the present conference, we would like to underpin the recent advances in biosensors based on enzyme inhibition field, focusing on the investigation of a new theoretical approach and the use of nanomaterials in order to improve the analytical performances of the enzymatic method.

In this lecture, the experimental results obtained with biosensors developed in our laboratory for the detection of pesticides aflatoxins, cyanide, sulfide, methylmercury, nerve agents, antibiotics, and various other drugs and toxins will be presented. These inhibitors were usually detected at levels of ppb. Given the low concentrations found of these contaminants in water samples, the Solid Phase Extraction is required prior to analysis and was commonly used in combination of biosensors for a wide range of compounds.

The diagnosis of type of inhibition greatly improves the sensitivity by a judicious choice of the enzyme concentration, substrate concentration and incubation time. A particular advantage of the reversible biosensors is that they offer the possibility of analysis in both batch and flow mode, allowing the use of these sensors for analysis of a large number of samples in a reasonable time interval. Irreversible biosensors, on the other hand, can be recommended for a single use with screen-printed electrodes.

Although the huge number of papers published in the enzymatic inhibition field, analyzing all reaction time-course of progress curve of enzyme inhibition is scarce. The advantages of progress curve analysis versus initial velocities will be highlighted in this lecture. Indeed, the plot of half time reaction versus inhibitor concentration allows determination of inhibitors with extended linearity [2].

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PL2

IMPRINTED POLYMERS IN BIOANALYSIS, BIOMARKER DISCOVERY AND IMAGING

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Artificial receptors in the form of molecularly imprinted polymers (MIPs) continue to gain ground in the analytical sciences, mainly as a low cost alternative to antibodies or other affinity reagents. [1] MIPs are prepared by a simple process from a limited number of synthetic monomers resulting in sturdy materials that can be designed to recognize a wide range of targets ranging from small apolar molecules over proteins to cells and microorganisms. With molecular recognition and size matching the performance of antibodies they are therefore often refered to as “plastic antibodies”. The role of the MIP is in most cases to enrich (capture-release) or to sense (capture-report) a specific known target (e.g. biomarker) or a class of targets. In spite of shortcomings, MIPs can here fill a gap in modern bioanalysis by providing artificial receptors for targets where no antibodies (e.g. phospho-peptides [2], sulfo-peptides [3], glycans [4], lipids [5]) are available or by allowing analysis to be performed under denaturing conditions. An alternative role of the MIP is to use it for the capture of previously unknown biological targets. [2,5] This can concern the identification of novel biomarkers or bioactive compounds and in turn the elucidation of signaling or biosynthetic pathways. Finally, a growing number of reports show MIPs to be a useful tool in cell biology e.g. for cell imaging of poorly immunogenic markers. [4] In the talk I will discuss some recent examples of the above applications in order to show what this technology can offer to the bioanalytical community.

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PL3

ENVIRONMENTAL CHEMOMETRICS

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Chemometrics has evolved and consolidated in a slow but sustained way in the research field and in its applications in applied and industrial sectors. This discipline is experiencing its biggest consolidation and expansion at present, because of the recognition of its role in the analysis of large volumes of data (big-data) and also due its success in the resolution of problems in various fields of application, like for example, in biological and environmental analytical sciences. This presentation will focuss on the description of the potential and applications of some chemometric methods in the investigation of some environmetal analytical problems, such as in environmental source apportionment problems, and in the investigation of the effects of chemical stressors on biological organisms using highthrougput untargeted analytical methods.

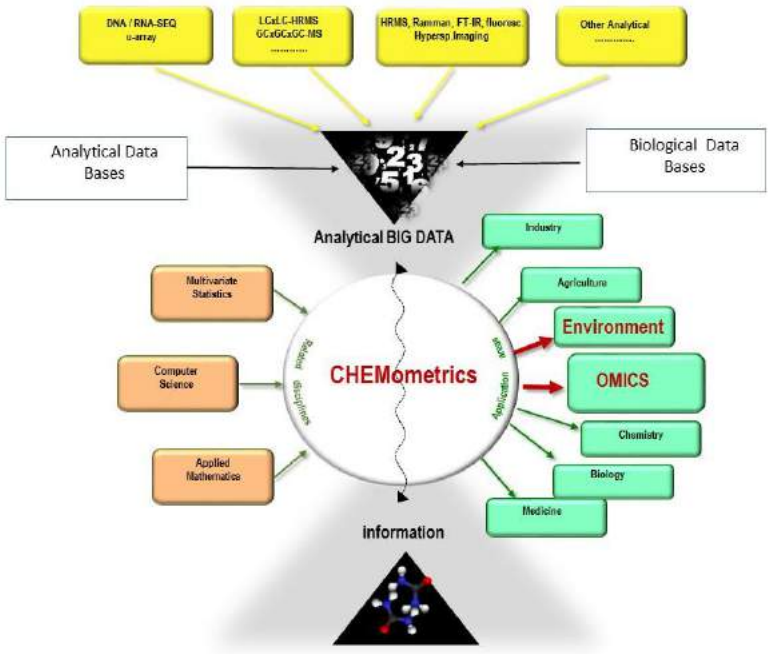

Figure 1. Chemometrics is an interdisciplinary field

LECTURE OF THE YOUNG RESEARCHER AWARD WINNER

GR

INNOVATIVE ANALYTICAL APPROACHES BASED ON MASS SPECTROMETRY TECHNIQUES AND IMMUNOSENSING DEVICES FOR FOOD SAFETY CONTROL AND CLINICAL DIAGNOSIS

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Impressive progress in analytical chemistry involves the introduction of novel methods and devices, allowing to expand applications to new scientific areas and sample types. An outlook is given on the fundamental role that mass spectrometry (MS) techniques and immunosensors play in food safety assurance and in clinical diagnosis. Among MS-based approaches, ambient ionization techniques, such as desorption electrospray ionization (DESI), have recently emerged as potent strategy able to successfully bridge the gap between the ambient environment and the vacuum system, allowing to perform screening analysis directly on native samples, since minimal or no sample preparation is required [1]. In addition, MS-imaging combines molecular mass identification with spatial information: the provided spatial distribution of selected compounds over tissue slices has enormous value mainly in biomedical research for biomarker discovery and detection [1].
Current analytical research is also moving towards the development of disposable immunosensor devices, able to meet the characteristics of operational ease, rapidity, cost-effectiveness for high-throughput screening that are typical of traditional immunological methods. Competitive or noncompetitive assays are implemented on the functionalized surface of proper transduction units, also exploiting multivariate experimental design for optimization [2]. However, awareness is required about the limitation due to cross-reactivity of antigen-antibody interaction that can impair analytical accuracy and reliability. For this reason, the development and availability of confirmatory methods based on MS techniques is required, taking advantage of high selectivity, identification power and multiplexing capabilities [3].

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KEYNOTES

KN1

Molecularly imprinted nanogel particles: tailor-made protein and peptide receptors for sensing and assays.

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Polymer biomimetics prepared by the technique of molecular imprinting (MIPs), i.e. a template assisted synthesis [1], are synthetic alternatives to natural receptors, that in principle possess recognition properties similar to the natural counterparts, i.e. antibodies and receptors, but share the robustness and the integrability to sensing devices and assays typical of the polymeric materials. MIPs can be prepared towards a wide spectrum of analytes, from small molecules to biomacromolecules [2]. MIPs can be prepared in different formats spanning from the micrometer to the nano-size (nanoMIPs).

Over the last few years the downsizing of the MIPs to nanoMIPs has shown to bring significant advantages in terms of binding kinetics, accessibility of the binding sites, homogeneity of the imprints, quasi-protein-sized dimensions, strengthening further their resemblance to natural receptors, hence the nanoMIPs are often referred to as “plastic antibodies” [3]. Moreover nanoMIPs find applications in sensors [4], assays and in vivo.

To contribute to the advancement in mastering and manipulating the nanoMIP recognition properties so gain the ability to custom-design these biomimetics, we investigated the process of stamping analytes of clinical relevance, such as protein and peptides, on protein-compatible polymers at the nanoscale. Polyacrylamide-nanogels were selected as suitable material and successfully imprinted obtaining highly selective and high affinity nanoMIPs for protein and peptide recognition. Both linear and structured peptides were imprinted, to better mimic protein recognition [5]. Plus we explored the possibility to integrate the nanoMIPs to assays and sensors by exploiting surface modification strategies. Overall these results contribute to define rules for the imprinting at the nanoscale, allow to modulate affinity, address the issue of their surface coupling, offering versatile custom-made recognition elements for analytical applications.

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KN2

FIELD-FLOW FRACTIONATION FOR NANOANALYTICS: FROM GENESIS TO REVELATION

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The micro-volume variant of flow field-flow fractionation that uses as fractionation channel a piece of polymeric hollow fiber (HF) of sub-millimetric radius shows performance comparable to that of conventional F4 techniques. The low sample volume required is a great advantage when scarcely available samples are analysed; and quality control performance is improved since cartridges are low-cost and potentially disposable [1]. Finally, when coupled with downstream characterization and detection methods such as MS, multi-angle light scattering (MALS), and fluorescence detection (FD), HF5 is able to separate, mass/size characterize, and quantify very/ultra-high molar mass proteins and nanoparticles [2,3]. HF5 based analytical platforms may significantly improve the knowledge and development of nanobased systems for bioanalytical applications, such as the analysis of different proteins and biologically relevant species, from protein drugs to bio-vesicles such as exosomes, and nanoparticles of biopharmaceutical interest. Examples are presented. Misfolded or aggregated proteins usually exhibit reduced or no biological activity, and in some cases stronger immunogenicity or toxicity. Protein drug aggregation monitoring then is major concern for biopharmaceutical companies. HF5 has also shown effective in monitoring high-level protein aggregation related to ageing [3]. The ability of separating and enriching biologically relevant nanoparticles, such as exosomes, is crucial to better investigate specific molecular and signaling patterns for human diagnostic and therapeutic applications. An ongoing challenge is the accurate size characterization and quantification of exosomes because of the lack of reliable characterization/isolation techniques. The use of a free-flow, non-invasive, and miniaturized separation device such is a key step [4]. A fractionation step to size-separate, characterize, and quantify exosomal subpopulations by HF5, coupled to a multidetection platform, then presents a useful solution. Quality control in the production of NPs with specific properties clashes with the lack of suitable techniques to provide characterization of the newly-produced materials. HF5 showed to be a key step on the development of a suitable analytical platform able to achieve a multiparametric assessment of NP suspensions, and its integration in the development of bioactive nanoproducts in a safety-by-design approach [5]. We have applied HF5 to the analysis and characterization of silver NPs, which are a promising tool to control bacterial infections.

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KN3

ADVANCED DIAGNOSTIC INVESTIGATIONS FOR THE STUDY OF ALTERED GILDINGS: NEW INSIGHTS INTO CIMABUE'S PAINTING TECHNIQUE

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This research was aimed at studying the painting technique adopted in the masterpiece *"Madonna Enthroned with the Child and Two Angels"* (figure 1) painted by Cimabue (1240-1302).

Cimabue can be considered as one of the most important and famous artist of the middle-age and his activity opened the door to the new artistic era. To the authors knowledge, a painting created by Cimabue was never submitted before to scientific investigations aimed at characterizing the execution technique. Particular attention was devoted to the characterization of the throne decorations, pointing out new questions on their originality. Analyses performed in situ and on cross sections by optical microscopy, SEM-EDX, micro-FTIR and micro-Raman spectroscopy permitted to identify an original paint layer which underwent to darkening and was probably repainted.

The original decorations were realized by mixing pigments containing arsenic sulfide, such as orpiment (As_2S_3) and metallic Ag. Synchrotron radiation-based μ-XRD mapping investigations in combination with μ-XRF and μ-XANES analysis at S K-, Ag L_3- and As K-edges performed at PETRA III-P06 beamline (Hamburg, DE) and the ESRF-ID21 beamline (Grenoble, FR) suggested that metallic silver might be actively involved in the alteration pathways of arsenic sulfide pigments, opening a possible explanation to the observed darkening.

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KN4

SEPARATION AND ENRICHMENT OF PEPTIDES AND AMINO ACIDS: A PIECE IN THE PUZZLE OF THE BIOACTIVITY OF PROTEIN DERIVATIVES

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The identification of peptides, first introduced as necessary step in proteomics for identification of proteins in biological samples, has slowly grown an importance of its own, becoming and independent field in the omics approaches usually referred to as peptidomics [1]. Peptides can be investigated in a variety of fields, from biomarker discovery with the identification of endogenous peptides in biofluids and tissues [2], to the application of bioactive peptide investigations, where endogenous peptides or protein hydrolysates are characterized in search of peptides with health-promoting activities, such as antioxidant, antihypertensive and antimicrobial properties, just to mention the most investigated ones [3]. In either field, the use of advanced analytical techniques for separation and identification of peptides is mandatory, but despite improvements by multidimensional chromatographic separation and high resolution mass spectrometry with database identification, challenges still exist. In particular, the low molecular weight window of the peptidome, especially shorter peptide sequences (< 5 amino acid long), and unusual amino acids remain under-investigated due to the lack of suitable chromatographic approaches for separation of very polar compounds and lack of bioinformatic software for spectra matching. Additionally, in most cases such compounds are also at low concentration, which in turn requires the use of enrichment strategies for identification. The recent developments in the research of bioactive peptides, especially short sequences, will be presented along with interesting examples of how new and improved separation approaches can help solving the investigations of bioactive short peptides and unusual amino acids.
Acknowledgments: The project was funded by Cariplo Foundation within the "Agroalimentare e Ricerca" (AGER) program. Project AGER2-Rif.2016-0169, "Valorizzazione dei prodotti italiani derivanti dall'oliva attraverso Tecniche Analitiche Innovative"-"VIOLIN"

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KN5

USE OF GANTREZ™ COPOLYMERS AS POTENTIAL CHELATING AGENTS FOR THE SELECTIVE SEQUESTRATION OF METAL IONS

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Natural organic matter is quite rich in carboxylic groups that act as binding sites for cations over a wide pH range. As regards most physical and chemical properties, humic substances can be regarded as high molecular weight polyelectrolytes. Many classes of polyelectrolytes were studied as model molecules of more complicated natural macromolecules; in particular, high molecular weight polycarboxylates represent a very good model for acid-base properties and for interacting capabilities with almost all cations.

Gantrez™ ligands are synthetic copolymers derivatives of the methyl-vinyl-ether and maleic anhydride or acid, widely employed in different industrial fields, in waste treatment, in pharmaceutical and medical purposes. Some applications are as base polymer for making polymer salts used as bioadhesives. Some Gantrez™ ligands are effective in delivery and retention of active ingredients including antimicrobials, flavors, coolants and medicants in toothpaste and mouthwash applications. These copolymers have also a main rule in the production of nanoparticles, since biocompatible and able to increase the bioavailability of some active molecules and the important capacity to control the release of the loaded drugs.

Owing to the absence of thermodynamic data in aqueous solution, a systematic speciation study on the behavior of three Gantrez™ copolymers of different molecular weights (AN169, S97 and S95) was carried out, determining the critical micelle concentration, the acid-base properties and the ability to form weak complexes with the alkaline cations (Na^+ and K^+) at different ionic strengths and temperatures. The complexing abilities towards different metal cations (Ca^{2+}, Mg^{2+}, Sn^{2+}, Zn^{2+}, Al^{3+}) in NaCl aqueous solutions at different ionic strengths and temperatures were studied by potentiometric technique. The stability trend of the species was: $Sn^{2+} > Al^{3+} >> Zn^{2+} > Ca^{2+} \approx Mg^{2+}$. The interactions with Zn^{2+} and Sn^{2+} were also investigated in a solution containing different amounts of fluoride, in order to investigate the formation of mixed metal-ligand'-ligand'' species.

The dependence of the stability constants on ionic strength and temperature was modeled by means of modified Debye-Hückel equations. From the gradient of the stability constants with respect to the temperature, rough enthalpy and entropy change values for the formation of the species were calculated, and results that the entropic contribution is the driving force of reactions.

The sequestering ability of the three Gantrez ligands towards the metal ions taken here in into account was evaluated by means of the $pL_{0.5}$ parameter. This allowed us to highlight a different ability of Gantrez ligands to sequester the metal ions, with differences in some cases of ~3-4 orders of magnitude, promoting these copolymers as chelating agent of metals in natural waters and biological fluids.

KN6

CHEMICAL COMPOSITION OF ATMOSPHERIC AEROSOL AND SURFACE SNOW AT DOME C (EAST ANTARCTIC ICE SHEET): AN OVERVIEW FROM 10-YR LONG RECORDS

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The knowledge of aerosol chemical composition in the Antarctic plateau is basic to achieve information on the main natural inputs, tropospheric transformation and long-range transport processes of the aerosol components. Moreover, chemical and physical processes occurring at the atmosphere-snow interface are not yet understood yet and further work is needed to assess the impact of atmospheric chemistry on snow composition and to better interpret ice core records there retrieved.

Station Concordia(Dome C, East-Antarctica, 75° 06' S, 123° 20' E, 3233 m a.s.l.) was chosen as one of the two drilling site in the EPICA project, yielding a 900 kyr long climatic and environmental record. But paleoclimatic and paleoenvironmental studies require to understand the present-day load and composition of atmospheric aerosol and gases at the same site and the processes occurring at the atmosphere/snow interface (such as wet and dry deposition, gas-adsorption, post-depositional re-emission or transformation, and migration or diffusion in the firn and ice layers of chemical species).

To achieve such information, a continuous all year-round sampling of atmospheric aerosol (bulk and size-segregated) and surface snow was carried out at Dome C continuously all year-round over the 2004-2013 period.

Aerosol and snow samples were analyzed for main and trace ion markers, which can be used as markers of environmental conditions (e.g.: hydrological conditions in the dust source area, sea level, sea ice extent, continental and marine biological activity, volcanic activity, atmospheric and oceanic circulation). A continuous high resolution record of those parameters allows studying the extent and timing of main aerosol sources as sea salt (open ocean/frost flowers/blowing snow), biogenic production, crustal input, as well as transport (e.g. free troposphere, stratosphere-troposphere exchange) and atmospheric reaction processes (such as neutralization, chemical fractionation).

A comparison with ozone and solar irradiance measurements, carried out continuously over the same time period, is also attempted to better understand the atmospheric processes involving the atmosphere-snow exchanges of N-cycle species.

KN7

Continuous, real-time measurement of a cancer chemotherapeutic in a living body using electrochemical aptamer-based sensors and a novel drift correction approach

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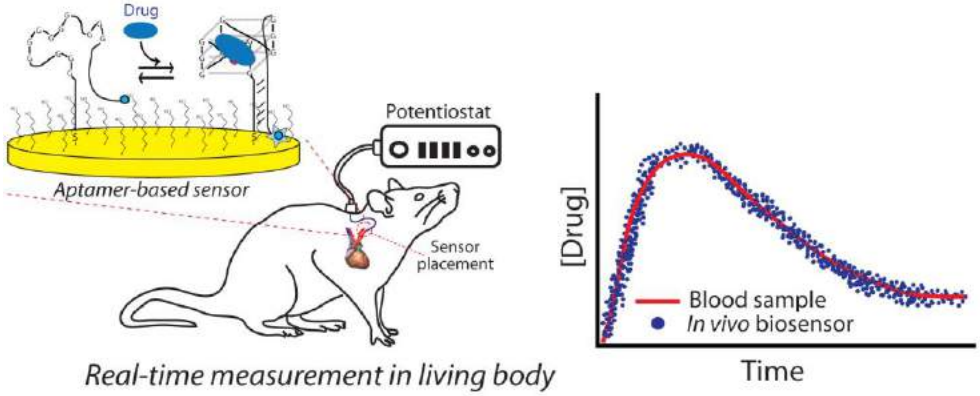
The development of sensors able to measure drugs in-situ in the body could revolutionize health care. Real-time monitoring of drug levels in blood, for example, would support the high-precision measurements of patient-specific pharmacokinetics and, ultimately, even closed-loop feedback-controlled drug delivery. Such personalisation of drug dosing would maximize drug efficacy while minimizing side effects. In response, we have developed electrochemical aptamer-based (E-AB) sensors, a modular sensing platform able to measure continuously and in real-time in the circulatory system of a living animal. Specifically, in this paper we rationally designed a new E-AB sensor against the chemotherapeutic drug camptothecin (CPT) and its derivatives. As the first step in this process we used an optical read-out to guide the re-engineering of the aptamer such that it undergoes a large conformational change upon target binding. We next converted this into an electrochemical read-out by attaching the re-engineered aptamer to an electrode and modifying it with a redox reporter. To ensure that E-AB sensors work in vivo in the veins of live animals we gave historically used a drift correction scheme termed "Kinetic Differential Measurements" (KDM) based on the different square wave frequency dependence of E-AB signaling. To exploit KDM approach, however, requires that the sensor exhibits a strong square-wave frequency response, which our re-engineered aptamer fails to do. To fix this we coupled the aptamer with a short, linear strand DNA that, together, generate the necessary frequency-dependence. Using this approach to KDM drift correction we are able to monitor in real-time the concentration of the camptothecin drug irinotecan in a living animal.



KN8

STRUCTURAL CHARACTERIZATION OF GLYCOSPHINGOLIPIDS BY MULTIPLE-STAGE LINEAR ION TRAP MASS SPECTROMETRY

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Glycosphingolipids (GSL) are glycolipids containing a ceramide with two hydrophobic chains (one amine-containing lipid referred to as the sphingoid base and one fatty acid tail) and a glycan head moiety (oligosaccharide). GSL are complex lipids due to the variability in the number and type of saccharides, the length, position, saturation, and configuration of the carbon chains of both the sphingoid base (SB) and the fatty acid tail. Some SB exist such as sphingosine [S], sphinganine or dihydrosphingosine [DS] and phytosphingosine (4-hydroxysphinganine) [P] [1], to which a long-chain fatty acyl (i.e., non-hydroxylated [N], α-hydroxylated [A], β-hydroxylated [B] or ester linked ω-hydroxylated) is attached through amide bonding. The polar head of GSL consists of one or more neutral or acidic monosaccharides which give rise to three main subclasses named as cerebrosides, globosides and gangliosides, respectively. Gangliosides are sialic acid-containing glycosphingolipids found throughout all eukaryotes and some prokaryotic organisms. Typically, GSLs are localized in the outer leaflet of the plasma bilayer membrane and are supposed to play an important role in transmembrane signaling events that occur at the cell surface [2]. Conceivably, several investigations intended at clarifying the molecular functions of glycosphingolipids have been reported [2].
In this contribution, a novel analytical approach based on hydrophilic interaction liquid chromatography coupled to ESI and multistage linear ion trap (LIT) mass spectrometry (HILIC-ESI-LIT MS) is proposed for GSL characterization. While MS/MS spectra mainly in negative ion mode by collisional-induced dissociation (CID) afford information on the type and saccharide number and ceramide moiety (i.e., N-acyl residue and long-chain base), CID-MS^3 spectra on the ceramide anions allow to recognize the sphingoid base. The occurrence of various SB as sphingosine (S), sphinganine (DS) and phytosphingosine (P) was inferred from the fragmentation patterns. The approach was successfully applied to samples of both biological (fibroblast cells) and food (donkey milk) origin [3].

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ORAL COMMUNICATIONS

O1 AB

DYNAMIC DNA AND RNA NANOTECHNOLOGY FOR BINDING-RESPONSIVE BIOMOLECULAR SENSING

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Inspired by the network of non-covalent interactions that nature harnesses to process information, nucleic acid nanostructures can be engineered into dynamic systems featuring programmable molecular motion and assembly. Nucleic acid actuators can be used to sense target biomolecules by means of binding-induced measurable outputs. We demonstrate that a co-localization mechanism can guide the assembly of a modular RNA system, performing detection of antibodies through a complementation assay.[1] We used antibodies to template the assembly of a split fluorescent Spinach aptamer, a synthetic RNA mimic of the Green Fluorescent Protein. We employed antigen-tagged RNA strands that, upon binding to target antibodies, reassemble into the native aptamer and yield a fluorescence output, showing high binding affinity, specificity for the target, and the ability to work in crude cellular extracts. Furthermore, we demonstrate that intracellular sensing can be achieved in a binding-responsive fashion. We implemented the use of a DNA molecular switch that enables probing of transcription factor binding activity directly in living cells in real time. Our strategy hinges on a DNA nanostructure that transduces, through a binding-induced conformational change, the recognition of a specific transcription factor into a fluorescence signal.[2] We monitored intracellular trafficking using super resolution microscopy, performed live cell imaging of transcription factor binding activity, and achieved relative quantification of intracellular transcription factor expression. On the whole, we highlight the potential of dynamic nucleic acid systems as innovative tools for bioanalytical chemistry and bioimaging.

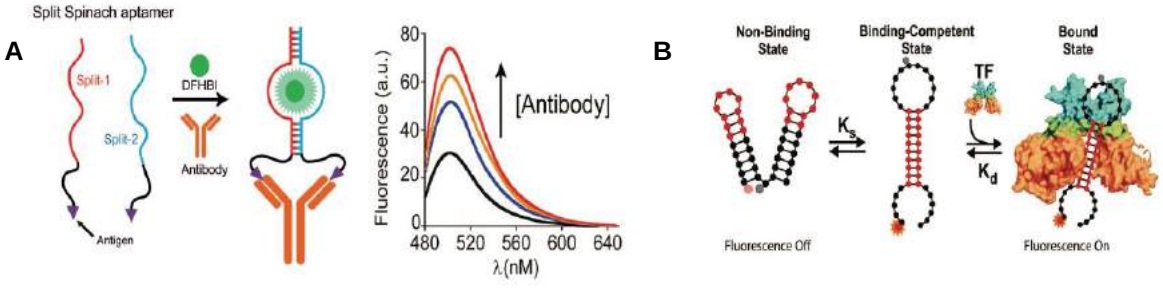

Figure 1. A) Antibody-based assembly of a fluorescent split Spinach aptamer; B) A DNA nanoswitch allows for detection of transcription factor binding activity through induced conformational motion

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O2 AB

A GC/MS APPROACH FOR THE SCREENING OF BIOACTIVE SECONDARY METABOLITES PRODUCED BY FUNGAL STRAINS

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Metabolomic studies of fungi allow to extrapolate novel biological data from the resulting metabolite profiles. Fungi are recognized as an important source of diverse natural compounds with potential biotechnological application. Hence, they are the subject of vigorous chemical investigation to be prime targets of the biosynthesis of natural products.
Advanced analytical strategies were developed to have a valid tool to achieve several aims: i) establish the fungal chemotaxonomy, ii) rapid identification and quantification of metabolites with biological activity, iii) distinguish among strains with different levels of bioactive compound production, iv) optimization of the growth conditions to increase the yield of interesting compounds. Gas Chromatography coupled to Mass Spectrometry (GC/MS) is a mature technology with valid criteria in a successful application for the detection of compounds. Here, we present some GC/MS applications to metabolome investigation of several fungal strains (e.g. *Talaromyces pinophilus, Lasiodiplodia theobromae*, *Aspergillus niger*) recovered from diverse hosts and habitat. However, the characterization of compounds not present in commercially available libraries, for example belonging to the classes of diketopiperazines, funicones, jasmonates, melleins, was made by implementing GC/MS results with other technologies (e.g. NMR spectroscopy, high resolution MS, optical rotation). Known and novel compounds have resulted from this work [1,2]. Most metabolites were isolated via conventional chromatographic techniques in order to test their biological activity. The bioactivities of fungal metabolites stimulate consideration for their industrial potential deriving from possible application in chemical and pharmaceutical industries.

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O1 AS

MORPHOLOGICAL AND COMPOSITIONAL ANALYZES OF SURFACES

Innocenti Massimo[a,b], Maurizio Passaponti[a], Emanuele Salvietti[a], Andrea Giaccherini[c], Walter Giurlani[a], Antonio De Luca[a], Roberto Felici[d], A. Lavacchi[b] and Francesco Di Benedetto[c]

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Thin films made of various materials are used in many scientific, technological and industrial environments. They are deposited through a variety of physical, chemical and electrochemical techniques. In all these fields, it is essential to measure the thickness, the colour, the morphological and compositional of the deposit because the properties of mechanical strength, corrosion, costs, optics and visual appearance depend on this feature.
We present a new method for thickness determination [1] of metal coating from galvanic industries. In the same field color measurement is one of the most important step in quality control at the end of the assembly line and in the research and development process for a variety of industrial applications printings, textiles, automotive and electroplating. Especially for electroplating, color inspection is a primary indicator of surface quality. Alteration of lightness, hue, and saturation are usually associated to surface defects or changes in galvanic baths composition and deposition efficiency. The purpose of our study is focused on the fashion applications, is to take an overview of conditions and techniques of color evaluation, effectively implemented from companies, and to find out the most accurate, and at the same time economically sustainable one [2]. Finally, for a simultaneous control of the morphological and structural growth of a film under the control of the potential, more complex techniques are needed. Some new experimental arrangements will be presented in the field of EC-SRM (Electrochemical-Synchrotron Radiation Methodologies) [3,4].

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Applied Surface Science 432 (2018) 53–59.

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Regione Toscana

O2 AS

THE UNCOMMON ELECTROCHEMISTRY OF COPPER NITROPRUSSIDE DISCLOSED BY SPECTROSCOPIC AND DIFFRACTION TECHNIQUES

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A rising class for insertion materials in lithium ion batteries is represented by Prussian blue analogues (PBAs). Copper nitroprusside $Cu[Fe(CN)_5(NO)]$, has been investigated for its interesting performances as cathodic active material [1]. *Operando* characterization [2] has been focused mainly on the first discharge process, during which the material experiences a deep structural and electronic modification. An approach consisting of multiple spectroscopic and diffraction techniques has been carried out to obtain a deeper insight into the redox mechanism. Both Cu and Fe are electroactive, as evidenced by *operando* XAFS measurements. Interestingly, nitrosyl ligand takes part in the first discharge process, as highlighted by both *ex situ* depth profiling XPS and *operando* IR. The reduction of nitrosyl group represents a unique case in PBA materials where a ligand is electrochemically active, beyond the metals' redox centers, contributing to a remarkable increase of specific capacity in the first discharge, fairly above the average among PBAs.

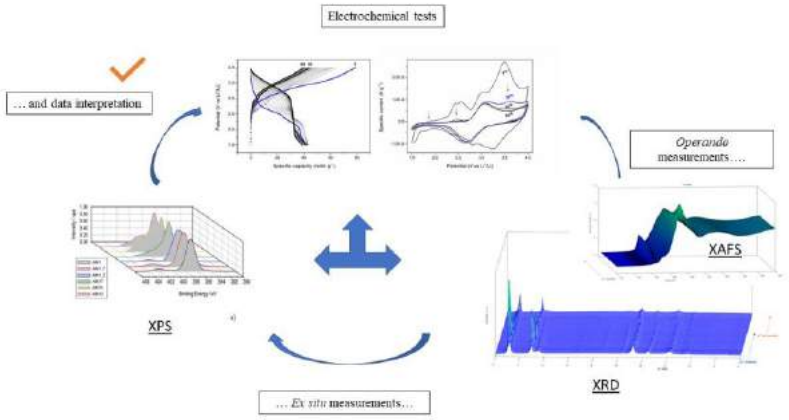

Figure 1. Main results in understanding the redox mechanism of copper nitroprusside.

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O3 AS

SURFACE CHARACTERIZATION OF NON-NOBLE METALS EMBEDDED IN N-DOPED CARBON CATALYSTS: THE IMPORTANCE OF HYDROPHILICITY ON OXYGEN REDUCTION REACTION ACTIVITY

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Oxygen reduction reaction (ORR) is a fundamental step in many electrochemical applications, e.g. fuel cells and zinc/air batteries. Being kinetically hindered, ORR requires efficient catalysts typically based on Platinum Group Metals [1]. Finding cheaper substitutes with similar or better electrocatalytic properties and stability is a challenge for the scientific community [2]. This works highlights the importance of the hydrophilicity of the catalyst active sites on oxygen reduction reaction (ORR) through an extensive study on catalysts based on nitrogen-modified carbon doped with different metals (Fe, Cu, and a mixture of them). Different analytical techniques, such as BET, XRPD, micro-Raman, XPS, SEM, STEM and hydrophilicity measurements were performed. In particular, XPS was used to assess the concentration and the chemical oxidation state of metal species. Moreover, N1s core level spectra were investigated to put in evidence different types of nitrogen-species on the surface of carbon catalysts, as well as C1s core level spectra to determine the total amount of carbon-oxygen functionalities (CxOy), considered as a measure of defects or edge sites in the graphene-like network [3]. From surface measurements, in combination with the results obtained from the other techniques, it was clearly demonstrated that the hydrophilicity of active sites plays a key role in electrocatalytic properties of ORR catalysts.

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O4 AS

XPS CHARACTERIZATION OF POLYDOPAMINE LAYERS FOR IMPROVING SURFACE BIOMOLECULE IMMOBILIZATION

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Polydopamine (PDA) films have attracted a rapidly increasing research attention during the last years due to its simple and rapid deposition under alkaline conditions in substrate independent manner providing a universal coating for materials with different chemical and physical properties [1]. Furthermore, this polymerized layer is enriched with functional groups that enable immobilization of primary amine or thiol-based biomolecules via a simple dipping process [2]. Although these fascinating aspects justify PDA wide and successful application as a versatile coating for biomolecule immobilization, several aspects have not been deeply investigated leaving some key details unclear and thus limiting PDA practical applications. A number of approaches are commonly used for the growth of PDA [3], but the effect of deposition conditions on film properties which in turn influence biomolecule immobilization has not been systematically investigated yet.
In the present work, a detailed investigation by X-Ray Photoelectron Spectroscopy (XPS) of PDA coatings deposited by different synthetic schemes (namely by autoxidation in air, under a pure oxygen environment, in the presence of a strong oxidizing agent for different time intervals (1, 3, 5, 8, 18, and 24 hours), and by electrochemical oxidation) is performed aimed at investigating film thickness and chemical composition as a function of polymerization conditions. Comparative spectroscopic analysis of PDA films revealed significant differences in terms of deposition kinetics and abundance of chemical components and allowed selection of synthesis conditions making PDA chemical structure richer in functionalities mainly involved in conjugation of biomolecules. The high suitability of the selected PDA film for bioconjugation was verified using a biomolecule conjugated to Horseradish Peroxidase or to fluorophore, obtaining also an estimation of immobilization time-stability within 4 weeks and a quantitative evaluation of immobilization extent. Moreover, further insight on biomolecule anchoring was provided by the comparison of XPS data on PDA samples before and after interaction with biomolecule [4].

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O5 AS

STREPTAVIDIN-COATED GOLD NANOPARTICLES: CRITICAL ROLE OF OLIGONUCLEOTIDES ON STABILITY AND LINEAR AGGREGATION

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Gold colloids have been the focus of research for many decades because of their intriguing electronic and optical properties, depending on the size and shape of gold nanoparticles (AuNPs)[1]. Strategies based on the combined use of Surface Plasmon Resonance Imaging (SPRI) and bioconjugated gold nanoparticles have been shown to produce an ultrasensitive detection of nucleic acids [2] which could lead to more reliable and sensitive diagnostics assays [3]. With the aim to provide fundamental information useful to improve performances of biosensing assays using biofunctionalized AuNPs, results from spectroscopic, dynamic light scattering (DLS), zeta-potential (ζ), transmission electron microscopy (TEM) and SPR investigations are here presented [4]. SA-coated AuNPs were modified with biotinylated oligonucleotides (ODNs) and spontaneously re-dispersed. The role of the oligonucleotide in the stabilization of the functionalized nanoparticle dispersion has been investigated by performing a competitive displacement of the biotinylated ODN through a ligand-exchange process with free biotin. Displaced biotinylated ODNs bring negatively charged strands in solution thus altering the balance between electrostatic and steric effects around colloidal NP and triggering the linear aggregation of nanoparticles.

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O1 CB

SO-COVSEL: A NOVEL METHOD FOR VARIABLE SELECTION IN MULTIBLOCK DATA

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Nowadays, with the development of new instrumentations, it is quite common to end up handling multi-tab data, i.e., measures obtained analyzing a specific set of samples with different analytical techniques. It has been proved that the simultaneous extraction of features from all the data-blocks, namely the application of data-fusion or multi-block methods, is much more profitable than modelling the individual sets of measures [1-2]. In literature, several multi-block approaches have been proposed, either for explorative analysis, classification or regression. Nevertheless, despite multi-block analysis involves a relatively high number of variables (compared to individual block modelling), not many feature selection methods have been proposed in this context. In the light of this, the feasibility of coupling a variable selection method, Covariance Selection (CovSel) [3] with a multi-bock regression method, Sequential and Orthogonalized-Partial-Least-Square (SO-PLS) [4], into a new approach called SO-CovSel, has been tested. The algorithm of the novel method follows the same scheme as SO-PLS but the feature reduction provided by PLS is carried out by CovSel. The resulting approach can be applied in regression and, by combination with discriminant analysis, also in classification. Concerning the regression context, SO-CovSel and SO-PLS gave comparable predictions; on the other hand, for what concerns their application in a classification framework (by combination with discriminant analysis) SO-CovSel provided equal or better results (from the prediction point of view) than SO-PLS-LDA.

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O2 CB

CHEMICAL MODIFICATIONS OF RICE GERM DURING STORAGE: FOCUSING ON WATER BY THE AQUAPHOTOMICS APPROACH

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The aim of this study is to investigate how different water activities affect rice germ shelf life. In fact, this matrix (a by-product of rice milling process) could be interesting for human nutrition but, for its composition characterized by unsaturated fatty acids, it undergoes rancidity during storage. Dried samples at different water activities (0.55, 0.45 and 0.36) were packed in air and stored at 27°C for 320 days (for a total of 7 sampling points). All the samples were analysed by FT-NIR spectroscopy in reflectance (in the 800 – 2780 nm spectral range) with a rotating sample holder, as a non-targeted analytical approach.
First of all, focusing on the Aquaphotomics approach, spectral analysis was done in the water first overtone range, 1300 and 1600 nm; then an exploratory principal component analysis (PCA) was performed, followed by a partial least squares regression method (PLSR) to understand the NIR spectral changes that characterize the differences caused by different water activity levels in rice germ during storage. In more depth, four wavelengths, essential for the description of this system, were found to define the so called water matrix coordinates (WAMACS): 1343 nm, associated with protonated water, 1392 nm, typical absorbance of trapped water, 1410 nm, the well-known band of free water and 1436 nm, the Zundel cation band ($H_5O_2^+$) and the respective WAter Spectral Patterns, WASP. Radial graphics of the normalised WAMACS absorbance values were built: such Aquagrams allow to understand the modification of different water molecular the structures along time, for each water activity under investigation.
Thanks to this state-of-the-art approach, the water molecular conformation changes related to different water activities in rice germ along the storage were discovered. These findings will open the venue of understanding the water molecular structure behind water activity in general.

Acknowledgment: the authors thank 'Rondolino - Società Cooperativa Agricola' for samples supply and economic support.

O3 CB

MULTIVARIATE CLASSIFICATION OF CHIANTI RED WINES BASED ON MASSIVE SAMPLING AND ICP-MS ELEMENT COMPOSITION

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Identification of the origin of wine got increasing interest in Europe and, for this reason, the European Union created systems known as PDO (Protected Designation of Origin) since 1992. Products, registered under this scheme, can thus be protected under frauds. Moreover, the identification of the geographical origin is of great interest for both wine consumers and producers [1].
In this study, a massive sampling of wine samples have been conducted to enhance the development of multivariate classification models for the identification of wines produced in the Chianti area. The aim of these models is the final industrial application for the reliable screening of the geographical origin of samples provided by suppliers.
The element content profile based on ICP-MS was determined on 639 red wine samples (125 belonging to the Chianti area and the other 514 representing the other major regions of production in Italy) and thus used as input for the subsequent calibration of multivariate classification models. Partial Least Squares – Discriminant Analysis [2] was carried out to establish relationships between the chemical profile and the geographical origin of wine samples. Classification models were properly validated through an external validation set of samples and demonstrated acceptable predictive performances, with sensitivity (% of correctly predicted Chianti samples) and specificity (% of correctly predicted non-Chianti samples) equal to 81% and 78%, respectively. Moreover, additional analysis for the identification of specific Italian regions with significant overlaps to Chianti have been conducted and sub-classification models were calibrated on samples belonging to these regions.

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O4 CB

SMARTPHONE-BASED DETERMINATION OF GRAPE PHENOLIC MATURITY

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In viticulture, the determination of the optimal moment for grape harvesting is a crucial aspect, which strongly influences the final attributes of the resulting wine [1]. In this context, phenolic maturity plays a paramount role on the organoleptic characteristics [2]. Generally, phenolic maturity is strongly connected with the amount of anthocyanins in the grape skin, which are responsible for wine colour, also strongly affecting its stability during aging. Currently, the determination of grape phenolic maturity requires expensive and time consuming analytical procedures, involving various steps for the extraction of the analytical sample and its subsequent analysis by UV-Visible spectrophotometry and HPLC. In this context the present study, developed in the frame of the POR-FESR research project SOSTINNOVI (www.sostinnovi.eu), was aimed at developing an alternative analytical method for the assessment of grape phenolic maturity directly in the vineyard, based on chemometric elaboration of RGB images of grape berries acquired with a smartphone. To this purpose, grape samples belonging to two different varieties of Lambrusco, Ancellotta and Salamino, were collected at different harvest times, from veraison until complete ripening. RGB images of the grape samples were acquired with a device designed *ad-hoc* for this application, consisting in a smartphone coupled with a specific 3D -printed plastic case containing a sample holder and a controlled illumination system. After image acquisition, the grape berries were also analysed by means of reference analytical methods for the determination of several analytical parameters usually employed for the assessment of phenolic maturity, such as colour index and the main anthocyanins content [3-4]. The RGB images of grape samples were converted into unidimensional signals named colourgrams [4], which were used to develop calibration models using Partial Least Squares (PLS) and interval PLS (iPLS) for the prediction of the analytical parameters related to grape phenolic ripening. The best performing calibration models have been implemented into a dedicated app, which easily allows to acquire the images on-site, visualize immediately the corresponding parameters of interest, and store the geolocalized data for further analyses using of a dedicated website.

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O5 CB

PREDICTION OF ODOUR CONCENTRATION BY USE OF SUPERVISED KOHONEN NETWORKS ON ELECTRONIC NOSE SIGNAL RECORDS OF ODORANT SAMPLES AND REAL ENVIRONMENT AIR SAMPLES

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Electronic noses are used for outdoor ambient air characterization to assess odour impacts on population but for air pollution studies and especially for odour concentration estimation, the relationship between sensor responses and odour is not trivial. A recent review [1] questioned the capability of some classic statistical elaboration tools for application to e-noses, highlighting how very few examples from field application are present in scientific literature. Moreover in 2015 the European Committee for Standardization started a working group (CEN/TC264/WG41) to draft a European Standard document about the "Instrumental odour measurement". One of the tasks of the group focuses on criteria for developing and validating mathematical models linking instrument metrics to odour [2]. Recently we published a study involving the use of Self Organizing Map algorithm to manage high-frequency e-nose data acquired at a receptor site near an industrial plant, identify the "air types" present and characterize them as "malodor" or "odor free" by linking the SOM output to independent odour concentration measurements according to EN 13725 (sensorial method) [3].

In the present study we propose a model for prediction of odor concentration of odorants (such as n-butanol and reduced sulfur compounds) and of mixture of odorants at different dilutions by use of supervised Kohonen networks [4] applied to electronic nose signal records, at a site impacted by multiple odour sources. The idea is that a specific calibration should be performed for each “air type” detected at the receptor site by the e-nose, since a single general “global” calibration linking odour responses from multiple sensors to different types of odorant mixtures appear intrinsically incorrect. We go for “local” calibration models, covering each type of odorous air detected at the receptor site. We discuss how to tailor the model parameters to produce site-specific odour estimation for air samples collected at receptors positioned near industrial plants. The model can be validated collecting air samples using a sampler that can be activated remotely when citizens signal odour nuisances and analyzing the samples both with the e-nose and according to the sensorial method EN 13725 to compare predicted and measured odour concentration.

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O1 EL

DETERMINATION OF ULTRATRACE IRON IN SEAWATER: NEW DEVELOPMENTS OF A CATALYTIC ADSORPTIVE STRIPPING VOLTAMMETRY METHOD

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Iron plays an important role in regulating the primary productivity of the oceanic systems: since 1990 (first iron hypothesis [1]) it is clear that its limitation has consequences on the regulation of the global climate due to a reduction of the phytoplankton activity which works as a sink for the atmospheric CO_2 [2]. Dissolved iron in seawater shows very poor solubility (nanomolar-picomolar level): researchers are challenged to study methods with high sensitivity and very low limit of detection, preventing the risk of sample contamination. Nowadays the best performing electrochemical method is the adsorption cathodic stripping voltammetry which uses 2,3-dihydroxynaphtalene as the complexant and atmospheric oxygen as oxidizing species for the catalytic enhancement of the signal: this method allows the use of 0.5-1 mL samples reaching a 5 pM limit of detection [3]. Aim of this discussion is to present the recent developments of this method. Two important modification were applied to the instrumental configuration: first the use of a silver wire as pseudoreference was introduced to limit the leaching phenomenon of the KCl solution through the septum into the sample as usual in the standard reference Ag/AgCl electrode. Pseudoreference was also introduced because it was more suitable for the small volume cell (0.5 mL) thanks to its small diameter of 1 mm. Atmospheric oxygen was firstly replaced with tank air (N_2-O_2 80%-20%) and then with an aerator pump. These modifications allowed to obtain very high sensitivity (i.e. about 30 $nA \cdot nM^{-1} \cdot min^{-1}$ for the ligand concentration of 30 μM). Moreover, some chemical aspects, as the complexant stability and the complex stoichiometry were studied in order to understand their importance for the analytical sensitivity of the method. Also the reaction rate of the electrode reaction and the catalytic constant in the presence of the oxidizing species were investigated to clarify the reaction mechanism.

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O2 EL

WIDE-SCOPE ENANTIOSELECTIVE VOLTAMMETRY: TESTING INHERENTLY CHIRAL SELECTORS WITH CHIRAL PROBES REPRESENTATIVE OF DIFFERENT STEREOGENIC ELEMENTS

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Enantioselective electroanalysis is an advanced, attractive target of high potential interest in applicative fields like *e.g.* the pharmaceutical one. Of course, since specular molecules have the same properties excepting when interacting with a chiral environment, enantiodiscrimination can only be achieved with the electron transfer process taking place at a chiral electrode|medium interphase. In this frame, remarkable performances have been recently observed employing selectors endowed with "inherent chirality", *i.e.* in which chirality and key functional properties originate from the same element. Successful chiral voltammetry tests have been obtained (a) on chiral electrode surfaces based on inherently chiral, electroactive heterocycle-based oligomers, including cyclic ones [1-4] and (b) on achiral electrodes in inherently chiral ionic liquids or achiral ionic liquids with inherently chiral additives [5].
An attractive feature of the above approach is its general validity. In fact, we have observed that a given inherently chiral selector can discriminate the enantiomers of even very different chiral probes (and, symmetrically, the enantiomers of a given probe can be discriminated by different inherently chiral selectors). Moreover, enantiodiscrimination by inherently chiral selectors is being tested with chiral probes representative of different classes of stereogenic elements. A selection of examples will be presented, compared and discussed.

The current support of Fondazione Cariplo/Regione Lombardia "Avviso congiunto per l'incremento dell'attrattività del sistema di ricerca lombardo e della competitività dei ricercatori candidati su strumenti ERC - edizione 2016" (Project 2016-0923) to our inherently chiral research is gratefully acknowledged.

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O3 EL

Multiple paper-based electrochemical biosensors for pesticide detection

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Pesticides are largely used at worldwide level to improve the food production, fulfilling the needs of the global population which is increasing year by year. Although persistent pesticides have been replaced (i.e. DDT) with the less persistence ones, the contamination of food, soil and water by pesticides remains an issue of public concern. The detection of pesticides is usually carried out by using liquid chromatography or gas chromatography coupled to mass spectrometric detection; however, these methods require laboratory set-up, expensive instrumentations, skilled personnel, and often organic solvents producing unsafe waste. In the last decade, paper-based electrochemical (bio)sensors have paved the way for sustainable measurements of pollutants, using the paper as active substrate where reagents are stored, electrodes are printed, real samples are analysed without any sample treatment and avoiding the use of organic solvents [1, 2].
In this work, the properties of the paper have been exploited to develop a multi-pad paper-based screen-printed electrochemical biosensing tool for the detection of pesticides. In detail, we developed an amperometric biosensing tool constituted of three paper-based biosensors based on the inhibition of three different enzymes namely: butyrylcholinesterase for the detection of paraoxon (an organophosphorus insecticide), tyrosinase for the quantification of atrazine (a triazinic compound), and alkaline phosphatase for the measurement of 2,4 dichlorophenoxyacetic acid (a synthetic auxin). To deliver a fast and easy measurement, all the required reagents are loaded on the paper-based patterns; thus, the operator needs only to add 5 µL of the real samples to carry out the measurement. This paper-based biosensing tool was successfully challenged in standard solutions as well in river water samples achieving detection limit at ppb levels.

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O4 EL

NANOSTRUCTURED TIO_2 ELECTRODES FOR PHOTOELECTROCHEMICAL BIOSENSING OF NUCLEIC ACIDS

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Recently, with the emergence of novel photoelectrochemically active species and new detection schemes, photoelectrochemistry has received increasing attention in biosensing of proteins as well as in the development of hybridization assays for the recognition of specific nucleic acid sequences. In this work, Au nanorods (NRs) modified nanostructured TiO_2/ITO electrodes have been fabricated and characterized, in order to develop a biosensing platform for the photoelectrochemical determination of microRNAs. The proposed method is based on the use of thiolated DNA capture-probes (CPs) immobilized onto Au NR surface. The Au NRs are chemically bound at the surface of TiO_2/ITO electrodes by means of the mercaptosuccinic acid linker. Subsequently, the DNA CPs are bound to the Au NR surface through the thiolate group, and reacted with the target RNA sequence. Finally, the obtained biosensing platform is incubated with alkaline phosphatase and L-ascorbic acid 2-phosphate (AAP) enzymatic substrate, for the in situ generation of ascorbic acid (AA). Such AA molecule, coordinating to surface Ti atoms, generates a charge transfer complex, that results in a shift of the UV-light absorption threshold of the nanostructured TiO_2 based electrode toward the visible spectral region and, hence, in the occurrence of an absorption band centered at 450 nm. The photoelectrochemical monitoring of the formation of the AA-TiO_2 complex, under the visible light illumination of a commercial LED light source, allows the selective and quantitative detection of the target microRNA strands.

O5 EL

PREPARATION AND CHARACTERIZATION OF NOVEL SONOGEL-CARBON ELECTRODES CONTAINING CARBON BLACK: APPLICATION AS AMPEROMETRIC SENSORS FOR DETERMINATION OF POLYPHENOLIC COMPOUNDS

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Amperometric sensors are very efficient devices widely applied to the measurement of concentration of different analytes thanks to their good sensitivities and wide linear ranges. Moreover, they can be low cost, they don't necessitate expensive instrumentation and are simple to use, so that they are diffused in different areas of chemical analysis among which food authentication or processing, environmental monitoring, medical applications and quality control. In the development of effective electrode systems, electrode materials play the most meaningful role, imparting the device specific physico-chemical properties and corresponding analytical peculiarities.

In this communication we present novel Sonogel-Carbon (SNGC) electrodes modified with a carbonaceous nanostructured material, namely carbon black (SNGC_CB). SNGC electrodes are characterized by robustness, coupled to reduced dimensions and good electrochemical efficiency, particularly as to sensitivity and reproducibility of the sensor. Moreover, through the inclusion of different components in the graphite phase, electrocatalytic processes can be activated. In this context, CB is particularly appealing due to its excellent conductivity and electrocatalytic properties.

SNGC_CB electrodes have been characterized by SEM, Raman spectroscopy, electrochemical impedance spectroscopy and cyclic voltammetry, showing good reproducibility and repeatability of the responses. The modified electrodes have shown improved efficiency with respect to SNGC electrodes in the individual and simultaneous detection of two isomers of dihydroxybenzene, namely catechol (CC) and hydroquinone (HQ), exhibiting wide linear ranges of the signals and low limit of detection. Moreover, the behavior of SNGC_CB electrodes has also been investigated with respect to the detection of caffeic acid (CA), viz. a molecule containing a catechol group, widely diffused in plants and fruits as well as in the derived beverages. Thanks to the satisfactory results obtained, an electrochemical method has been developed for the rapid estimation of the overall content of chlorogenic acids, among which CA, in several instant coffee samples. Finally, preliminary tests performed in matrices rich of natural antioxidants species, such as different wines, suggest that, under proper conditions, SNGC_CB electrodes can be successfully used for the detection of the main families of anthocyanins.

O6 EL

Layered double hydroxides as electrode modifiers for (bio)sensing applications

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Our group has been extensively used layered double hydroxides (LDHs) to modify conductive supports with the aim to develop electrochemical sensors.
Their general formula is: $[M^{II}_{1-x}M^{III}_{x}(OH)_2]^{x+}(X_q^{-x/q})\cdot nH_2O]$. Firstly, the properties of anionic exchange of LDHs were exploited to develop potentiometric sensors for the detection of chloride, sulfate, and phosphate. Even if LDHs can be considered non-conductive materials, if a transition metal which undergoes a reversible redox reaction is present in the LDH brucite layers, the material becomes conductive and can be exploited to electrocatalyse the oxidation of many compounds. Ni and Co based LDHs were used as electrode modifiers for the development of amperometric sensors to detect alcohols, sugars, phenols, amines, salicylic acid, glyphosate, and glufosinate [1]. Until 2004, the LDHs were chemically synthesised and the conductive supports were modified by casting. In the following, we developed an electrochemical synthesis based on the generation of an alkaline pH next to the electrode (generally Pt or GC) in the presence of the bivalent and trivalent cations which allowed to obtain a tunable control of the thickness of the LDH film and a better adhesion of the same on the electrode. In such a way, the modified electrodes were used as detectors of sugars in flow systems without detachment of the films for long periods [2]. A pH sensor was fabricated with a Co/Al LDH coating GC which displayed a super-Nernstian response and was particularly suitable to operate in strongly alkaline solution. The same LDH electrodeposited on ITO was exploited for the development of an optical sensor for glucose due to its reversible electrochromic behavior. Electrodes modified with conductive or not conductive LDHs were also proposed as biosensors for glucose and lactate. Very recently, our research has focused on three issues: i) to get an amplified signal in respect to the one of a typical amperometric sensor: to this aim the same configuration used for the development of glucose biosensors has been embedded in the architecture of an organic electrochemical transistor; ii) to improve the electrocatalytic activity of Ni centres synthesising LDHs containing Fe instead of Al, as trivalent cation, or composites based on Au nanoparticles uniformly dispersed on a nanosized Ni/Al LDH matrix; iii) to improve LDH electrical conductivity by carrying out the LDH electrosynthesis on GC electrodes modified with carbon nanomaterials so obtaining better performing sensors.

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O1 BO

IDENTIFICATION OF AUTISM SPECTRUM DISORDER BIOMARKERS BY LIQUID CHROMATOGRAPHY COUPLED WITH MASS SPECTROMETRY

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It is recognized that *any perturbation of a biological system is expected to give rise to changes in the abundance and/or composition of the lipid pool* [1]. Autism spectrum disorder (ASD) is a heterogeneous group of neurological developmental disorders affecting approximately 0.63% of children worldwide; ASD indicators arise early in childhood and involve social skills, communicative language and imagination, as well as narrowness of focus resulting in rigidity, anxieties, repetitive movements and speech [2]. Presently, a medical test to diagnose autism unequivocally does not exist; the only system in use consists of an interview performed by specialized physicians and psychologists for autism-specific behavioral evaluations.

To identify and characterize early biomarkers for ASD, lipid levels and their composition in lymphocytes have been investigated. The study has been performed on samples obtained from patients affected by ASD without any pharmacological treatment. ASD individuals were categorised on a disease severity degree from 1 to 3 according to *Diagnostic and Statistical Manual of Mental Disorders* (DSM-5) and from their unaffected brothers or sisters, considering participants with age between 3 and 16 years.

The lipid extract obtained following the Bligh & Dyer protocol [3] has been analyzed by *hydrophilic interaction liquid chromatography* (HILIC) coupled with electrospray ionization high-resolution/accuracy Fourier-transform mass spectrometry (ESI-FTMS) [4]. To manage the large amount of data obtained using an *untargeted lipidomic approach*, different metabolomic and lipidomic software performances, e.g, Lipid Data Analysis [5] and XCMS [6] have been compared; in the first software package, a database containing more than 25000 lipid species, each with different ionization ability both in positive and negative ion mode has been written. Statistical approaches have been applied to discover plausible ASD lipid biomarkers; MS/MS and MS^n have been performed to obtain lipid species identification. In this communication, we provide a preliminary description of how some of the main software packages work, which may help lipidomic data analysis as an integrated technology in the clinical medicine of patients affected by ASD.

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O2 BO

Hydrogel Extraction Surface Analysis (HESA): an option for shotgun quantitative proteomics from cardiac myxoma FFPE biopsy

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The Hydrogel Extraction Surface Analysis (HESA) is an analytical method for histology-directed on-tissue protein digestion coupled with mass spectrometry for both qualitative and quantitative analysis. The HESA is based on the use of a miniaturized enzyme delivery platform, called hydrogel, which is fabricated as a microwell (e.g., 3mm Ø). The whole strategy is characterized by minimum sample manipulation and minimum biopsy material needs: a tissue section is cut (12 µm), the hydrogels are properly activated (by swelling with 0.125 µg of trypsin buffered solution) and placed onto one or more regions of the tissue surface according to the histology (e.g., tumor/adjacent area). After *in situ* digestion (2min, microwave), peptides are TMT labeled, solvent extracted, and LC-MS/MS analyzed (Figure 1).

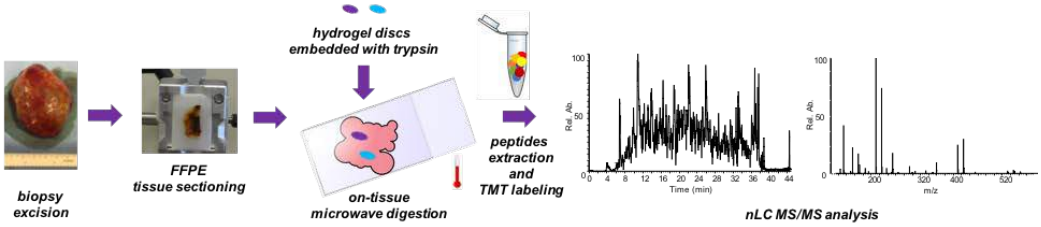

Figure 1. HESA workflow for on-tissue protein digestion, peptides extraction, TMT labeling and LC-MS/MS analysis for protein quantification from two myxoma tumor regions.

Since proteins are extracted from the area covered by the disc, the tissue section is not destroyed by the whole process. So, the tissue can be further used for staining or immunohistochemistry. The HESA concept was early introduced on fresh-frozen tissues for qualitative proteins localization [1], then implemented for quantification [2]. Here, the HESA was successfully applied for protein quantification for the first time to a FFPE biopsy from a cardiac myxoma patient. A total of 1869 proteins (FDR 0.01, min. 2 peptides) were localized and quantified from myxoma vascularized (V) region and the adjacent hypo-cellulated (H) area in sample limited conditions (12µm tissue thickness; 7mm^2 tissue area; 40-100ng protein recovery). The repeatability in protein recovery was demonstrated (R^2=0.985, V; R^2=0.975, H). Finally, differentially expressed proteins were identified (11 over-expressed in V; 4 in H).

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[2] D. Taverna, C. Mignogna, C. Gabriele, G. Santise, G. Donato, G. Cuda, M. Gaspari, An optimized procedure for on-tissue localized protein digestion and quantification using hydrogel discs and isobaric mass tags: analysis of cardiac myxoma. Anal. Bioanal. Chem. 409 (2017) 6935-6944.

O3 BO

URINARY STEROIDAL PROFILE AS INNOVATIVE TOOL FOR THE SCREENING OF PROSTATE DISEASES

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The screening procedures presently used to detect prostatic diseases, involve PSA measurement and digito-rectal exploration, but results in excessive false positive findings. These induce the execution of useless biopsies (invasive, expensive, stressful both physically and psychologically) on healthy men. The present study proposes the use of an extended urinary steroid profile (USP) as new screening tool for the detection of prostatic carcinoma. The whole profile includes 18 androgens, detected by GC-MS, plus 5 steroid concentration ratios. The analytical procedure and instrumentation has limited costs and wide availability, making it suitable for broad-spectrum screening application. A total of 300 urinary samples from men affected by benign prostatic hypertrophy (BPH) and prostatic carcinoma (CAP) were collected. The USPs were used to build a PLS-DA classification model, subsequently submitted to external validation using the 20% of the data. It produces a slightly better sensitivity (81% *versus* 78%) and much better specificity, i.e. 84% *vs* 55%, with respect to the PSA cut-off of 4 ng/mL (PSA performances have been calculated over our dataset). To obtain a stratification of the response, useful for personalized prevention medical programs, regression and likelihood ratio tools have been applied to the class probability scores.

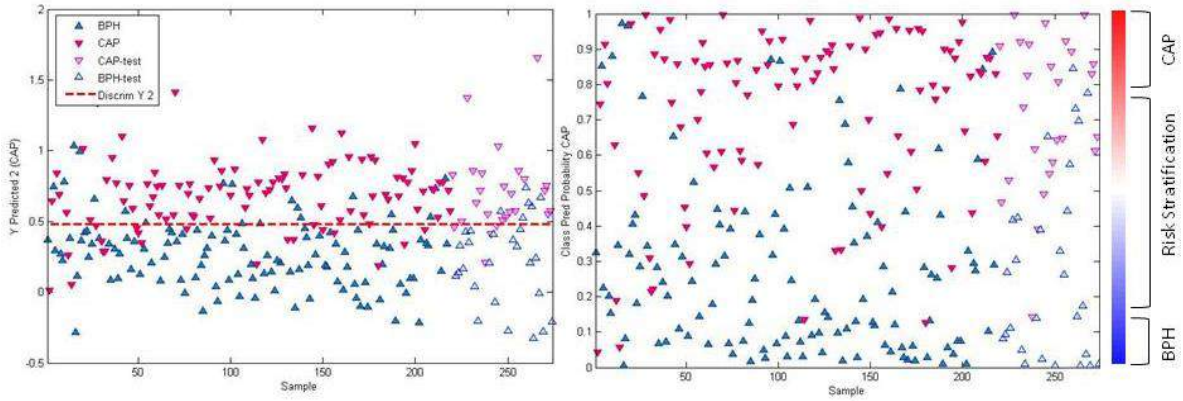

Figure 1. Scores plot representing the Y predicted for the training and evaluation sets with respect to the threshold (left) and class probability for each sample (right). Moreover, a qualitative representation of the stratification of the response is given (color-bar).

O4 BO

MICRO EXTRACTION BY PACKED SORBENT COUPLED TO LIQUID CHROMATOGRAPHY-TANDEM MASS SPECTROMETRY FOR THE ANALYSIS OF PROSTANOIDS AND ISOPROSTANOIDS IN DRIED BLOOD SPOTS

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The current pharmacological treatment in preterm newborns suffering from Patent Ductus Arteriosus is based on prostaglandin-E_2 suppression by cyclooxygenase inhibitors (e.g. ibuprofen, acetaminophen) and is far from being optimal due to possible adverse effects and frequent failures. Monitoring inflammation and oxidative stress mediators, such as prostanoids and isoprostanoids in blood, could assess their potential role as predictors of response to therapy [1].

In this work a very innovative procedure, based on micro-extraction by packed sorbent (MEPS) coupled to liquid chromatography-tandem mass spectrometry (UHPLC-ESI-MS/MS), was developed for the determination of prostaglandin-E_2, 8-iso-prostaglandin-$F_{2\alpha}$ and 8-iso-prostaglandin-E_2 in dried blood spots (DBSs). The chromatographic separation of the analytes was achieved in less than 10 minutes on a reversed-phase Polaris-C18 column by a gradient elution, using aqueous formic acid (0.1%) and a mixture of acetonitrile:methanol (50:50 v/v). Detection was carried out on a triple quadrupole mass spectrometer operating in ESI(-) and MRM mode. A novel and fast (< 10 min) MEPS procedure was optimized for the clean-up and pre-concentration of the analytes extracted from the DBS (50 µL) by a methanol:water mixture (70:30 v/v). The analytical method was validated and showed LODs below 20 pg/mL, linear calibration range (R^2 > 0.99) over three orders of magnitude, satisfactory recovery (> 70%) and very good overall intra- and inter-day precisions (RSD < 10%) for all the analytes. The labelled internal standard (i.e. 8-iso-prostaglandin-$F_{2\alpha}$-d4) was successfully laid on the filter paper instead of the common addition to the extraction solvent [2], in order to control both storage and extraction steps. Analytes stability was also investigated. The method was successfully applied for the fast and non-invasive monitoring of preterm newborns.

[1] J. X. Chen *et al*., Isoprostanes as physiological mediators of transition to newborn life: novel mechanisms regulating patency of the term and preterm ductus arteriosus. Pediatr. Res. 72 (2) (2012) 122-8.

[2] N. E. Bastani *et al*., Dried blood spot (DBS) sample collection for determination of the oxidative stress biomarker 8-epi-PGF_{2a} in humans using liquid chromatography/tandem mass spectrometry. Rapid Commun. Mass Spectrom. 26 (2012) 645–652.

O5 BO

IMPROVING LC-MS DETECTION OF PHOSPHOLIPIDS BY MOLECULARLY DESIGNED CLASS SELECTIVE SPE SORBENTS

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Lipids play several essential roles in human physiology by means of a variety of distinct structural lipid classes. The huge diversity of structural isomers and isobaric compounds makes confident identification a challenging task. There are as many as 180,000 different lipid molecular species that can be found in a narrow mass range thus requiring some kind of separation prior mass spectrometric. Common strategies for improving LC-MS detection in lipidomics are 2D-LC chromatography, use of chiral columns, SPE fractionation and chemical derivatization. Among others, the bioactive sphingolipid metabolite Sphingosine 1-phosphate (S1P) is a phospholipid that is formed in the intracellular environment and has important mitochondrial and nuclear targets and on the cell membrane where specific receptors are present. [1] According to recent studies, S1P levels are strictly regulated by the balance between synthesis and degradation thanks to the activity of three specific enzymes: kinase, phosphatase and lyase. [2] In order to quantify S1P in human plasma and serum, it has been shown that the platelets, after their activation, release large quantities of it, so changes in the levels of sphingosine 1-phosphate in the circulatory stream, due to an upregulation of sphingosine kinases, may be related to clinical disorders. [3] S1P is currently recognized as a critical regulator of many physiological and pathophysiological processes [4], including inflammation, tumors and neurodegenerative diseases. Based on previous results [5], in this study we present a new material able to enrich and capture the phosphorylated molecule S1P as well as the new drug Fingolimod Phosphate and its pro-drug Fingolimod in complex matrices. The resin was synthesized using bis-imidazolium functional monomer and divinylbenzene (DVB) in a porogen environment consisting of toluene:methanol (1:1) mixture. The selective SPE greatly simplify LC-MS detection of these metabolites. The sorbent materials were characterized using several techniques including optical microscopy, SEM, BET, IR spectroscopy and thermogravimetric analysis. Sorbents selectivity was evaluated on different solvents and real plasma samples.

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[2] S. Spiegel, S. Milstien; Nat. Rev. Molecular Cell Biology, 4 (2003) 397-407.
[3] Y. Yatomi et al.; J. Biochem. 121 (1997) 969-973.
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O1 EC

INVESTIGATING SYNTHETIC POLYMERS IN HERITAGE OBJECTS: A MULTI-ANALYTICAL APPROACH FOR THE STUDY OF POLYURETHANE FOAMS IN 1960S SCULPTURES

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Synthetic materials of new formulation have influenced contemporary artists since the beginning of last century; consequently, the conservation of synthetic polymers in modern and contemporary art is, at present, a matter of great importance.
Among the wide variety of synthetic polymers that can be encountered in XX century art, the family of polyurethanes (PU) can be found in works of art as flexible and rigid foams, or in design furniture as upholstery foams. Polyurethane was first synthetized in 1937 in Germany; however only in the late 1960s artists approached this new material, appealed by its peculiar properties, such as lightness and softness.
Nowadays, conservators have to face the limited durability of polyurethane foams: they already show degradation phenomena affecting the stability of artworks after a few decades from their production. The limited amount of data about long-term stability of polyurethane foam, along with the existence of a wide variety of possible types and compositions for these materials, make the preservation of PU foams in artworks a critical issue.
This work aims at evaluating the composition and the state of preservation of the PU foams constituting the 1960s Italian pop-art sculpture "Disgelo" (1968) by Piero Gilardi and "Contenitoreumano n.1" (1968) by Ico Parisi (1916-1996) and Francesco Somaini (1926-2005).
In order to obtain a full picture of the composition of the two PU sculptures, evolved gas analysis/mass spectrometry (EGA-MS) and pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS) with multi-shot technique were applied to define the chemical composition of the PU foams, paint and organic pigments. The two analytical approaches were applied on micro-samples of the PU foam with different states of preservation, in order to obtain a picture of the degradation processes of the PU, based on its thermal degradation behaviour. The two approaches were applied in this study for the first time in the characterisation of PU in cultural heritage.
Moreover, high-performance liquid chromatography with diode-array detection (HPLC-DAD) analyses were performed to confirm the identification of the organic pigments in the Gilardi's work of art.

EMISSIONS FROM PELLETS COMBUSTION: A STUDY ON STOVES TO EVALUATE THE IMPACT ON ATMOSPHERIC AEROSOL

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During recent years, the use of biofuels as energy source has raised significantly in Europe, due to its limited cost, availability, and being a renewable energy source. According to the European Commission, solid biofules combustion in households accounts for about one third of all PM emissions. Similarly, in Italy, wood combustion accounts for one third of PM emissions as well, with the largest part attributed to open and closed fireplaces and traditional stoves. Recently, combustion of wood logs in traditional appliances has been replaced in several areas by combustion of wood pellets. Still limited knowledge exists on wood pellet combustion emissions, and their contribution to ambient particulate matter (PM). In the framework of a project carried out in collaboration with Innovhub-Stazioni sperimentali per l'industria, we analyzed the main pollutants emitted by pellet combustion. Two types of stoves and two types of pellets were tested: overall four stoves, two high and two low performing appliances were powered with high and low quality pellets. The impact of combustion appliance ageing on emissions was investigated over one year. Stoves emissions were collected with a dilution tunnel both at the beginning and at the end of the project. Furthermore, daily PM2.5 and PM10 samples were collected nearby the chimneys of pellet stoves. All the samples have been analyzed for organic and elemental carbon, by thermo-optical analysis, for water-soluble inorganic species, by ion-chromatography, and for levoglucosan concentration, by ion-chromatography with amperometric detector [1].
The analysis of stoves filters shows that the pellets quality has a stronger impact on OC emissions than the appliance performance level: a high performance stove burning low quality pellets emits higher OC amounts than a low performance stove burning high quality pellets. Ambient PM samples have been divided into 3 categories, depending on meteorological parameter and stoves working conditions: 1) stoves off; 2) stoves on and samplers intercepting chimneys emissions; 3) stoves on and chimneys emissions not impacting samplers. As regards ambient samples we observed that pellet stoves didn't impact on levoglucosan concentrations, in agreement with laboratory observations showing that levoglucosan emissions from pellet burning are negligible compared to wood log burning. On the other hand, water soluble potassium can be considered a good marker for pellet combustion. The chemical speciation of pellet combustion emission during this study will support the improvement of local emission inventories to better understand the impact of biofuel use at local and regional scale.

[1] A. Piazzalunga, V. Bernardoni, R. Vecchi, P. Fermo, Optimisation of analytical procedures for the quantification of ionic and carbonaceous fractions in the atmospheric aerosol and applications to ambient samples. Anal Bioanal. Chem. 405 (2013) 1123-32.

O3 EC

UNVEILING RISKS CONCEALED IN TEXTILES

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The textile industry is often referred as one of the most polluting productive activity because of the large use of water and highly toxic compounds. Thousands of chemicals are involved in the manufacturing steps including fibers production, bleaching, dyeing and finishing. Over the years there has been growing concern about the environmental impacts of textile industry, and EU authorities are pushing toward more sustainable productions within REACH and Ecolabel criteria [1]. On the other hand, several risks for human health might be still present in the finished product. Recent results demonstrated that small amounts of potentially harmful compounds might be released from common consumer products [2].
In order to evaluate the risk of exposure and the threats to human health, efficient analytical procedures for a broad range of compounds are necessary [3]. Explorative non-targeted screening analysis of textile materials in common clothing revealed the presence of thousands of compounds. According to frequency of occurrence, skin penetrating properties and toxicological data, analytical methods were developed for their extraction and quantification, with focus set on four groups of compounds: benzothiazoles, benzotriazoles, quinolines and aromatic amines.
This presentation will report the analytical procedures developed as well as the results obtained so far in the search for the chemicals occurrence and the evidence for potential risks.

[1] 2014/350/EU: Commission Decision of 5 June 2014 establishing the ecological criteria for the award of the EU Ecolabel for textile products (notified under document C (2014) 3677) Text with EEA relevance, 2014.
[2] G. Luongo, Chemicals in textiles: A potential source for human exposure and environmental pollution, Ph.D. thesis, Stockholm University (2015).
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O4 EC

SELECTIVE EXTRACTION OF WATER-SOLUBLE THALLIUM FRACTION FROM CONTAMINATED DRINKING-WATER DISTRIBUTION NETWORKS: OPTIMIZATION OF THE PROCEDURE AND EXTRACTS SPECIATION

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Metallic pipes in drinking water (DW) distribution networks are able to retain some elements over time that may be subsequently released into the water. In September 2014, researchers from the Department of Earth Sciences (University of *Pisa*, Tuscany, Italy) reported the presence of thallium in water samples collected from *Pietrasanta* DW wells (*Lucca*, Tuscany, Italy) at concentrations (up to 10 µg/L) much higher than US-EPA max contaminant level goal (2.0 µg/L).
So far, there is no analytical sequential extraction procedure to selectively distinguish between the fraction released into DW, characterized by health and hygiene relevance, and the remaining insoluble one, strongly retained on the pipe inner surface. In 1992, Community Bureau of Reference (BCR) published an extraction procedure to be applied to sludge and sediments, in which four extracting solvents with increasing reactivity were sequentially made to come into contact with the sample. In particular, an acetic acid solution was used to dissolve the water-soluble fraction at weakly acid pH during the first extraction step. The procedure, optimized for fine powdered solids that are dispersible in the extracting solvent by mechanical stirring, is not suitable for thick alternating layers, which could cover the inner surface of pipe core samples.
Starting from the BCR method, we have developed an innovative procedure to determine the thallium water-soluble fraction retained by contaminated pipe core samples. The target fraction is solubilized in acetic acid solution by means of consecutive sonication treatments (at least, five) carried out after changing the aliquot of the extractant. All the working conditions (such as, solvent volume and concentration, sonication time) have been optimized while the number of extraction steps required to ensure the complete dissolution of the water-soluble fraction has been calculated. The obtained extracts were analyzed by ICP-MS and subsequently speciated by polarography with a dropping mercury electrode (DME) and by HPLC - ICP-MS, as well. The procedure applied to a number of pipe core samples collected from a thallium-contaminated DW network showed the presence of the water-soluble fraction in a percentage of 5-9 % of the total quantity detected, mainly coming from the release of Tl(I)-enriched layers.

O5 EC

MICROPLASTIC POLLUTION IN ICE, SNOW AND SEDIMENTS FROM VESIJÄRVI AND PIKKU VESIJÄRVI LAKES, FINLAND

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Microplastics (MPs) have been identified as contaminants of emerging concern in aquatic environments. In the last few years, several studies have investigated MPs in marine ecosystems, but data on freshwater environments are still scarce [1]. The present study aims to investigate the occurrence, distribution and sources of MP pollution in Vesijärvi and Pikku Vesijärvi Lakes, near the city of Lahti (Finland).

Sediment, snow and ice-core samples were collected near the shore of the two lakes. MPs in snow and ice-core samples were filtered on glass fibers, while MPs in sediment samples were first extracted through a density separation. MPs were analyzed and identified by a non-invasive method consisting in a Fourier Transform Infrared Spectroscopy (FTIR) 2D Imaging. Lake Vesijärvi is known to be a great example of lake restoration in Finland [2] and a big attraction for tourists and citizens of Lahti going there for skiing, skating, sledging and walking on the frozen surface in winter. These activities could represent a remarkable source of MPs that end up in the freshwater environment posing a risk for the biota and likely entering the food web.

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O6 EC

ISOTOPIC ANALYSIS OF ANTARCTIC SNOW BY QUADRUPOLE INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY USING A TOTAL-CONSUMPTION SAMPLE INTRODUCTION SYSTEM

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The determination of Pb and Sr isotope ratios in snow and ice from polar areas can provide useful information on the sources of both natural and anthropogenic atmospheric inputs, the relative contributions of these sources over time and the corresponding transport routes. However, precise and accurate determination of isotope ratios is quite challenging, due to the low analyte concentration (typically at the pg/g level), thus requiring ultra-clean collection, storage and treatment procedures. In addition, the limited amount of sample typically available can prevent the application of efficient preconcentration approaches and the identification of short time-scale events. Finally, these studies generally make use of high-priced instrumentation, such as thermal ionization mass spectrometry (TIMS) and multi-collector inductively coupled plasma mass spectrometry (MC-ICP-MS), whereas cheaper techniques such as quadrupole ICP-MS would be advantageous.
In order to overcome these limitations for the analysis of snow samples, we applied a simple preconcentration procedure in combination with quadrupole ICP-MS equipped with a total consumption sample introduction system. This apparatus, called torch-integrated sample introduction system (TISIS) [1-2], consists of a PFA micronebulizer coupled to a heated single-pass evaporation chamber, with a sheathing gas stream protecting the aerosol from impacts against the chamber walls. The main advantages of this system include an increase in sensitivity and the capability of working at very low sample consumption rates (20 µl/min), allowing to preconcentrate the samples to small volumes (200 µl) and so achieving high preconcentration factors.
Different analytical methods were optimized for Pb and Sr to obtain the best conditions of sheathing gas flow rate and main instrumental parameters. Then, they were characterized in terms of working range, precision, accuracy, limit of detection and isotope fractionation. Finally, they were applied to the analysis of snow samples collected from the Antarctic plateau in the context of the Italian National Research Program in Antarctica. In order to improve the confidence in the developed methods, data were compared to those obtained by a reference method (MC-ICP-MS).

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O7 EC

MINIATURIZED BIOSENSORS TO PRESERVE AND MONITOR CULTURAL HERITAGE: FROM MEDICAL TO CONSERVATION DIAGNOSIS

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We design and develop portable and reliable analytical systems, which can be used on site by not specialized operators, supporting restoration campaigns at a limited cost. Thus, these tools would allow restorers to rapidly obtain information to guide their restoration strategy. The proposed devices exploit the lateral flow immunoassay (LFIA) system to obtain maximum user-friendliness, as the operator does not need to manipulate any reagent.
For the first time, multiplex LFIA biosensors were designed for in situ analysis of historical materials allowing simultaneous detection of collagen and ovalbumin. The two biosensor formats differ from one another by the detection principle: CL reaction catalyzed by enzymes in one case and AuNP colorimetric approach in the other. Their performances have been evaluated for the in situ identification of ovalbumin and collagen in microextracts obtained from 0.5 mg of paint samples. The detectability of the chemiluminescent system was two times higher than that of the colorimetric system. The CL-LFIA method requires a multistep analytical protocol with sequential addition of sample and reagents. To simplify the procedure, we designed a disposable analytical cartridge containing the LFIA strip and all the necessary reagents. Thus, only the sample must be added. In addition, to keep the device small, we used a "contact imaging" configuration, in which the CL signal is conveyed to the CCD sensor by a fiber optic faceplate (Fig. 1). These results point to the enormous potential of these cheap, easy-to-use, and minimally invasive diagnostic tools for conservators and restorers in the cultural heritage field.

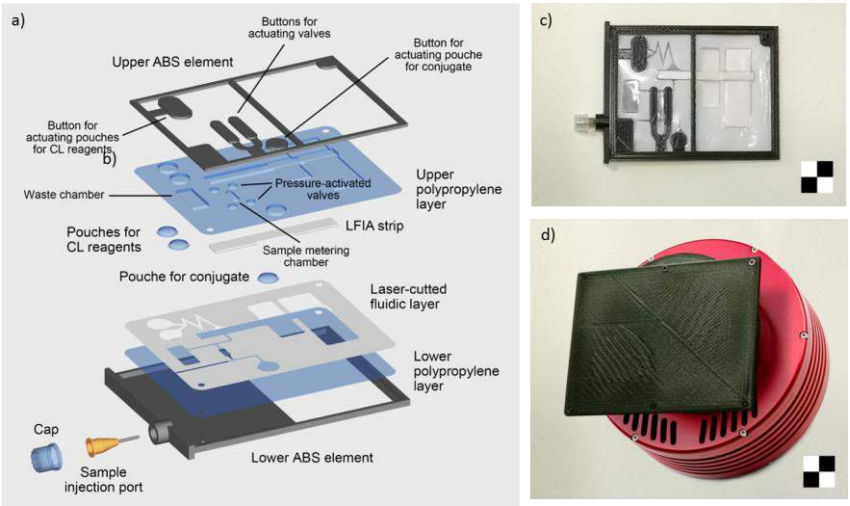

Figure 1. a) Layout and b) Image of the disposable analytical cartridge; c) CCD camera with 3D-printed box. Scale checkerboard is 2x2 cm.

O8 EC

CHARACTERIZATION AND TEMPORAL EVOLUTION OF THE ELEMENTAL COMPOSITION OF PM_{10} COLLECTED AT NY-ÅLESUND (THE ARCTIC)

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In this study, the elemental composition of PM_{10} samples collected in Ny-Ålesund (Norwegian Arctic) in the sampling campaigns 2010-2013 was investigated, with the purpose to identify the PM sources and to understand short- and long-range transport processes [1]. Enrichment factors were calculated for all elements with respect to the mean values for the Earth's crust reported by Wedepohl [2] and to the mean abundances in sea water reported by Goldberg [3], in order to distinguish elements having natural, anthropic or mixed origin. The results obtained so far evidence a remarkable seasonal trend for most of the investigated elements. For both geogenic and anthropogenic elements, concentrations are generally higher in March and April, when the ground is almost entirely covered by snow and ice, suggesting that long-range transport processes might be taking place. On the other hand, the elements typically deriving from marine aerosol (i.e. Mg and Na) present higher concentrations in late spring and summer, together with Co, Ni and V, typical anthropogenic metals related to ship emissions. From the Kruskal-Wallis and Conover-Iman tests it emerged that, for most of the analytes, the four campaigns are not significantly different; therefore, in the studied period, the composition of PM_{10} in Ny-Ålesund did not vary remarkably. Principal Component Analysis allowed us to better understand the sources of different elements and to lay the basis for an interpretation of the chemical and physical processes concerning the Arctic atmosphere. Airborne pollution deriving from ship fuels, local vehicle and continental emissions resulted to be the main sources of anthropogenic elements.

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O9 EC

REMOVAL OF HEAVY METALS FROM CONTAMINATED ZEOLITIC TUFF WITH (S,S) ETHYLENEDIAMINE-**N,N'**-DISUCCINIC ACID

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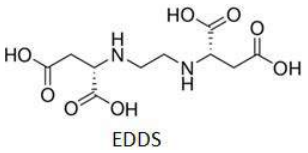

EDDS

Soils contaminated by heavy metals, including some toxic, pose a danger to public health (as they are involved in the food chain). Their remediation through minimally invasive technics is still an open problem. The use of biodegradable complexing agents with high sequestering capacity towards toxic metals is a sustainable technique that modifies little of the ecosystem (soil washing).[1] (S,S) Ethylenediamine-N,N'-disuccinic acid (EDDS) represents a valid candidate, due to its biodegradability (*half–life* of 4.2 days) and low toxicity (LD_{50} (rat) = 2700 mg/kg). Aim of present work is to study the sequestering capacity of the EDDS ligand on the volcanic tuff of zeolitic matrix (Neapolitan yellow tuff variety), very common in the Phlegrean area, contaminated by heavy metals. In the first phase the characterization of the acid base properties of the solid phase surface has been conducted, through potentiometric titrations carried out at 25° C in 0.1 M $NaClO_4$. Furthermore, complexation reactions of EDDS towards some heavy metals (such as Pb(II) and Gd(III)) have been studied. Subsequently a model of speciation of the adsorption of metals in the presence of EDDS is proposed. The stoichiometric of the metal-ligand species in solution has been validated through spectroscopic measurements (UV-VIS, CD-UV and ^{1}H-NMR). Finally, the efficiency of the removal of heavy metals from a sample of contaminated tuff has been obtained at 25° C (by determining the amount of analyte adsorbed per gram of solid depending on the pH and the EDDS concentration. Information on the solid-metal interaction mechanism is obtained by measurements in function of time.

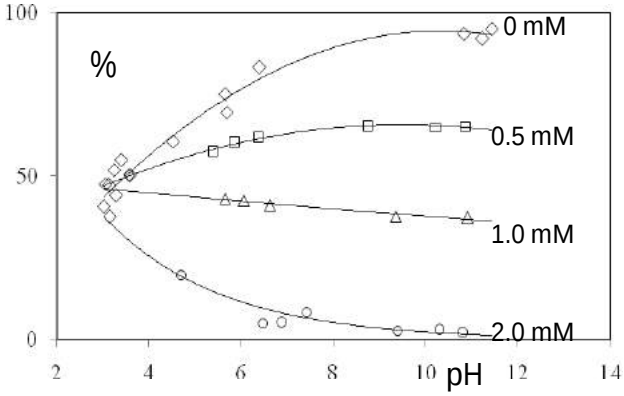

Fig. % Pb adsorption onto yellow tuff in function of pH at different EDDS concentrations (value indicated near curve) at 25° C in 0.1 M $NaClO_4$.

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O10 EC

IDENTIFICATION AND QUANTIFICATION OF SYSTEMIC INSECTICIDES AND THEIR METABOLITES BY UHPLC-HRMS

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Systemic insecticides are widely used for pests control and their success is due to their ability of protect the whole plant from roots to the upper leaf. In particular, seeds coating technique is very popular and it is applied to many crops (e.g. corn). However, the use of high amount of Active Ingredient (AI) for seeds coating is causing concern about negative effects to non-target animals. Pollinators insects are exposed to contaminated pollen and nectar, but also herbivore insects are exposed through contaminated leaf. In addition, these insecticides can leach from fields and contaminate wild plants or waterbodies. Therefore, also aquatic species are exposed to insecticides pollution and vertebrates like birds and small mammals could be exposed through coated seeds, seedling and insects [1].
The aim of this study was to develop an UHPLC-HRMS method for the identification of insecticides and their degradation production in corn guttation drops. Particular attention was posed to metabolites, because few information is available in the literature about their presence in relevant matrix for eco-toxicological studies [2]. In addition, some metabolites may have greater toxicity if compared with their parent compounds. In particular, neonicotinoids imine metabolites are characterized by an inversion of selectivity between insects and mammals. Therefore, they can be more toxic for mammals if compared to the neonicotinoids AI [3].
Several metabolites were identified in corn guttation and an extraction procedure based on QuEChERS strategy coupled with a target UHPLC-MS^2 method was developed and validated for the quantification of these compounds in corn leaf. High concentration of neonicotinoids thiamethoxam, clothianidin and thiacloprid were observed in corn seedling. Concerning the carbamate methiocarb, the AI was observed only at low concentration, but its metabolites were present at µg/g level. Particularly interesting was the presence of methiocarb sulfoxide, because this metabolite is more toxic of the parent compounds for some species.
In conclusion, guttation analysis with UHPLC-HRMS is a powerful technique in order to assess the presence of insecticides metabolites in plants treated with systemic AI. However, UHPLC-MS^2 still provide better performance for quantitative analysis, in particular for complex matrices as corn leaf.

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[3] M. Tomizawa e J. E. Casida, NEONICOTINOID INSECTICIDE TOXICOLOGY: Mechanisms of Selective Action. Annu. Rev. Pharmacol. Toxicol. vol. 45, n. 1, pagg. 247–268 (2005).

O11 EC

EXPERIMENTAL METHODOLOGY TO MEASURE THE REACTION RATE CONSTANTS OF PROCESSES SENSITIZED BY THE TRIPLET STATE OF 4-CARBOXYBENZOPHENONE AS PROXY OF THE TRIPLET STATES OF CHROMOPHORIC DISSOLVED ORGANIC MATTER

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By combination of transient absorption spectroscopy (Laser Flash Photolysis) and steady-state irradiation experiments, we investigated the transformation of phenol and furfuryl alcohol (FFA) sensitized by irradiated 4-carboxybenzophenone (CBBP). The latter is a reasonable proxy molecule to assess the reactivity of the excited triplet states of the chromophoric dissolved organic matter (^{3}CDOM*) that occurs in natural waters and that plays often an important role in the photochemically activated self-depollution ability of water bodies.[1,2] The main reactive species for the transformation of both phenol and FFA was the CBBP triplet state (^{3}CBBP*), despite the fact that FFA is a commonly used probe for singlet oxygen ($^1O_2$). In the case of FFA it was possible to develop a simple kinetic model that fitted well the experimental data obtained by steady-state irradiation, in a wide range of FFA concentration values. The GC-MS analysis carried out with a SPME fiber coated showed that furfural was the only detected FFA transformation intermediate. In the case of phenol the model was made much more complex by the likely occurrence of back reactions [2] between radical species (e.g., phenoxyl and superoxide). This problem can be tackled by considering only the experimental data at low phenol concentration, where the degradation rate increases linearly with concentration.
We do not recommend the use of $^1O_2$ scavengers/quenchers such as sodium azide to elucidate CBBP photoreaction pathways, because the azide provides misleading results by also acting as a triplet state quencher. Based on the experimental data, we propose a methodology for the measurement of the CBBP triplet-sensitization rate constants from steady-state irradiation experiments, allowing for a better assessment of the triplet-sensitized degradation of emerging contaminants in irradiated natural waters.

[1] D. Vione, M. Minella, V. Maurino, C. Minero, Indirect photochemistry in sunlit surface waters: Photoinduced production of reactive transient species. Chem.-Eur. J. 20 (2014) 10590-10606.
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O12 EC

FRAGRANCES AS NEW ENVIRONMENTAL CONTAMINANTS

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Fragrance Materials (FMs) are ubiquitous components of household and Personal Care Products (PCPs), whose environmental fate is still largely unknown. We chose 17 among the longest-lasting and most stable fragrance ingredients that are commercially available (Givaudan®: Amberketal, Ambrofix, Amyl Salicylate, Benzyl Salicylate, Bourgeonal, Dupical, Hexyl Salicylate, Isobutavan, Lemonile, Mefranal, Myraldene, Okoumal, Oranger Crystals, Pelargene, Peonile, Sandalore, Ultravanil) to assess their persistence, distribution and transport in the ecosystem. A new analytical method was developed to quantify FMs in water samples using Oasis HLB SPE followed by HRGC-LRMS (7890A-5975C, Agilent Technologies).

The selected fragrances were found as contaminants in the Venice Lagoon: urban sewages largely emit these FMs into the surface seawater, reaching total concentrations higher than 10 μg L-1 in the innermost urban canals [1]. This pilot study reported the first detection in environmental samples for most of the selected FMs. The distribution of these FMs was later studied in the coastal seawater of the Ross Sea, Antarctica [2] and in snow samples from the Svalbard Islands. Local emission of FMs from the research bases was revealed, together with evidences of a long-range atmospheric transport (LRAT) of these substances. These compounds were also detected in open sea areas of the Mediterranean, highlighting the role of mesoscale hydrodynamics and LRAT as key factors [3]. In each of the investigated environments the allergenic and oestrogenic Salicylate compounds resulted in general the most abundant and widespread components, probably due to their large global consumption. These findings support the hypothesis of the environmental persistence of the selected FMs, highlighting future research priorities.

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[2] M. Vecchiato, E. Gregoris, E. Barbaro, C. Barbante, R. Piazza, A. Gambaro, Fragrances in the seawater of Terra Nova Bay, Antarctica. Sci Total Environ 593–594 (2017) 375–379.

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O13 EC

CHEMICAL COMPOSITION OF ATMOSPHERIC AEROSOL IN ANTARCTICA

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Within the framework of the Italian National Programme for Antarctic Research (PNRA) six PM10 aerosol samples were collected at Faraglione Camp, 3-km far from the Italian station "M. Zucchelli" (Terra Nova Bay, Ross Sea), from December 1, 2013 to February 2, 2014. A PM10 high-volume sampler and precleaned cellulose filters were used, with a sampling strategy of 10-day exposure time. A two-step sequential extraction procedure was applied to separate the water soluble and the insoluble (dilute HNO_3- extractable) fractions. Major (Al, Fe) and trace (Cd, Pb and Cu) elements were determined by Square Wave Anodic Stripping Voltammetry (SWASV) [1,2] and by Graphite Furnace Atomic Absorption Spectrophotometer (GF AAS). The aim was to determine the distribution and the summer seasonal evolution of these elements, providing a better understanding of the metal sources.
Total Atmospheric concentration of the elements ranged as follow: Al 20-30 ng/m³, Fe 16-28 ng/m³, Cd 0.55-1.9 pg/m³, Pb 9.4-21 pg/m³ and Cu 30-56 pg/m³. Al, Fe and Pb were mainly found in the insoluble fractions, whereas Cd and Cu in the soluble fraction.
The summer seasonal evolution showed a substantial constant trend for total concentration of Al and Fe; Pb total atmospheric content increased at the beginning of the season, and then remained constant in the following months; Cd and Cu total content showed a bell-shaped trend with a maximum in mid-summer.
Enrichment factors (EF) indicated an anthropogenic origin for Cd and Cu, whereas Pb and Fe appeared mainly related to natural/crustal origin.
Aerosol studies on polar and uncontaminated regions are a valuable instrument to assess the global environmental pollution.

[1] S. Illuminati, A. Annibaldi, C. Truzzi, G. Libani, C. Mantini, G. Scarponi, Determination of water-soluble, acid-extractable and inert fractions of Cd, Pb and Cu in Antarctic aerosol by square wave anodic stripping voltammetry after sequential extraction and microwave digestion. J. Electroanal. Chem. 755 (2015) 182-196.
[2] C. Truzzi, A. Annibaldi, S. Illuminati, C. Mantini, G. Scarponi, Chemical fractionation by sequential extraction of Cd, Pb, and Cu in Antarctic atmospheric particulate for the characterization of aerosol composition, sources, and summer evolution at Terra Nova Bay, Victoria Land. Air Qual. Atmos. Health. 10 (2017) 783-798.

O1 EQ

CURCUMIN AS POTENTIAL CHELATING AGENT TOWARDS Al(III) AND Fe(III)

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The thermodynamic study of curcumin (HL, Figure 1) as a ligand towards some metal cations was previously reported only in a few works. In this study, the first under physiological conditions (*i.e.*, 37°C and 0.16 M NaCl), the complexation of curcumin with Al(III) and Fe(III) is reported.

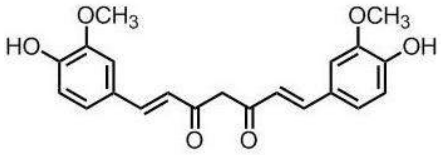

Figure 1. Structure of curcumin.

The reason for choosing the aluminium cation is mainly due to the fact that human exposure to aluminium does not serve any essential function in human biochemistry. Al(III) can enter the brain where it persists for a long time causing neurotoxicity [1]. Some of the aluminium toxicity can be reduced by chelation, for this reason it was interesting to explore the sequestering ability of a natural product such as curcumin to coordinate the Al(III) ion. The choice of the iron was related to the role that it plays in the biological systems and to its significant concentration in the body. Curcumin is a natural antioxidant and it has been employed in the treatment of cardiovascular and arthritic illnesses. Presently, it is also used as anti-inflammatory, antioxidant and anticarcinogenic [2]. The thermodynamic approach provides, first of all, the determination of the solubility and of the acidic constant of ligand under the selected experimental conditions. Then the formation constants of metal/ligand complexes were determined evaluating the competition between the proton and the metal cations towards ligand. The investigated equilibrium can be expressed according to the following general equation:

$$pM^{3+} + qOH^- + rL^- \rightleftarrows M_p(OH)_q(L)_r^{(3p-q-r)+} \qquad \log \beta_{p,q,r}$$

The speciation model, based on the potentiometric results, was in agreement with data obtained from the mass spectrometry and cyclic voltammetry studies.

[1] C. Exley, Human exposure to aluminium. Environ. Sci.: Processes Impacts 15 (2013) 1807–1816.
[2] M. Bernabé-Pineda, M. T. Ramirez-Silva, M. Romero-Romo, E. González-Vergarac, A. Rojas-Hernández, Determination of acidity constants of curcumin in aqueous solution and apparent rate constant of its decomposition. Spectrochimica Acta Part A 60 (2004) 1091–1097.

O2 EQ

INORGANIC ARSENIC SPECIATION IN WATER SAMPLES: AN ULTRAFAST METHOD BASED ON FRONTAL CHROMATOGRAPHY/ICP-MS.

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Arsenic is an ubiquitous an toxic element that can be introduced in the environment both through natural and anthropogenic routes. Its toxicity strictly depends on its chemical form, with inorganic species (iAs), arsenate (As^{V}) and expecially arsenite (As^{III}), being classified as much more toxic than organo-arsenic compounds. Due to the wide distribution of iAs sources, the only way to face this problem is to develop suitable and sustainable abatement processes at the point of use of water. Almost all the strategies so far reported for iAs abatement implies the pre-oxidation of As(III) to As(V). This pre-oxidation is fundamental because: i)As(III) is much more toxic than As(V); ii)it is easier to remove As(V) rather As(III) from contaminated waters. The most promising route to perform such pre-oxidation relies on the development of (photo)catalytic processes: the research in this field is still in its pioneering age, and the assessment of the kinetic behaviour of developed catalysts strongly needs a suitable high-throughput method for iAs speciation. In the literature are reported several works about the speciation of arsenic (both inorganic and organic species) in water and food,[1] all based on chromatographic separation coupled with different detection techniques such as inductively coupled plasma mass spectrometry (ICP-MS), graphite furnace atomic absorption spectrometry (GFAAS) or flame atomic absorption spectrometry (FAAS). All the reported methods are able to efficiently separate As^{III}, As^{V} and some methylated forms of As^{V}, but none of them is optimized in terms of time of analysis for the separation and determination of iAs: to the best of our knowledge the fastest technique reported in the literature takes almost 5 minutes for a complete analysis.[2]
The aim of this work is to go further developing an ultrarapid, easy and cheap method suitable for iAs speciation in water samples coming from catalytic abatement studies.
The here presented method is based on a frontal chromatography approach for the separation of iAs (using a strong anion exchange resin) coupled to ICP-MS for the detection of As.
The resulting method combine very short analysis times (around 120 seconds for each sample, i.e. less than a half of the times necessary for a complete analysis with the fastest method reported in the literature [2]), with no need of additional pumps or injection valves for the chromatographic separation. Problems encountered during the development of the method will be critically discussed.

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[2] B. P. Jackson, Fast ion chromatography-ICP-QQQ for arsenic speciation. J. Anal. At. Spectrom. 30 (2015) 1405

O3 EQ

EXPLORING VARIOUS LIGAND CLASSES FOR THE EFFICIENT SEQUESTRATION OF STANNOUS CATIONS IN THE ENVIRONMENT

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Metal pollution, coming from both natural and anthropogenic sources, has become one of the most serious environmental problems. Various strategies have been tested with the aim of removing heavy metals from environment. In this contribution, containing a robust experimental work together with a critical literature analysis, the sequestering ability of a variety of ligands towards Sn^{2+} cation will be evaluated in the conditions of several natural fluids, *i.e.* sea water, fresh water, human blood plasma, urine and saliva. 13 structural and 11 thermodynamic descriptors will be selected for a total of thirty-eight molecules belonging to different classes (carboxylic acids, amines, amino acids, phosphonates, polyelectrolytes etc…). For the filling of those missing data relative to the 11 thermodynamic descriptors, different strategies will be adopted, including simple correlations and Nipals algorithm.
The evaluation of the sequestering ability of the ligands is assessed in terms of estimation of $pL_{0.5}$ (total concentration of ligand required to bind the 50% of metal in solution), an empirical parameter that takes into account all the side reactions in solutions and does not depend on the speciation scheme.
Partial least square calculations were performed to model the $pL_{0.5}$ and to determine its correlation with the abovementioned descriptors.
The possibility to design and build up new tailor-made molecules capable of effectively sequester Sn^{2+} in various conditions is crucial for practical applications in biosphere, hydrosphere and lithosphere.

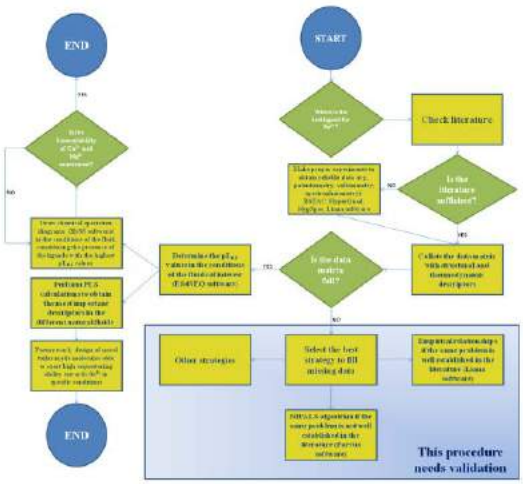

Figure 1. Flow-chart describing the methodological approach of this work.

O1 FO

MULTIVARIATE DATA ANALYSIS STRATEGIES FOR FIRE DEBRIS INVESTIGATION

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The possibility of recognizing whether the collected evidence is related to the occurrence of an arson is a largely investigated issue in the field of fire debris investigation [1]. Traditionally, data from GC/MS analyses performed on the fire debris recovered on the fire scene are compared to those from known ignitable liquids (e.g. gasoline, diesel fuel or the ones, for instance, found in possession of a suspected arsonist). In the present study several diesel fuel and gasolines samples from different gas stations located within the area of the city of Turin were analyzed by a validated Solid-Phase Micro-extraction (SPME)-GC/MS method [2]. In particular, samples were analyzed both as pure liquids and as mixtures of fresh and weathered mixtures at different percentages (i.e. 25%, 50%, 75%, 95% and 99%), as suggested by the American Society for Testing and Materials (ASTM) 1618 protocol. The collected mass chromatograms were subsequently interpreted using a variety of targeted and untargeted approaches of multivariate data analysis, involving both raw and semi-quantitative data. A data set including more than 150 GC/MS analyses relative to more than 30 gas stations was used for multivariate analysis. Several multivariate data analysis procedures were tested and their results were compared. The use of chemometric strategies allowed the building of explorative, classification, and likelihood ratio models. These allowed us to obtain probability values regarding the usage fire accelerants to set the fire. Principal Component Analysis arranged the fresh gasoline and diesel fuel samples according to their origin (i.e. the different gas stations). N-way, Self-Organizing Maps and Discriminant Analysis strategies were also tested to assess the occurrence of fire accelerant in an arson scene. Similar investigative approaches have been used with the integration of Bayesian's logic, by means of multivariate feature-based and score-based likelihood ratio models. Even if in a preliminary stage, this study emphasize the employment of multivariate strategies aimed at potentially helping analysts during the interpretative process of fire debris investigations.

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O1 FN

DEVELOPMENT OF A REFLECTANCE SMARTPHONE PAPER-BASED CHEMOSENSOR FOR THE QUANTIFICATION OF TOTAL POLYPHENOL CONTENT IN EXTRA VIRGIN OLIVE OIL.

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Features that characterize the quality of extra virgin olive oil (EVOO) such as antioxidant activity, free acidity, and total phenolic content, are usually determined by expensive laboratory procedures. Thus, simple, rapid and low-cost analytical techniques to be used "in situ" and ''in real time'' would be greatly beneficial for controlling the quality of EVOO. We propose a "point-of-need" paper-based chemosensor, exploiting the Folin-Ciocalteu colorimetric reaction (FC) and light reflectance measurement, for quantifying the total polyphenol content in extra virgin olive oils [1]. The device was fabricated with a black acrylonitrile-butadiene-styrene (ABS) polymer using a low-cost 3D printing technology and includes a disposable analytical minicartridge, a mini dark box to avoid interference from ambient light and a holder to connect the dark box to a smartphone. A Samsung S8 with a BI-CMOS sensor was used as detector, the smartphone flash acting as light source. The disposable analytical cartridge contains four reaction chambers (one for the sample, two for low and high concentration reference standards and the last for blank), in which all the FC reagents necessary to complete the analysis were adsorbed on 1 cm^2 cellulose paper. Quantitative color analysis was performed using a dedicated software (ImageJ v.1.46). Under the optimized conditions, reflectance decrease is proportional to the polyphenol content, expressed as equivalent of gallic acid (µg/mL), with a linear range from 100 to 750 µg/mL and a limit of detection (LOD) of 26,5 µg/mL. The extreme simplicity of the assay (no reagents need to be added) together with the high versatility make our chemosensor suitable for point-of-need testing with an "all in one" device able to detect phenolic content in a large variety of foods.

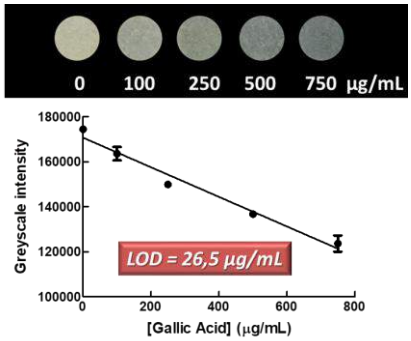

Figure 1. Calibration curve obtained for gallic acid (range 100-750 µg mL^{-1}).

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Acknowledgments: The project was funded by Cariplo Foundation within the "Agroalimentare e Ricerca" (AGER) program. Project AGER2-Rif.2016-0169, "Valorizzazione dei prodotti italiani derivanti dall'oliva attraverso Tecniche Analitiche Innovative (VIOLIN)"

O2 FN

DETAILED PROFILING OF EXTRA-VIRGIN OLIVE OILS BY USING COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY WITH DUAL QUADRUPOLE MASS SPECTROMETRY AND FLAME IONIZATION DETECTION

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The present investigation is focused on the development of a comprehensive two-dimensional GC (GC×GC) method, with dual quadrupole mass spectrometry/flame ionization (QMS/FID) detection, for the qualitative and quantitative analysis of the fatty acid and of the unsaponifiable fractions of extra-virgin olive oil.
In particular, the unsaponifiable fraction forms a minor, highly specific part of extra-virgin olive oils, and can be used as an indicator of genuineness and to highlight subtle intra-sample (*e.g.*, different geographical origin) differences. The column set used consisted of a low-polarity first dimension, and a medium-polarity secondary one, both characterized by a high thermal stability. The use of dual detection enabled the attainment of both mass spectral information and % FID data.
The complexity of the fingerprint, generated by the unsaponifiable fraction, fully-justified the employment of the two-dimensional GC technology. Furthermore, two other GC×GC benefits contributed greatly to the attainment of promising results, namely sensitivity enhancement and the formation of group-type patterns. The method herein proposed could potentially open a new opportunity for the more-in-depth knowledge on the composition of extra-virgin olive oils and for the purpose of fingerprinting.

Acknowledgement
The research was performed within the context of the project AGER2-Rif 2016-0169,
"Valorizzazione dei prodotti italiani derivari dall'oliva attraverso tecniche analitiche innovative Violin"

O1 GC

PHOTOCATALYTIC HYDROGEN EVOLUTION FROM (WASTE) AQUEOUS BIOMASS UNDER SIMULATED SOLAR LIGHT: TITANIUM DIOXIDE VS. GRAPHITIC CARBON NITRIDE

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Aim of this work is to study and compare P25 titanium dioxide (TiO_2) and oxidized graphitic carbon nitride (o-g-C_3N_4) for photocatalytic H_2 evolution from water containing various sacrificial biomasses. o-g-C_3N_4 was prepared by HNO_3-refluxing of bulk g-C_3N_4 produced by thermal condensation of dicyandiamide, and presently it has been neither tested in presence of waste biomass nor critically compared to P25 TiO_2. Basing on these considerations, the two catalysts have been studied, coupled with of Pt or Cu-Ni as the co-catalysts, under simulated solar light. The preliminary experiments were run in water samples containing soluble starch (4.5 g/L), chosen as model polysaccharide biomass, under 6 h radiation (500 W/m^2). Results showed that H_2 production was affected by catalyst concentration, and co-catalyst type and loading, giving hydrogen evolution rates (HER) up to 450 and 800 µmoles/g/h using TiO_2 (0.25, 1 g/L) decorated with 3 wt% Cu-Ni and 0.5 wt% Pt, respectively. Using o-g-C_3N_4 (0.25 g/L), coupled with 3 wt% Cu-Ni or 3 wt% Pt, HERs up to 170 and 590 µmoles/g/h were observed, respectively. Under the most convenient conditions, H_2 evolution was also explored in water samples containing glucose, lactose, maltose or galactose (4.5 g/L), achieving HERs in the range 500-1170 µmoles/g/h for 1 g/L TiO_2 (0.5 wt% Pt) and 340-910 µmoles/g/h for 0.25 g/L TiO_2 (3 wt% Cu-Ni). The o-g-C_3N_4 systems proved to be efficient as well, with HERs in the range 90-610 µmoles/g/h. The best performing systems were then tested for each catalyst in brewery and dairy factories wastewaters rich in maltose and lactose, respectively. Despite the samples turbidity and filtering effect on the incident light, appreciable H_2 production (up to 286 µmoles/g/h) was achieved (Fig. 1), with apparent quantum yields up to 1.1%.

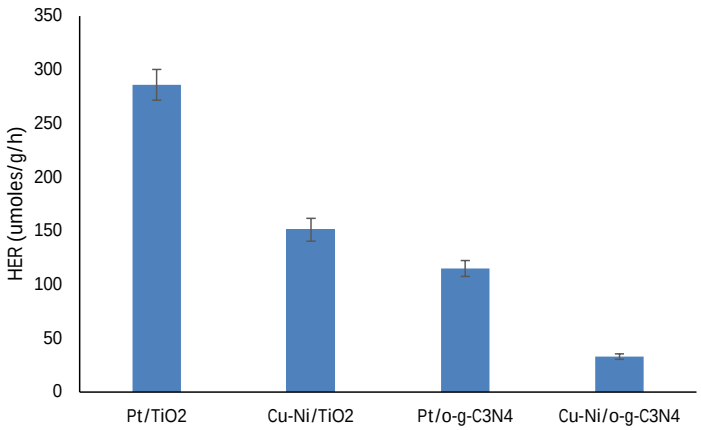

Figure 1. H_2 evolution obtained from brewery wastewater under simulated solar light (*n*=3).

O1 MS

FAST DILUTE-AND-SHOOT APPLICATIONS USING AN LEI LC-MS INTERFACE

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Food safety, forensic analyses and quality control in personal care products (PCP) are analytical fields where mass spectrometry (MS) plays a fundamental role, especially when focused on a targeted approach. Most protocols are based on LC-ESI MS; however, the broad variability of this matrices need a dedicated method for every sample with an increase in complexity, time and material consumption. Liquid-EI (LEI) is an LC-MS interface for coupling liquid chromatography and electron ionization mass spectrometry. LEI provides the "fingerprint" spectrum of electron ionization (EI) for polar and non-polar analytes in absence of matrix effect. Its highlights are of great potential for flexible and direct targeted and non-targeted approaches. Parabens are conservative compounds widely present in cosmetics, food and beverages. Together with dimethyl phthalate, their chronic exposure is hazardous for the human health. On the other hand, drug facilitated crimes (DFC) are violence and robberies performed adulterating beverages with psychoactive substances. The "Mediterranean diet" is a healthy eating habit widely studied and known for reducing cardiovascular risks and other metabolic diseases. Extra Virgin Olive Oil (EVOO) is the most used fat in the Mediterranean diet. It is mainly made of mono-unsaturated fats but it also contains other precious nutraceuticals such as anti-oxidative polyphenols like tyrosol and hydroxytyrosol. The quantification of this molecules is fundamental to assess product safety or quality or to identify a DFC. Conventional approaches based on LC-ESI are rigid making a fast and affordable determination of this compounds a challenging real-world application. In these applications the LC apparatus is directly connected to the MS capillary and all the injected molecules go inside the ion source together. An Agilent 1290 Infinity UHPLC fitted with an Agilent UHPLC Nanodapter coupled to 7010 QQQ triple quadrupole mass spectrometer equipped with a High Efficiency Ion Source (HEIS) (Agilent Technologies Inc., Santa Clara, CA) is used. UHPLC Nanodapter primary flow: 90 µL/min, flow on column: 525 nL/min. Injection volume: 10 nL. Mobile phase: 90:10% ACN:H_2O. Ion source temperature: 280 °C. Vaporization micro-channel temperature: 350 °C. Data acquisition: MRM. The samples are diluted (if needed) and analyzed in FIA mode without preliminary extraction. The MRM signal of the target compound is directly correlated to its concentration, regardless the composition of the sample, thanks to the absence of matrix effect. This advantage permits a dilute-and-shoot approach with an appreciable time and material saving. Parabens and dimethyl phthalate are directly determined in commercial merchandise, whereas flunitrazepam are dissolved in beverages to simulate equal-to-real samples. Finally, the direct determination of tyrosol and hydroxytyrosol in extra virgin olive oil is presented.

O2 MS

LIPIDOMIC ANALYSIS OF TISSUE FROM HIGH FAT AND HIGH FRUCTOSE DIET TREATED MICE

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In the last decades the study about human diseases has had some new key players: the lipids. These latter were recognized not only as the bricks of cellular membrane, but also, and more notably, as the fundamental players in a broad range of biochemical processes, such as calcium homeostasis and membrane trafficking [1, 2].
It was recently understood that aberration in lipid metabolism caused many human diseases, and the most studied pathologies related to a high fat containing-diet are obesity and prediabetes syndromes [3]. Ceramides and phosphosphingolipids, both belonging to the sphingolipids family, are involved in such disorders [4, 5]. There are four major pathways to synthetize ceramides that involve many enzyme families, starting from glycosphingolipids, sphingomyelin, and ceramide-1-phosphate, and finally a de novo synthesis that involves serine and palmitate. Phosphosphingolipids are metabolized from ceramide, through the alkanolamine sphingosine (2-amino-4-octadecene-1,3-diol). All the mentioned enzyme-catalyzed reactions are reversible.
Pathological diseases disquiet the enzymatic equilibrium between ceramides, sphingosines and phosphosphingolipids leading to oxidative stress and metabolic cellular damage. Some vitamins, such as pyridoxamine, an analog of vitamin B6, can bring back the equilibrium.
In our project livers from mice fed with different diets were analyzed using UPLC coupled with a triple quadrupole mass spectrometry (MRM mode).
We developed a novel UPLC-MRM method for targeted lipidomics characterization of rat liver tissue. We stressed the attention on the differences between control and treated groups in distribution of ceramides, sphingosines, glucosyl ceramides and glucosyl sphingosines. We focused on a peculiar biomarker of hepatic steatosis, the sphingosine-1-phosphate, and monitored its concentration in different diets with the aim to characterize lipidomic of diet induced obesity.

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O3 MS

LC-MS BASED STRATEGIES FOR THE COMPREHENSIVE ANALYSIS OF MARINE TOXINS IN ENVIRONMENTAL AND FOOD MATRICES

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Microalgae are vitally important to marine ecosystems and most of the microalgal species are not harmful. However, an important number of species produces potent, heat-stable toxins. Concomitantly to harmful algal blooms (HAB), these toxins can be transferred to humans mainly through the food web but also through other exposure routes, such as aerosol and/or skin contact, or even cause mortality of aquatic organisms. These events result in adverse effects and sanitary problems, as well as in significant economic losses related to aquaculture, fishery and tourism sectors.

Efficient analytical strategies are thus required to detect toxins in the environment and in food supply to the final aim of protecting human health and guaranteeing seafood safety and quality. Selection of the appropriate instrumental technique may be challenging because marine toxins are a heterogeneous group of structurally complex compounds, usually contained at sub-mg levels in complex matrices in the form of a wide array of different congeners. In addition, certified reference material of individual toxins is in some cases unavailable, which hampers full validation of analytical methods. The combination of liquid chromatography with mass spectrometry (LC-MS) is pointed by official organizations, such as the European Food Safety Authority (EFSA), as the most promising instrumental technique for the monitoring of marine toxins in the environment and in seafood.

Several MS-based approaches employing either tandem MS or high resolution MS^n have been developed so far for the detection of both the regulated and the emerging toxins, validated, and eventually used as an effective alternative to animal based methods in official monitoring of marine toxins in seafood. They allowed to disclose the presence of known and unknown toxins in the Mediterranean area and even to structurally characterize new congeners based on the interpretation of their fragmentation patterns [1].

An overview of the different experimental strategies used to discover marine toxins, determine toxin profile and content of algal and mussel samples, and elucidate the structure of new low-, mid- and high-MW congeners will be presented. Although LC tandem MS proved useful to face most of the HAB-related outbreaks occurred so far due its high sensitivity, selectivity and reproducibility, in some cases it lacked in providing a comprehensive overview of the toxin profile of a real sample. That's where high resolution MS^n played a key role, proving to be the most desirable approach to avoid underestimation of sample toxicity.

[1] C. Dell'Aversano, L. Tartaglione, MS-based methods for the structural characterization of marine toxins. Comprehensive Analytical Chemistry. Recent Advances in the Analysis of Marine Toxins. CAC Elsevier, Eds. J. Diogene and M. Campas. 78 (2017) 193-209.

O4 MS

HIDDEN SOURCES OF BISPHENOL A FROM FOOD CONTACT MATERIALS

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The new European Regulation 2018/213 further restricts the use of bisphenol A in food-contact materials, reducing the SML from 0.6 mg/kg to 0.05 mg/kg and establishing an SML of non-detect (detection limit = 0.01 mg/kg) for materials and articles specifically intended for infant or baby food. However, all analytical systems of control are aimed at identifying and quantifying the molecules of bisphenol A without taking in consideration the possible presence of species originating from material degradation and able to follow an *in-vivo* hydrolysis providing bisphenol A generation. Thus, the presence of oligomers of polycarbonate deriving by unreacted species or polymer degradation, as recorded in previous works [1,2], can be considered a hidden source of several bisphenol A units that remains outside the control of legislation and should be considered of high concern.
This work was focused on the identification and the description of kinetics of release of different molecules migrating from polycarbonate food contact materials to simulants and to a model food sample such as melted chocolate. Analyses were performed by UHPLC system coupled to a Q-Exactive mass spectrometer.
Targeted and untargeted analysis through data dependent acquisition mode [2] allowed to detect the occurrence of several species (Figure 1) deriving from polycarbonate, and permitted to investigate the polymer degradation pattern and explore the correlation of the recorded amounts of each product with age, hours of usage, and washing cycles of the plastic articles. The detection of common plastic additives and dyes was also achieved.

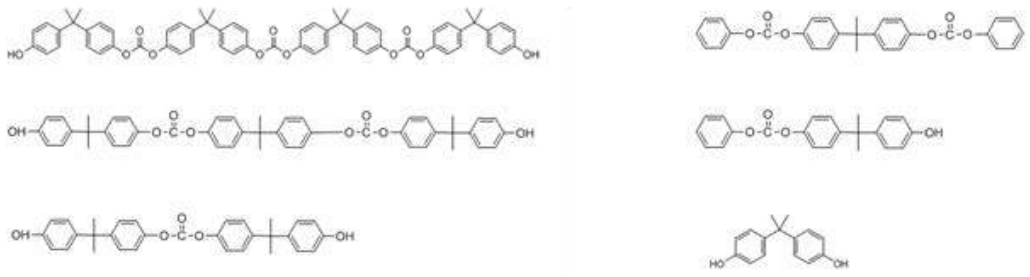

Figure 1. Molecules migrating from food contact articles to simulant and chocolate.

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O1 SB

SINGLE MOLECULE DETECTION OF MARKERS IN REAL BIO-FLUIDS WITH A LABEL-FREE ELECTRONIC SENSOR

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Digitizing biomarkers analysis by quantifying them at the single-molecule level is the new frontier for advancing the science of precision health. It is also the frontier-line beyond which analytical chemistry simply cannot go. The enhancement of the technical capabilities of analytical bio-electronics systems, by giving clinicians the possibility to rely on biomarkers quantifications down to the single-molecule, holds the potential to revolutionize the way healthcare is provided. Such an analytical tool will indeed enable clinicians to associate a biomarker tiniest increase to the progression of a disease. This would be extremely useful particularly when a disease is in its early stage. Eventually, physicians will be able, by quantifying extremely small amount of a given bio-marker, to identify the very moment in which the illness state begins. Such an occurrence will enormously enhance their ability of curing diseases by supporting better prognosis and permitting the application of precise treatment methods.

Thin-film transistors integrating biological systems have been shown to result in highly performing bioelectronic devices capable to accomplish tasks such as sense bio-species as well as transduce the electrical activity of cells or even organs such as the brain. The scientific activity developed within the exciting and fast developing field of printable bio-electronics, has been centred on the use of organic or printable transistors as electrodes or as sensitive and selective analytical biosensors. Prof. Torsi is acknowledged for being one of the initiators of the electronic biosensing field and, besides the analytical applications, the group has always paid attention to the fundamental understanding of the sensing mechanisms underpinning the device extremely high performance level. Eventually, they lately managed to demonstrate single molecule detection of immunoglobulins, peptides, proteins and DNA markers even in whole serum using a printable millimeter-sized transistor that integrates a layer of the biological recognition elements capable of selectively binding a given bio-marker. This sets a world record in label-free single molecule detection and puts these research activities headed by prof. Torsi at the fore-front in single molecule detection analytical technologies. Moreover, because the platform is label-free, it is also fast and can detect both proteins and gene markers, hence it holds the potential to revolutionize the present approach to point-of-care testing and well-being.

O2 SB

CHAMELEON PROBES FOR CHROMOGENIC SENSING OF VOLATILE SPOILAGE PRODUCTS OF CHICKEN MEAT

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The methods commonly employed to evaluate the meat quality could be instrumental or microbiological analysis and sensory evaluation, but they all require specialized people and are time and cost expensive.
Automated techniques and/or methods that allow a continuous and simple monitoring, for in-field application, like home setting, supermarket, store, are strongly demanded. Included in this category there are biosensors, electronic devices and colorimetric sensors.
Colorimetric sensors, based on colorimetric indicators, are capable of changing colour due to a reaction with volatile compounds produced on packaged meat samples. Either included directly on packaging, or attached with on-package sticker, they offer the simplest, practical, instrumentless way for monitoring meat freshness, directly detected using naked eye.
We focused our attention on chicken meat, following the spoilage aerobically at ambient and at domestic fridge temperature. Indicator dyes with different pK_a values were embedded into an anion exchange cellulose sheet, CC, to obtain colored spots (0.5 cm diameter), reported in Fig 1. Color image analysis was chosen for the colorimetric analysis.
An array of 6 different spots was placed over the tray containing a sample of the skinless chicken beast, but under the PVC package, avoiding direct contact with meat. Photos of the array were acquired for each sample as function of time, RBG index was used for monitoring the spoilage, Principal Component Analysis to model the data set: three clusters of three different degradation step, an early spoilage, an intermediate spoilage and the final spoilage were identified.

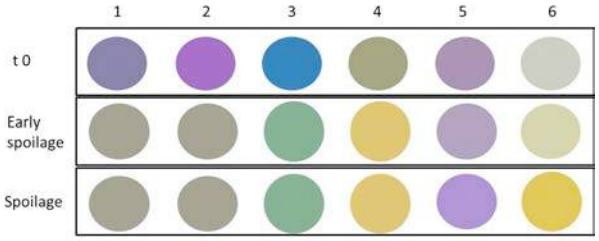

Figure 1 – Pictogram of evolution of sensing spots over poultry meat sample. Namely, ***1***: *m*-cresol purple-CC@, ***2***: *o*-cresol red-CC@, ***3***: bromothymol blue-CC@, ***4:*** thymol blue-CC@, ***5***: chlorophenol red-CC@, ***6***: Ellman's reagent-CC@.

Ultimately, not more than three dyes will be selected and included, not simply in cellulose spots, but directly into PVC or PE sheets, in a project with colleagues of Organic Chemistry and of the R&D laboratory&technical support special films of ITP (Industria Termoplastica Pavese), extremely interested in developing new tailored materials in food packing.

O3 SB

A NEW CELL-BASED BIOLUMINESCENT ASSAY FOR REAL-TIME DETECTION OF ANDROGENIC ACTIVITY IN LIVING CELLS

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Living cells used as sensing systems have proved to be valuable for prediction of the physiological response to drugs, chemicals, and samples in complex matrices, whose toxic effects and specific biological activity can be evaluated in an easy and straightforward manner. Thanks to their easy implementation into high-throughput screenings and portable analytical platforms, cell-based assays are versatile tools for bioanalytical applications, including drug screening, environmental monitoring, and pathophysiological studies providing functional information about hundreds of compounds. Since altered protein–protein interactions (PPI) may result in pathological cellular processes, one of the major targets of the drug discovery pipeline is the investigation of protein networks through the development of reporter protein complementation assays. In this work a new bioassay for real-time monitoring of homo-dimerization of human Androgen Receptor (hAR) based on split complementation of Nanoluc was developed. NanoLuc luciferase is the smallest (only 19KDa) and brighteest BL protein commercially available (150-fold brighter than firefly luciferase); moreover, thanks to the absence of post-translational modifications, Nanoluc can be genetically fused to target proteins without modifying its structure and function. Human embrionic kidney cells (HEK293) were genetically engineered to express a novel splitted NanoLuc Luciferase (NanoBiT) composed by two chimeric halves: a large domain fused to hAR (LgBit-hAR) and a small domain fused to hAR (hAR-SmBit) under the control of constitutive promoter (SV40 or Tk). The correct folding and homodimerization of the chimeric protein have been checked upon induction by different concentration of testosterone (in the range 0.01-100nM), selected as model analyte. In optimized conditions, the developed bioassay is able to obtain a rapid response (30 min) obtaining a Limit of Detection (LOD) of $3.69 \pm 0.23 \times 10^{-11}$ M and EC50 of $8.64 \pm 0.57 \times 10^{-10}$ M, demonstrating the suitability of the assay for analysing molecules with androgenic activity, including new drugs or endocrine disrupting chemicals. This performance was obtained with real-time measurements using a nonlytic assay format obtaining quantitative investigation of protein interaction dynamics under relevant physiological conditions. Benefiting from the small size and bright luminescence of NanoLuc, it provides detection at low intracellular concentrations with minimal steric interference on appended target proteins.

O4 SB

SURFACE PLASMON RESONANCE TRANSDUCTION ON OPTICAL FIBER AS A LOW COST ALTERNATIVE TO THE KRETSCHMANN CONFIGURATION

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Surface-plasmon resonance (SPR) is a label-free technique for monitoring specific receptor/substrate interactions. The popularity of this technology has grown rapidly since the 1980s. Nevertheless, the development of biosensor based on SPR has lagged significantly behind research output, due primarily to both technical and cost issues. This is mainly ascribable to the particular configuration required to obtain the information, i.e. the Kretschman configuration which is at the same time bulky and rather expensive. Recently it has been shown that optical fibers enable much cheaper and smaller experimental set-ups [1]. Plastic optical fibers (POF) are especially advantageous in this aspect [2].

In the present work the possibility of applying SPR sensors based on POFs configuration instead of much more expensive SPR devices is investigated in the case of furfural (furan-2-carbaldehyde, 2-FAL). 2-FAL is widely present in food and in the environment, so that its determination in different matrices is of high interest.

Here a previously described SPR platform is considered, with a peculiar D-shaped profile[2], which enables SPR measurements in the visible range from 400 to 950 nm (normalization against the transmission spectrum of the same platform in air) in a very convenient way.

The combination of the template molecule (2-FAL) with the specific sites in the MIP produces a variation of the refractive index of the polymeric layer, which is measured as a shift of the surface plasmon resonance wavelength (Δλ). The function Δλ against 2-FAL concentration can be fitted to the Langmuir isotherm, and can be used for quantitative determinations.

Typical parameters obtained in water are: affinity constant K_{aff}=1.09 10^6 mol^{-1} L; $\Delta\lambda_{max}$=2.73 nm; sensitivity al low concentration= 1.8 10^7 nm mol^{-1} L; LOD=3.5 10^{-7} mol L^{-1}. K_{aff} is only slightly lower than 5 × 10^6 mol^{-1} L obtained from a completely different matrix, i.e. mineral oil. Opposite, much lower K_{aff} (about 10^{-4} mol^{-1} L) were obtained by a parallel sorption characterization by batch experiment at higher 2-FAL concentrations. This shows that interaction sites with different affinity are formed in MIP, but that only the strongest ones produce the SPR signal, i.e. a variation of the refractive index of the MIP layer when the corresponding substrate combines.

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O5 SB

DISSIPATIVE DNA-BASED NANOMACHINES

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Over the past decades supramolecular chemistry has permitted enormous advancements in the fields of nanotechnology to form functional structures that typically reside at thermodynamic equilibrium. Although this is a favourable property for many applications, it also poses an intrinsic limitation to reproduce other properties [1]. Here, we demonstrate that DNA is ideally suited for programming synthetic out-of-equilibrium dissipative systems that can have applications in sensing or drug delivery [2]. Advantages of the DNA-based systems presented in this study include a perfect control over the activation site for the chemical fuel in terms of selectivity and affinity, highly selective fuel consumption that occurs exclusively in the activated complex, and a high tolerance for the presence of waste products. Finally, it is shown that chemical fuels can be used to selectively activate different functions in a system of higher complexity embedded with multiple response pathways.

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O6 SB

A SMARTPHONE-BASED THERMOCHELUMINESCENT IMMUNOSENSOR FOR VALPROIC ACID DETECTION

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Biosensors for Point-of-Care (POC) applications, strongly demanded to enable rapid and on site analysis, should provide high assay detectability and robustness employing and easy-to-use analytical devices. Recently, smartphones and other portable electronic devices have been proposed as suitable platforms for developing ready-to-use biosensors usable by everyone at the point of need. Herein, we propose for the first time a smartphone-based immunosensor employing a paper-based format and thermochemiluminescence (TCL) detection, that was optimized for valproic acid (VPA) in blood and saliva samples. TCL is a chemical luminescence phenomenon in which photons are emitted upon thermally-induced fragmentation of a suitable molecule, with production of a moiety in its singlet electronically excited state [1]. Its peculiar characteristics make it a suitable detection principle for smartphone's-based biosensing, thanks to its high detectability and reagent-less nature of the measurement. A vertical flow immunoassay (VFIA) format was exploited to develop a rapid and one-step competitive immunoassay for VPA detection, employing silica nanoparticles doped with a TCL 1,2-dioxetane derivative as a label. The VFIA sensor is a stack of paper-based layers, in which reagents are stored in a stable form, therefore the immunoassay protocol could be completed in a very short time after the addition of the sample. Suitable accessories were developed using a bench top 3D printer in order to adapt the analytical protocol to the smartphone platform which was exploited as a multi-tasking tool, providing a power source for the heat shock required to trigger the TCL reaction and a sensitive camera for emitted photons measurement. The developed biosensor allowed to quantify VPA in blood and saliva, with limits of detection (4 and 0.05 μg mL^{-1} respectively) and dynamic ranges (4-300 and 0.05-20 μg mL^{-1}) suitable for therapeutic monitoring purposes. The integrated device offers an innovative analytical platform for rapid one-step biosensors exploitable in a variety of point-of-care applications.

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O7 SB

NEW ANTIFOULING PLATFORM FOR DNA DETECTION IN HUMAN PLASMA BASED ON MODIFIED POLY-L-LYSINE POLYMERS WITH ANIONIC PEPTIDE

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Antifouling surfaces are required for many biotechnological applications to prevent the non-specific protein/cell adhesion and detect biological targets, such as cancer biomarkers, circulating in complex natural media (e.g., blood plasma or serum) [1]. Accurate quantification of nonspecific protein adsorption is crucial for the evaluation of their antifouling activities [2]. Here, we present an innovative, rapid and simple method for surface modification based on cationic poly-L-lysine (PLL) polymer functionalized with an anionic oligopeptide, in order to obtain a mixed-charge polymer with antifouling property. PLL polymer was synthesized with different percentages (y%) of maleimide-NHS ester chains (PLL-mal(y%)), and the anionic oligopeptide structure (CEEEEE) with five negative charges was attached to the PLL-mal(y%) polymers on gold sensors through the thiol–maleimide Michael-type addition. Contact angle and PM-IRRAS data indicated the successful monolayer formation of the modified PLLs. Antifouling properties of peptide-PLL surfaces were evaluated in adsorption studies using Surface Plasmon Resonance Imaging (SPRI). PLL-mal(26%)-CEEEEE exhibits excellent antifouling property in single-protein solutions, and relevant low-fouling capacity in human plasma samples. The new PLL-mal(y%)-CEEEEE polymer offers a prominent resistance to protein fouling in complex media compared to conventional non-fouling materials, and allows to have a critical control over the biosensing interfaces by creating mixed monolayers with different functionalities.

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O8 SB

ALL-IN-PAPER (BLUE): SYNTHESIS, MATRIX PURIFICATION, REAGENT-FREE DETECTION. BLOOD GLUCOSE AS CASE OF STUDY.

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Paper is establishing itself as one of the most intriguing materials of the 21th century, being adopted in various fields, as paper is used in applications such as building batteries, amplifying nucleic acids, remediating pollution, and fabricating low-cost diagnostics. Moreover, in the era of sustainability, environmentally friendly synthesis pathways for preserving the environment and minimizing waste are strongly required. For the first time, we propose filter paper as a convenient scaffold for chemical reactions. To demonstrate this novel approach, Prussian Blue Nanoparticles (PBNPs) were synthesized on filter paper by utilizing a few µL of its precursors without external inputs, i.e. pH, voltage, reducing agents, and without producing waste as well. The functional paper, named "Paper blue", is successfully applied in the sensing field, exploiting the artificial peroxidase properties of PBNPs to electrocatalyze the reduction of hydrogen peroxide at low applied potential. The eco-designed "Paper blue" was combined with wax- and screen-printing to manufacture a reagentless electrochemical point-of-care device for diabetes self-monitoring, by using glucose oxidase as the biological recognition element. Blood glucose was linearly detected for a wide concentration range up to 25 mM (450 mg/dL), demonstrating its suitability for management of diabetes and glucose-related diseases. The Paper blue-based biosensor demonstrated a correlation coefficient of 0.987 with commercial glucose strips (Bayer Contour XT). The achieved results demonstrated the effectiveness of this approach, which is also extendible to other (bio)systems. This work opens to a plenty of different applications based on paper. It might serve as a reactor to create different nanomaterials, i.e. gold nanoparticles, as platforms for both electrochemical and colorimetric assays. It can serve as a remediation-active material, for instance by functionalizing with a heavy metal-adsorbent material: one can imagine to remediate and detect the heavy metal with the same platform. Again, different functional paper sheets can be assembled with the possibility to create 3D integrated multiplexed tools.

O9 SB

SIMULTANEOUS DETERMINATION OF GLUCOSE AND FRUCTOSE IN SYNTHETIC MUSTS BY SONOGEL-CARBON AMPEROMETRIC SENSORS

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Glucose and fructose are commonly present in fruits and fruit drinks. For this reason their determination is important for quality control, nutritional purposes and for monitoring the ripening of fresh fruits. In particular, in grapes the predominance of glucose in the first stage of maturation is compensated by a greater fructose production in the following stage, so that at full maturation the glucose/fructose ratio is close to 1. The variations of glucose and fructose contents can be then considered as an index of the maturation level of grapes.

The most common analytical instrumentation for the quantification of glucose and fructose in grapes is liquid chromatography. As a more rapid approach for the in situ monitoring of sugars content, we propose here an amperometric sensor based on Au nanoparticles (AuNPs) embedded in a Sonogel-Carbon electrode [1]. The rigid inorganic matrix can stably incorporate AuNPs, allowing the activation of electrocatalytic processes in charge of sugar oxidation [2]. Furthermore, the electrode surface can be very simply and rapidly renewed by means of electrochemical cleaning procedure.

The electrochemical responses of glucose and fructose in standard solutions evidence the presence of electrochemical processes peculiar for the two singular analytes, suggesting us their possible simultaneous quantification when present in the same solution. This can be achieved by chemometric analysis of the whole voltammetric signals collected in solutions containing the two analytes. The effectiveness of this amperometric sensor for simultaneous glucose and fructose determination has been tested in synthetic musts mimicking red grapes at different maturation degree.

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O10 SB

DEVELOPMENT AND CHARACTERIZATION OF A NEW BETAINE / PT ELECTROCHEMICAL SENSOR FOR DETECTION OF B GROUP VITAMINS

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In recent years, noble metal nanomaterials have received much more attention in electroanalysis owing to their unique optical, electrochemical and electronic performances. In particular, Pt nanoparticles have been used increasingly in many electrochemical applications [1]. In this study an interesting strategy of electrodeposition of Platinum has been developed using a glassy carbon electrode coated with betaine (Be). Betaine is a neutral compound having an NH_4^+ quaternary amino group and a negatively charged functional group away from the cation site. It has a molecular structure very similar to choline, an organic substance that can play a significant role in the preparation of nanoparticle surface structures formed through quaternary group interactions with complex anionic metal species [2]. The aim of this work is to define an experimental route for electrochemical and morphological preparation and characterization of an innovative electrode material based on betaine and defined GC/Be/Pt. The electrode modified preparation comprises of two steps: first, the betaine film is electrodeposited on the GC by cyclic voltammetry or by pulse electrodeposition technique in a neutral solution containing Be 1,5 mM. The betaine modified electrode is denoted as GC/Be. The second one involves an electrodeposition of Na_2PtCl_6 2 mM on the substrate GC/Be by voltammetric procedures and the obtained electrode is denoted as GC/Be/Pt. The effects of several experimental conditions such as potential applied, pulse waveform, time of electrodeposition, etc. on the kinetics of electrodeposition and film morphology are considered and critically evaluated. The use of betaine represents an element of strategic importance in the making of electrodic material through electrodepositing meso/nano Pt particles in the potential range between 0.4 V and 0.1 V. Morphological analysis of the electrode material surface (GC/Be/Pt) by Scanning Electron Microscopy (SEM), showed the presence of stable Pt globular shape structures homogenously distributed on GC/Be substrate. Therefore the use of betaine allows a better modulation of platinum electrodeposition conditions on traditional electrode substrates. Additional attention has been paid to the electroanalytical/amperometric characterization of the GC/Be/Pt sensor through the electrooxidation of molecules of biological and pharmacological interest such as B group vitamins.

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O11 SB

HIERARCHICAL NANOSTRUCTURES COMPOSED BY Ag NANOSTARS ON Au/Cu NANOWIRES AS SERS SENSORS FOR PAINTING MATERIALS

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Surface enhanced Raman spectroscopy (SERS) is a powerful spectroscopic technique particularly suitable to study molecules adsorbed or bound onto nanostructured interfaces. SERS has been recently applied in the field of Cultural Heritage to study organic substances such as dyes and lakes. Aim of the present research is the preparation and characterization of nanoparticles (NPs) and nanomaterials suitable for the application of the SERS technique directly on samples of paintings or other works of art. To this aim we prepared hierarchical nanostructures made of metal nanowires on which star-shaped silver nanoparticles are immobilized. The Ag nanostars (AgNSs) are prepared using a one-pot synthesis method based on the reduction of the metallic precursor ($AgNO_3$) by a reducing agent (hydroxylamine) in the presence of a capping agent (trisodium citrate) and additives (NaOH) [1]. The metal nanowires (NWs) are obtained in the shape of ensembles of nanoelectrodes by templated growth in nanoporous membranes. We prepared and compared both Au-NWs and Cu-NWs. The Au-NWs are synthesized by electroless deposition in track-etched polycarbonate membranes [2], while the CuNWs are produced by electrochemical deposition both in polycarbonate and anodic aluminum oxide (AAO) membranes. After the deposition, the membranes are chemically etched. Finally, the anchoring of the AgNSs on the AuNWs is obtained by the use of bifunctional thiols, able to bridge together the two different nanomaterials. The Raman spectra of organic molecules (thiophenol as well as some organic dyes used in painting layers) bound onto the surface of the so obtained hierarchical nanostructures are significantly enhanced, so allowing the sensitive detection of several analytes of interest in the field of cultural heritage.
A synergetic Raman amplification effect related to the simultaneous presence of NWs and AgNSs is observed experimentally and simulated on the basis of theoretical models.

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O12 SB

MICRONEEDLE-BASED BIOSENSOR FOR MINIMALLY-INVASIVE LACTATE DETECTION

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Microneedle arrays for minimally invasive continuous sensing in the dermal interstitial fluid (ISF) have been demonstrated in both amperometric [1,2] and potentiometric [3] modes, however there are no publication where microneedle arrays have been shown to function as second generation biosensors [4].
To further demonstrate the capability of microneedle arrays as mediator-based biosensors we have modified metalized polymer solid microneedles with multiwalled carbon nanotubes (MWCNTs) at which mediated electron transfer of lactate oxidase takes place.
The gold surface of the microneedles has been modified in 3 subsequent steps: i) electrodeposition of Au-MWCNTs; ii) electropolymerization of the mediator, methyleneblue; iii) immobilization of the enzyme lactate oxidase by drop-casting procedure.
The resulting microneedle-based enzyme biosensor displays an interference-free lactate detection without compromising its sensitivity, stability and response time.
The performance of the microneedle array second generation biosensor for lactate detection was assessed in artificial interstitial fluid and in human serum.
The results reveal that the new microneedle lactate sensor holds interesting promise for the development of a real-time monitoring device to be used in sport medicine and clinical care.
The biosensor will be further optimized for “in vivo” measurements through clinical studies in healthy volunteers.

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O13 SB

DISPOSABLE pH BIOSENSOR FOR UREA MEASUREMENT

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Cost and reliability represent major determinants for introducing new technologies in clinical settings. In this study, we present the fabrication, testing and validation of cheap and disposable potentiometric sensors to measure pH and urea concentration. The first sensor, exploiting graphene oxide sensitivity to pH, is also used to measure the local variations of acidity due to the reaction of urease with urea. The same scheme, i.e. pH sensor modified with an enzyme, can be used to detect a variety of different compounds and represents for this reason a very general platform.

A graphene oxide dispersion in water was prepared by a modified Hummers' method and deposited onto graphite working electrodes previously screen printed on a PET film. A solution containing urease was then drop cast on activated (EDC/NHS) working electrodes. The open circuit potential existing between each working electrode and a reference silver/silver chloride electrode was measured by a potentionstat/galvanostat (Palmsens 4).

The pH sensor was calibrated using certified buffer solutions, whereas solutions at different urea concentrations in the range (25 - 500 μM) were used for the urea sensor. In-vitro validation with model solutions established accuracies of ±0.2 pH units (range 3-10 pH units) for the pH sensor, whereas the urea sensor's intra-day and inter-day precisions in model solutions were 5 and 10% respectively. The sensor showed a detection limit of 25μM.

The sensor capability to monitor the efficiency of dialysis was tested with plasma samples collected from patients undergoing this treatment. Sensor measurements were in good agreement with values supplied from the analytical chemistry laboratory, with an average deviation of about 5%. The efficiency of dialysis as measured from KT/V, i.e. the reference parameter representing the treatment capability to remove uremic toxins, was estimated with an uncertainty of 5%.

The combination of a pH sensitive material and enzymes catalysing reactions producing acidic or alkaline species can be exploited to develop large arrays of sensors. The simple and reproducible fabrication procedure is suitable for scaling at an industrial level, to obtain cheap sensors to be disposed after single use.

O14 SB

PROXIMITY-BASED OPTICAL AND ELECTROCHEMICAL PLATFORMS FOR THE RAPID, SINGLE-STEP DETECTION OF ANTIBODIES IN BODILY FLUIDS

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Antibody detection is crucial for the diagnosis of many human disorders including infectious, autoimmune, and oncological diseases. Moreover, since immunotherapy represents nowadays the frontier to fight cancer, the detection of monoclonal antibodies becomes of paramount importance to correctly monitor the progression and efficacy of such therapies. To allow early diagnosis, prompt therapeutic actions and efficient immune-based therapy antibodies detection methods should be sensitive, quantitative and specific but also rapid and easy to use. Unfortunately, however, current methods routinely used for this purpose in clinical settings either require reagent-intensive laboratory-based techniques, multiple time-consuming incubation steps and/or sophisticated equipment.
Here we show a nucleic acid nanoswitch platform able to measure Immunoglobulins of type G and E (IgG and IgE) levels directly in blood serum and other bodily fluids in few minutes and without washing steps.[1] The system couples the advantages of target-binding induced co-localization and nucleic acid conformational-change nanoswitches. This novel sensing programmable platform can be adapted to the detection of any antibody for which the recognition element that can be coupled to the nucleic acid anchoring strand. We also demonstrate a clinically relevant application of our detection method monitoring Trastuzumab concentration, a monoclonal antibody widely used for breast cancer therapy. We were able to measure quantitatively and quickly drug levels directly in blood serum.
To allow the system development as a powerful diagnostic platform both for POC applications and large-scale analysis, we recently developed the sensing in an electrochemical format.

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O15 SB

AN INTEGRATED IOT-WIFI BOARD CONNECTED WITH AN INNOVATIVE IMMUNOSENSOR FOR REMOTE DATA ACQUISITION. CASE OF STUDY: DIAGNOSIS OF CELIAC DISEASE

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A new compact device exploiting the integration of screen printed electrode-based immunosensors and remote-controlled IoT-WiFi acquisition board has been realized and validated for the diagnosis of Celiac Disease as case of study [1]. The immunodevice is based on chemisorption of open tissue transglutaminase (Open-tTG) on the surface of gold nanoparticles-functionalized carbon screen printed electrodes [2]. IgA and IgG anti-Open-tTG antibodies are recognized by the immobilized bioreceptor as highly specific biomarkers related to Celiac Disease. The signal from the amperometric sensor is acquired and processed through on-purpose developed IoT-WiFi integrated board, allowing for real-time data sharing on cloud services to directly notify all users on the device outcome. The proposed solution does not require customized hardware or software. The analytical performances of the immunosensor were optimized by experimental design, achieving diagnostically useful results in terms of limit of detection (LOD) and limit of quantitation (LOQ) values (LOD_{IgA} = 3.2 AU·mL^{-1}; LOD_{IgG} = 1.4 AU·mL^{-1}; LOQ_{IgA} = 4.6 AU·mL^{-1}; LOQ_{IgG} = 2.3 AU·mL^{-1}) as well as good intermediate precision (RSD < 5%). Finally, the high discrimination capability between positive and negative serum control is suitable for diagnostic purposes, with strong statistical significance (*p<0,001*)

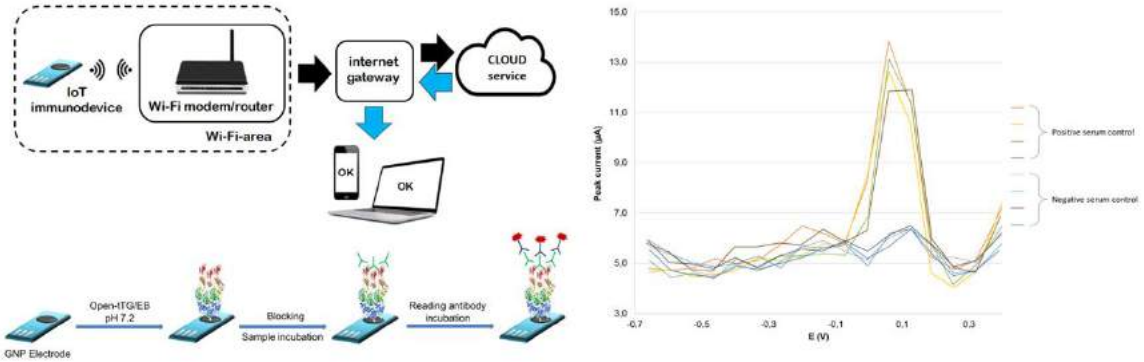

Figure 1. Schematic representation of the immunosensor set-up and of the acquisition and processing system

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O16 SB

NON-SPHERICAL GOLD NANOPARTICLES: A VERSATILE COLORIMETRIC PROBE FOR AGGREGATION-BASED ASSAY AND POINT-OF-NEED TEST

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Spherical GNPs are largely employed as sensitive signal reporters for developing colorimetric (bio)sensors. GNP-based colorimetric assays are built on a unique phenomenon that leads to a color change from red to blue when spherical GNPs aggregate [1]. They have been used for the detection of small molecules, proteins, DNA, and metal ions. The extremely high extinction coefficients of GNPs make them highly sensitive; the color change can be detected by the naked eye, though visual interpretation is complicated by the need of distinguish among similar color shades. Non-spherical GNPs show a color change from blue to colorless when aggregate that simplifies the visual detection and also enables the easy quantification of the aggregation by means of a common colorimeter. Based upon antibody functionalized ns-GNP, we designed a one-step colorimetric method in which ns-GNPs undergo analyte-dependent aggregation. Advantages of ns-GNPs are illustrated by a quantitative assay for monitoring aflatoxin B1 (AFB1), a potent fungal toxin. Aggregation of ns-GNPs is triggered by a multivalent antigen; AFB1 inhibits ns-GNP aggregation and leads to a proportional blue color typical of ns-GNPs (Fig 1). The colorimetric assay based on ns-GNP aggregation guarantees simplicity and rapidity (signal generation is achieved within 10 minutes) joined to sensitivity (estimate LOD value 0.3 ng/ml) and quantitation ability.

Figure 1. Color change triggered by aggregation for non-spherical (blue) GNPs

Spherical (red) GNPs are also the preferred probes for colorimetric lateral flow assays (LFAs). Thanks to the unique shape of ns-GNPs, their surface plasmon resonance band is largely red-shifted so that ns-GNPs appear blue-colored (fig 1). Therefore, combining red (spherical) and blue (non-spherical) GNPs, we designed a novel visual multiplex LFA that uses a single multicolor Test line with a color code for the interpretation of results. The strategy is exemplified by simultaneously detecting aflatoxin B1 and fumonisins in cereal-based food. Images of LFA strips, acquired by means of a common smartphone, also provided (semi-)quantitative information about the analytes through RGB data analysis.

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O17 SB

Carbon Black -MoS_2 nanocomposite as novel screen-printed electrodes modifier

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Carbon Black (CB) is a nanostructured material with comparable electrochemical properties to carbon nanotubes and graphene. However, its low cost makes it very appealing in the fabrication of composite materials. Good examples are reported in the literature on the use of CB modified electrodes for electrochemical sensing of antioxidants [1]. On the other hand, Transition Metal Dichalcogenides (TMD) have emerged as electrode material for analytical purposes due to large available surface area and structural versatility [2]. Particularly, MoS_2 as graphene analogue have been widely used in combination with different carbon and metallic nanostructures for sensing and for (bio)sensing in food analysis, biological and environmental samples [3]. The combination of CB and MoS_2 is reported here for the first time. Different amounts of CB and MoS_2 were studied in terms of electrochemical performance, assessed by CV and EIS using redox probe $[Fe(CN)_6]^{3-/4-}$. The best combination (SPE modified with a mix of CB-MoS2 75:25, v/v) showed an enhanced electrocatalysis towards classic electroactive molecules such as dopamine, uric acid, caffeic acid, coumaric acid and different polyphenols, compared to CB and MoS_2 alone. The obtained electrochemical performance is attributed to the synergistic effects between MoS_2 and CB, and it may open new gates for (bio)sensors tuning and design.

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O1 SS

AN EFFICIENT STRATEGY FOR MOLECULARLY IMPRINTED SOLID PHASE EXTRACTION OF AILANTHONE FROM LEAVES OF AILANTHUS ALTISSIMA

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Ailanthus altissima is used in traditional chinese medicine to treat cold and gastric diseases. The biological activity of its extracts is mainly due to the presence of ailanthone, a compound belonging to the quassinoid class. Over the past two decades, several studies have demonstrated anti-tuberculosis and anti-malarial activity. Moreover, recently, special attention has been paid to the cytostatic activity of ailanthone itself. In spite of the spread of A. altissima in a wide variety of environments, the extraction of ailanthone is a very long and demanding procedure preventing its use in medical pratice.

Due its molecular structure and polar character, ailanthone can be considered a difficult molecule to be molecularly imprinted. To overcome this drawback, we used a preliminary screening of a polymeric library of non-imprinted polymers in order to select polymers capable of significant interactions towards ailanthone. Starting from several monomer-crosslinker combinations selected, we identified two possible MIPs formulations, based on divinylbenzene (DVB) or trimethylolpropane trimethacrylate (TRIM) as cross-linkers and 4-vinylpyridine (4VP) as functional monomer. Their binding properties were investigated by equilibrium binding experiments performed in acetonitrile, methanol and water. The best binding properties compared with the correspondent non-imprinted polymer were obtained with 4VP-TRIM polymer.

The selected MIP was used to set up a solid phase extraction protocol for the extraction of ailanthone from leaf extracts. A complete extraction protocol was developed by optimizing the sample loading, the washing steps and the elution conditions to recover ailanthone from dried leaves.

In conclusion, through the screening of a non-imprinted library it is possible to identify an optimal formulation to prepare an ailanthone-imprinted polymer, and a simple and rapid approach to solid phase extraction of ailanthone from *A. Altissima* was successfully achieved, paving the way to the development of an efficient method to isolate this molecule from its natural source.

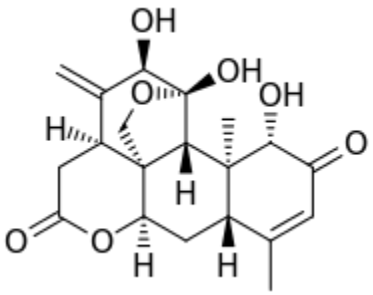

Figure 1. Ailanthone.

O2 SS

UNMATCHED KINETIC PERFORMANCE IN ENANTIOSELECTIVE SUPERCRITICAL FLUID CHROMATOGRAPHY BY COMBINING LATEST GENERATION WHELK-O1 CHIRAL STATIONARY PHASES WITH A LOW DISPERSION IN-HOUSE MODIFIED EQUIPMENT

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Supercritical Fluid Chromatography (SFC) has become one of the preferred techniques for chiral analysis and purification in the pharmaceutical industry, representing a "greener" and faster alternative to common reversed- or normal-phase separations. Despite latest generation chiral stationary phases (CSPs) are characterized by extraordinary efficiency and performance, the extra-column dispersion of commercial SFC equipment (generally around 90 μL^2 vs. 1-2 μL^2 of modern UHPLC chromatographs) is still too large for their satisfactory employment in SFC [1,2].
In this work, a commercial SFC instrument has been in-house modified to reduce its extra-column volume by a series of technical adjustments including the replacement of (i) standard tubings with shorter and narrower capillaries; (ii) the 8 μL flow-cell with a 3 μL one; (iii) the injection system with a 200 nL fixed-loop external one and (iv), finally, by using an *ad hoc* designed external column oven. The extra-column variance was reduced by more than 230% in comparison to the original configuration, from about 85 to slightly more than 2 μL^2 (measured at 2.0 mL/min). This study demonstrates that the dramatic increase of performance in the modified equipment was achieved thanks to the development of turbulent regime inside capillaries at significantly smaller flow rates than in the original configuration. Ultra-high efficiency chiral columns of different geometries in-house packed with latest generation sub-2μm Whelk-O1 CSP have been employed under SFC conditions. By carefully modulating the length of connecting tubings in function of column geometry, efficiencies of roughly 300,000 theoretical plates/m have been obtained on 4.6 mm ID chiral columns. Remarkably, for 3.0mm ID columns, a gain in efficiency greater than 90% for compounds with retention factor of 1 was achieved by using the low dispersion configuration with respect to the standard one.

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O3 SS

DISPERSIVE MAGNETIC SOLID-PHASE EXTRACTION USING GRAFENE@Fe_3O_4 NANOCOMPOSITE FOR THE UHPLC-PDA ANALYSIS OF THE NEW ORAL ANTICOAGULANT DRUGS (NAOCs) IN HUMAN PLASMA

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Despite the development and the improvement of the analytical instrumentation over the last decades, sample preparation plays a key-role in the identification and measurement of the analytes.

Recently, the development of microextraction techniques such as microextraction by packed sorbent (MEPS), solid phase microextraction and dispersive liquid-liquid microextraction have become increasingly popular for the NSAIDs analysis due to the high recoveries, high enrichment factors and the possibility of combining with chromatography or spectroscopy techniques.

Graphene (G), an emerging carbon material, has gained a lot of importance in analytical chemistry in which it has been used as sorbents in sample extraction due to its ultra-high surface area, its hydrophobicity as well as the possibility of establishing π-π interactions thanks to its delocalized electrons. However, graphene is difficult to handle, it is completely insoluble in water, it is difficult to obtain in a high yield and tends to stack to other graphene layers via π-π interactions.

In order to overcome these drawbacks, reduced graphene oxide (rGO), obtained by oxidation of graphite and subsequent reduction, is preferentially used because it is easy to process, it is easily exfoliated, it is more soluble in water and some organic solvents than pure graphene and keeps the high aspect ratio that characterizes graphene. The possibility to combine the magnetic materials with graphene has become a research hotspot. The combination of Fe_3O_4-graphene allows to obtain an efficient adsorbent with high adsorption capacity of graphene and separation convenience of magnetic materials.

The present study focused on the synthesis of a graphene based magnetic nanocomposite (G/Fe_3O_4) as a newly designed material for MSPE and investigated its performance for adsorption of new oral anticoagulant drugs (NAOCs) in human plasma. The results showed that the proposed method was easier and more sensitive compared to the existing method for the determination of NAOCs.

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O4 SS

THE "RACEMIC APPROACH" IN PHARMACEUTICAL ANALYSIS: A SELECTION OF LABORATORY STUDIES

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Two alternative approaches can be pursued for the preparation of enantiomerically/stereomerically pure compounds: the "chiral approach" in which the desired enantiomer/stereoisomer is obtained through dedicated asymmetric synthesis protocols, and the "racemic approach" where the stereoisomer mixture is submitted to chromatographic resolution. The latter case, represents the elective choice at the discovery stage, when preliminary biological tests with single stereoisomers have to be carried out. In this scenario, the (semi-)preparative-scale stereoresolution of pharmaceutically relevant compounds is usually performed with either low- or high-molecular weight chiral selectors (SOs) grafted onto chiral stationary phases (CSPs).
Starting from the studies in which my research group has been historically and is still involved, mainly focused on the domain of chiral ligand exchange chromatography, the use of an amino acid-based SO in the eluent was applied in the reversed-phase (RP) mode for the first time at a preparative scale, to obtain both 1 enantiomers in sufficient amounts for following functional activity tests. As a result of these experiments, only the (*S*)-isomer resulted a potent and mGluR1 subtype selective antagonist. A low-molecular weight SO, based on a *Cinchona* alkaloid derivative, was successfully used in the semipreparative scale enantioseparation of 2, a potent *S. aureus* NorA efflux pump inhibitor when tested as racemate. Interestingly, the isolation of 2 enantiomers under polar ionic (PI) conditions, revealed the prominent contribution of the (*R*)-isomer to both the EtBr efflux inhibition and synergistic effect with ciprofloxacin against SA-1199 B (norA+/A116E GrlA). The same family of SOs was used in PI mode, to get all four diastereoisomers of cyclopropyl dafachronic acid derivatives 3 in sufficient amount for their appraisal towards DAF-12 receptor. The application of the "racemic approach" through the use of polysaccharide-based CSPs, in normal phase (NP) conditions, allowed to evaluate the inhibitory potency of the 5-lipoxygenase-activating protein (FLAP) by 4 enantiomers. As a result, a negligible effect of individual enantiomers over the racemate occurred. The same class of high-molecular weight SOs allowed to obtain pure enantiomers of the BK channel opener 5. The evaluation of the vasorelaxing potency and efficacy of its enantiomers indicated that the absolute configuration at the C-2 position does not play a role in defining the biological activity.

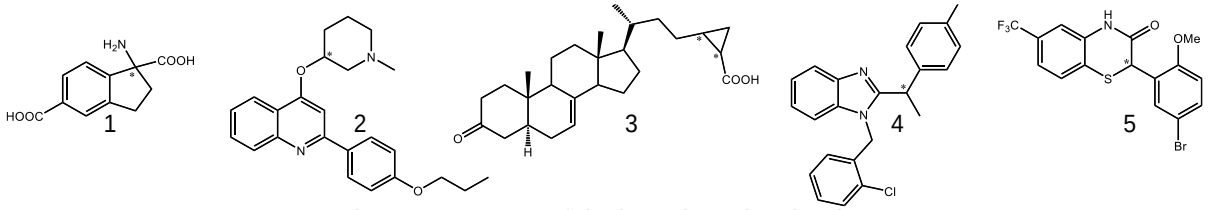

Figure 1. Structure of the investigated molecules

O5 SS

THERMALLY CONDENSED HUMIC ACIDS ONTO SILICA AS SPE FOR MULTI-CLASS PRECONCENTRATION OF STEROID HORMONES FROM ENVIRONMENTAL WATERS FOLLOWED BY HPLC-ESI-MS/MS

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Steroid hormones are an important group of active molecules involved in various physiological functions, but also largely employed in human and veterinary medicine. Nowadays, natural and synthetic steroids are considered pollutants of great concern due to their potent endocrine disrupting activities in aquatic systems [1]. The aim of this work is the application of a new carbon-based sorbent to be used for solid-phase extraction (SPE) of three classes of steroid hormones: oestrogens, progestins and androgens in natural waters. Humic acids were selected as the carbon source in the sorbent due to their low cost, green aspect and macromolecular base structure consisting of hydrophobic frameworks and abundant hydrophilic groups that make them prone to be converted into a mixed-mode carbonaceous material, by a simple pyrolytic treatment (N_2 flow,600°C, 1h). A full characterization of the obtained material (HA-C@silica) demonstrated the presence of sp^2 hybridized carbon and polar groups, both essential for the adsorption and concentration of analytes [2]. Pre-concentration tests were undertaken on tap water samples (500 mL) enriched with 0.05-1 µg/L of each hormone (estrone, 17β-estradiol, 17α-ethinyl estradiol, progesterone, hydroxyprogesterone, medroxyprogesterone acetate and testosterone) using 200 mg of sorbent packed in 3 mL SPE tubes. Quantitative adsorption was observed at the sample native pH for all analytes, and a sequential elution with MeOH and ACN provided good recovery (80-115%) and enrichment factor (EF) up to 200. After SPE, hormones were separated and quantified by HPLC-ESI-MS/MS, with high selectivity guaranteed by Multiple Reaction Monitoring (MRM) mode. Further tests are ongoing on river water and wastewater treatment plants effluents exploring the applicability of the proposed sorbent material to various/complex environmental matrices. The overall performance obtained in terms of recovery, EF, selectivity, sensitivity, precision and cost will be evaluated, and the final analytical method will be applied to the analysis of actual-world water samples.

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O6 SS

DEVELOPMENT OF A FAST AND SIMPLE METHOD FOR THE ASSAY OF URINARY PHTHALATE MONOESTERS BY SOLID-PHASE MICROEXTRACTION-GAS CHROMATOGRAPHY-TRIPLE QUADRUPOLE MASS SPECTROMETRY

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Phthalates esters are industrial compounds that derive from phthalic acid. They are used for a variety of products such as personal care products, medical devices, pharmaceutical and packing materials. Due to the large use, phthalates have become ubiquitous environmental contaminants. They are not chemically bounded to the products and for this they are easily released into the environment. These compounds are hazardous to human health, they affect development and reproductive functions because they act as endocrine disrupting agents. They have also carcinogenic and hepatotoxic effects. Phthalates esters are rapidly metabolized through hydrolysis to their respective phthalates monoesters, which are excreted through urine in their free or glucuronide-conjugated forms. To monitor the exposure to phthalates esters their urinary metabolites are generally used as biomarker [1]. The main purpose of the present work was the development of a fast and simple method for the quantification of monomethyl phthalate, monoethyl phyhalate, monoisobutyl phthalate, monobutyl phthalate, monocyclohexyl phthalate, monoethylhexyl phthalate, monoisononyl phthalate, monooctyl phthalate and monobenzyl phthalate in human urine. The method provided aqueous derivatization based on alkyl chloroformate [2], followed by solid phase microextraction-gas chromatography-triple quadrupole mass spectrometry (SPME-GC-QqQ-MS) analysis. The signals were recorded in selected reaction monitoring (SRM) acquisition mode that allows the achievement of high specificity by selecting appropriate precursor–product ion couples. The derivatization reaction was directly carried out in urine with propyl chloroformate in order to obtain a fast and simple protocol. The extraction ability of five commercially available SPME fibers was evaluated in univariate mode, while the variables affecting the SPME analysis and the derivatization reaction were optimized by the multivariate approach of "Experimental design" (DoE). Finally, the developed SPME-GC-MS/MS method was evaluated in terms of linearity, accuracy, precision, limit of detection and matrix effect.

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O7 SS

QuEChERS EXTRACTION FOLLOWED BY LIQUID CHROMATOGRAPHY COUPLED WITH TANDEM MASS SPECTROMETRY FOR PERFLUOROALKYL ACID DETERMINATION IN STRAWBERRIES IRRIGATED WITH TREATED WASTEWATER

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Agriculture is typically characterized by a high-water demand, since about 70% of worldwide freshwater (FW) withdrawals is used for agricultural irrigation. On the other hand, limited FW availability is a problem of increasing concern and the reuse of treated wastewater (TWW) for irrigation could be an efficient tool of reducing water shortage. However, the TWW reuse is currently far to be fully realized, due to several barriers, such as potential risks for the environment and the human health in the reuse of wastewater improperly treated, due to residual concentrations of priority and/or emerging (e.g. perfluorinated compounds) organic micropollutants. In this regard, this work focused on the development of an analytical method for the identification and determination of selected linear perfluoroalkyl acids (PFAAs) in strawberries irrigated with TWWs. The method is based on the QuEChERS approach, which include the liquid/liquid partition of analytes between salty water and acetonitrile, combined with dispersive solid phase extraction (d-SPE) as clean-up step, followed by liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) analysis. Different d-SPE sorbent phases and their mixtures (e.g. C18/PSA 90/10 w/w) were tested in order to evaluate the best compromise between matrix effect (ME%) and analyte recoveries. Satisfactory recovery values were obtained for all selected PFAAs using C_{18} sorbent (92% - 108%). ME% and apparent recoveries (AR%) of the adopted extraction and clean-up procedure were evaluated through the fortification of sample extracts at the following concentration levels of target analytes: 50, 100, 250 and 500 ng L^{-1}. For the majority of the investigated analytes |ME%| decreased adopting d-SPE procedure, confirming the importance of this step; among the selected analytes, only perfluorodecanoic acid showed a higher absolute value of matrix effect (|ME%|=34%) in cleaned-up extracts, compared to untreated ones. The proposed analytical method exhibited better analytical performances than those published in the literature until now, in terms of analysis time and/or sensitivity, achieving method quantification limits in the range of 7.4-184 *pg* g^{-1} level, with a whole analysis time of about 35 min per sample. Based on the results obtained, this method could represent a valid and effective tool to be used for monitoring also other micropollutants in strawberry and, more in general, other water-rich food matrices. Future studies are necessary for the evaluation of the method applicability to non-aqueous food matrices (e.g. olive) and soil in order to allow the monitoring of the whole agricultural production chain linked to TWW reuse.

FLASH
COMMUNICATIONS

F1 AB

AN ANALYTICAL STUDY OF THE INFLUENCE OF CHITOSAN FEATURES ON THE CHEMICAL, PHYSICAL AND MECHANICAL AND IN-VITRO PROPERTIES OF 3D PRINTED SCAFFOLDS

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Tissue engineering is a promising field of regenerative medicine that relies on the interaction of three main elements: a supporting material, growth factors, and cells to develop a biological substitute for the replacement, restoration or regeneration of damaged tissues and organs [1]. A relevant task of tissue engineering is focused on 3D printing as innovative technologies drawing tremendous attention from both academia and industry for their potential applications in regenerative medicine and pharmaceutical drug delivery [2-3]. Although 3D printing presents revolutionary capabilities, the design and fabrication of 3D devices is critical.
Among biomaterials, chitosan has been widely envisioned, but, to date, not much attention has been given to the relationship between the effects of the physicochemical properties of the raw material and the final 3D product characteristics such as, morphology, mechanical strength and swelling properties. Therefore, in this work, in order to close the existing gap, the relation within the physicochemical features of the polymer as molecular weight and degree of deacetylation to the degree of protonation of the final product has been investigated. Further, the effect by using three different acids as acetic, lactic and ascorbic has dissolution media to prepare the 3D ink has been tested. Then, a relation among these features and the swelling ability of 3D chitosan scaffolds, fabricated by a home-made 3D printing technique, has been revealed. I*n-vitro* culture studies on human skin cell growth are reported to demonstrate the cytocompatibility of the 3D printed scaffolds.
In conclusion, this research lead promising and innovative perspectives to design improved 3D chitosan-based supports for regenerative medicine applications.

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F1 AS

INSIGHTS INTO THE INHIBITION OF *P. FLUORESCENS* BIOFILM FORMATION VIA AFM AND ATR-IR CHARACTERIZATIONS

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Metal nanoparticles are providing new routes to fight the increase of diseases caused by antibiotic-resistant microorganisms. In particular, the interest about nanoantimicrobials is being focused on their efficiency against bacterial biofilm formation [1]. Silver-fluoropolymer (Ag-CF_x) nanomaterials are based on the encapsulation of the active nanophases into a proper dispersing matrix, such as a thin CFx coating. Hence, they offer a controlled release of biocidal ions, and prevent NP from being directly released in the environment. In this work, we prepared Ag-CF_x thin films by ion beam co-sputtering (IBS) [2]. The IBS experimental conditions were chosen in order to obtain nanocomposite films with a silver volume fraction of 0.25 [2]. Samples were characterized by Atomic Force Microscopy (AFM), X-ray Photoelectron Spectroscopy (XPS) and Transmission Electron Microscopy (TEM). Release kinetics of antibacterial silver ions were evaluated in physiological solution by Electro-Thermal Atomic Absorption Spectroscopy (ETAAS). Thin film swelling properties in aqueous environment were measured in an AFM liquid cell, at different sampling times. A comprehensive ATR-IR study was performed to evaluate the effectiveness of Ag-CF_x nanocomposites towards biofilm inhibition. ZnSe crystals modified with Ag-CF_x nanocomposites were mounted into a flow cell with an internal volume of 1.75 mL and a surface contact area of 5.2 cm^2.

While in previous studies we focused on short-term exposure experiments (within 8 hours) [2], in the present study we explored much longer contact times (2 days). AFM and ETAAS measurements on swollen nanoantimicrobial coatings outlined an abrupt change in the ionic release kinetics, under prolonged contact conditions, providing an unprecedented efficiency in the delivery of Ag^+ species. ATR-IR data showed that the biofilm grew for the first 5 hours and remained steady until 20 hours. Around a contact time of 30 hours, Amide I band and Amide II band started to slightly increase while EPS increased dramatically. We interpreted this evidence as an attempt of recolonization by bacteria after 30 hours of contact with the antimicrobial surface.

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F1 CB

Near-Infrared based detection of insects infestation in rice samples

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Rice is one of the most widely consumed cereal in the world and it has to be stored for long periods, so it is very important to protect it from animal attacks, in particular from insects infestation. The high risk due to the possible presence of food pests makes sure that rice must be continuously checked by producers and/or retailers.
Many methods have been proposed in literature to detect food pests, but they are destructive and/or invasive, thus provoking high product and, therefore, economic losses. Under this perspective, the aim of the present work is to develop a methodology for detecting pests infestation in stored rice by Near-InfraRed (NIR) spectroscopy coupled with discriminant and class-modelling classification methods in order to propose a rapid, cheap, green, non-destructive and non-invasive alternative to the conventional methods. To achieve this goal, many rice samples coming from six different Countries were considered, both "edible" and "infested"; after carrying out the NIR analysis, Partial Least Squares-Discriminant Analysis (PLS-DA) [1] and Soft Independent Modelling of Class Analogies (SIMCA) [2] were performed to distinguish between infested and edible samples.
38 parcels of rice have been analysed: 23 were infested and 15 were suitable for human consumption. For each parcel, about 40 individual grains were scanned by means of an integrating sphere (Thermo Scientific Inc., Madison, WI) for a total amount of 1525 spectra. To perform the external validation of the predictive models, measurements have been divided into a training set, consisting of 1025 samples, and a test set, consisting of 500 samples: 181 of "edible" rice and 319 of "infested" rice.
Subsequently to the application of different data pretreatments, the best one was chosen for each of the two models: both for the discriminant and for the modelling approach, the classification error is around 3%.

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F1 EL

SINGLE CELL ELECTROCHEMILUMINESCENCE IMAGING: FROM THE PROOF-OF-CONCEPT TO DISPOSABLE DEVICE-BASED ANALYSIS

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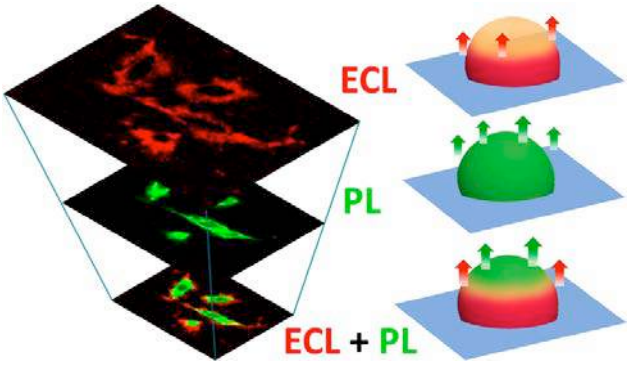
Electrochemiluminescence (ECL) is a leading technique in bioanalysis.[1] Since the excited species are produced with an electrochemical stimulus rather than with a light excitation source, ECL displays improved signal-to-noise ratio compared to photoluminescence. The peculiar analytical performances in terms of high detectability of conventional chemiluminescence (CL) are retained and, in addition, the electrochemical trigger of the reaction allows controlling the time and position of light emission from ECL probes. These properties make ECL systems particularly attractive also for microscopy imaging techniques.
Here we present the application of optically transparent electrodes based on carbon nanotubes materials to ECL, demonstrating the electrocatalytic superiority of such materials *vis-à-vis* ITO electrodes. The employ of carbon nanotubes resulted in a ten times higher emission efficiency compared to commercial transparent ITO electrodes.
Finally, we present the potential diagnostic applications of our approach thought the direct ECL imaging of overexpressed proteins on tumor cells. [3]



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F2 EL

OPTIMIZING THE ELECTRODEPOSITION PROTOCOL OF ENANTIOSELECTIVE INHERENTLY CHIRAL ELECTRODE SURFACES: A MULTI-TECHNIQUE INVESTIGATION

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We have recently introduced "inherently chiral" enantiopure electrode surfaces of outstanding chirality manifestations, including circularly polarized luminescence, reversibly potential-driven circular dichroism, and large potential differences for the enantiomers of chiral probes in voltammetry experiments performed on such surfaces. [1-3]
The outstandingly powerful "inherent chirality" concept implies a molecular structure where the stereogenic element does not consist in an isolated stereocentre or an external chirality source, but originates from a tailored torsion in the whole main backbone endowing the molecule with its key functional property (here electroactivity).
A key issue is now to investigate the enantioselection mechanism and to optimize the experimental protocols for the deposition of our inherently chiral surfaces. For both aims it is important to study the thickness and regularity of the chiral oligomer films as a function of the experimental conditions. We started a systematic profilometry study correlated to electrochemical impedance spectroscopy measurements of the oligomer films obtained by carefully controlled electrodeposition, varying one by one different experimental parameters. The study is also important to properly compare enantioselection by films prepared from different inherently chiral monomers, including *e.g.* bisindole and tetrathiahelicene ones.

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F1 EC

INVESTIGATING PAINT MATERIALS IN STREET ART MURAL PAINTINGS BY ANALYTICAL PYROLYSIS BASED TECHNIQUES

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Different forms of urban art and street art, intended as contemporary visual artworks located outdoor in urban contexts, are quickly developing heritage status. The need to preserve urban contemporary art in the context where it was created is widely recognized, however its preservation and conservation raises severe issues to conservators, conservation scientists and heritage managers. The paint materials of contemporary art, e.g. acryl, alkyd and vinyl paints, and synthetic organic pigments, pose challenges only recently faced in heritage science. An improved knowledge of the factors influencing the stability and degradation processes of street art paint materials is needed to assess the impact of the environmental factors in the constantly changing urban landscapes, and to plan effective preventive conservation strategies.

To achieve this target suitable analytical tools needs to be developed , evaluated and applied. This study explores the potentialities of analytical pyrolysis based analytical methods in investigating the synthetic paint materials used in a series of street art artworks. The characterised paint materials include both XX century public paintings by word reknown artists as Alvaro Siqueiros and Keith Haring, and contemporary street art works which conservation is object of ongoing research, in addition to reference paints.

Analytical pyrolysis coupled with gas chromatography and mass spectrometry (Py-GC/MS), with and without thermally assisted in situ derivatisation of pyrolysis products , was used as an effective approach to characterise at a molecular level the complex mixtures of polymeric paint binders and additives which constitute the paints used by street artists, by direct analysis of a solid micro samples without any pre-treatment. Recent developments of analytical pyrolysis as multi-shot Py-GC/MS and evolved gas analysis mass spectrometry (EGA-MS) allowed us to investigate components with different molecular weight/volatility in the same micro-sample with high chemical resolution, such as polymers, plasticizers and organic dyes.

The investigations were carried out in collaboration with conservators and conservation scientists from the Accademia delle Belle Arti di Verona , University of Urbino, University of Udine, with LANCIC - Laboratorio Nacional de Ciencias para la Investigación y Conservación del Patrimonio Cultural in Mexico City and with the private conservator Antonio Rava. The results were exploited or are currently exploited to plan conservation intervations of the murals, and the objectives of the reserahc where both assessing the full potential of innovative analytical techniques in the study of synthetic paint materials, both going towards the creation of a data base of the street art paint materials, containing inormation on binders, pigments and additives.

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F2 EC

POTENTIALLY HARMFUL ELEMENT (PHE) OCCURRENCE AND PHASE PARTITIONING IN THE RIVER MOUTHS OF THE GULF OF TRIESTE (NORTHERN ADRIATIC SEA)

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Potentially harmful elements (PHEs) are supplied to estuarine environments in association with freshwater inputs affected by several anthropogenic sources [1]. The present work aims to understand the PHE (Pb, Hg, Cs, As, Zn, Cu, Ni, Co, Fe, Mn, Cr) partitioning between particulate (> 0.45 µm), colloidal (0.45 µm - 10 kDa) and dissolved (< 10 kDa) fractions in river mouths of the Gulf of Trieste (northern Adriatic Sea). In order to achieve these objectives, CTD (Hydrolab H_2O Multiprobe) vertical profiles of salinity, temperature and turbidity were recorded before sampling to identify the water masses. The surface samples were collected at variable depth, according to the salinity trend and along the salinity gradient, whereas the bottom water samples were representative of salt water intrusion. In addition, the main physico-chemical parameters (T, pH, Eh, DO and EC) were measured *in situ* (pH-meter PH25, Conductivity-meter CM35+ by Crison Instruments). Samples were filtered through 0.45 µm filters (Millipore HA, Ø 47 mm) to isolate the particulate fraction which was acid-digested through a total dissolution in a closed microwave system (Multiwave PRO, Anton Paar). The filtrate samples were ultrafiltered through 10 kDa membranes (Vivaflow 200, Sartorius). All sample aliquots were analysed for PHE determination by means of Inductively Coupled Plasma Mass Spectrometry (Nexion 350x Perkin Elmer), whereas Hg was analysed via Cold Vapor Atomic Fluorescence Spectrometry (Mercur Analytic Jena). Hydrodynamic conditions at the river mouths showed the presence of two distinct layers due to the freshwater input and salinity vertical profiles displayed a sharp halocline or mixing layer depending on the river discharge. Elevated PHE contents were detected in the particulate and dissolved fractions and in some parts, PHEs seem to be associated with the colloidal fraction. As expected, Hg reaches elevated values in the particulate fraction of the Isonzo River [2]. The Timavo River samples showed elevated concentrations of PHEs, most likely due to wastewater discharge from a paper mill located near the river mouth. Information on PHE mobility can be provided by the correlations observed between PHE content and salinity, which appear to have an important role in PHE phase partitioning.

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F3 EC

USE OF NANO-STRUCTURAL MATERIALS FOR ABATEMENT OF NITRATES IN NATURAL AND WASTE WATER

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Intensive agricultural crops demand the use of specific fertilizers with advanced nutritional properties. Among these products, the most efficient and functional are slow release fertilizers which guarantee a constant nutrition over time.
A real problem of the Italian environment is the leaching of nutrients brought into the soil, such as nitrates. These compounds haven't enough time to be assimilated by plants, but they end up directly in the groundwater or in natural waters. In addiction high level of nitrates in waste water from different industrial processes is a real problem. For this reason the study has been focused on innovative nanostructured materials (such as nanosponges) for the abatement of nitrates in waters.
These nanosponges arise from biopolymers, especially based on maltodextrins. Maltodextrins are a family of oligosaccharides get from starch of different biomass (potatoes, corn, peas). Starting from the starch, it is possible to get both cyclic and linear maltodextrins through an enzymatic conversion or a partial hydrolysis processes. Specific cross-linking agents allows to achieve a hyper-crosslinked biopolymer, with an eco-compatible and biocompatible polymeric structure. The main nanosponges characteristic is their hydrophilicity and modular electrical charge. It is possible to have a high exchange capacity for the absorption and release of compounds, changing some parameters of the synthesis.
Therefore, laboratory tests were carried out both to assess the potential retention of nitrates and to evaluate their future use as fertilizer. To this end the synthesis was developed changing the amount of charge into the nanosponges and using water in the reagent environment as solvent. Other organic solvents were totally avoided. Several batch and continuous analytical tests were performed, changing experimental conditions. The results achieved were in a range from 50% up to 80-90% of nitrate abatement.
So these nanosponges are definitively an innovative, biodegradable and environmentally friendly material (based on sugar structure). They have shown a considerable potential for the abatement of nitrates. Moreover these nanosponges charged with nitrates could be used as slow release fertilizer. With the degradation of the sugar structure, there would be an enrichment of the both of nitrate and carbon into the soil. Tests in the field must be eventually carried out to validate its functioning as a totally biodegradable fertilizer.

F1 EQ

CALIXARENE-BASED SUPRAMPHIPHILES IN NEUTRAL BUFFERED SOLUTION: DETERMINATION OF CMC AND ΔH_{mic} BY A SINGLE EXPERIMENT

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Surfactants have widespread applications in fine chemical industry, detergents, personal care and cosmetics, agrochemicals, pharmaceuticals and food processing. Conventional surfactants consist of a polar or an ionic head group connected to a hydrophobic alkyl chain by covalent bonds. A new class of amphiphilic systems, called supramolecular amphiphiles or supramphiphiles, in which the hydrophilic and hydrophobic components are held together by non-covalent interactions, has gained increasing attention in recent years. Different types of interactions, such as metal-ligand coordination, hydrogen bonding or host-guest formation, can be employed to drive the assembly of supramolecular amphiphiles [1]. In particular, the interaction/encapsulation of appropriate long-tailed guests with the cavity of suitable receptors, such as calixarenes, has been reported to afford new and efficient supramolecular amphiphilic adducts [2].
The aggregation of supramphiphiles based on host-guest complexes formed by water soluble calix[n]arenes and cationic organic guests has attracted the interest of some research groups [3]; however, a quantitative characterization of the binding features and driving forces of the host-guest formation and micellization processes occurring in buffered aqueous solution has not been reported yet.
Isothermal titration calorimetry (ITC) is an invaluable technique for the study of both the host–guest complex formation and the self–organization of surfactants into micellar aggregates. This technique allows for the accurate determination of key parameters, such as critical micelle concentration (CMC) and enthalpy of micellization (ΔH_{mic}), through one single experiment.
In this work, complex species, binding constants and forces driving the formation of supramphiphiles made of a *p*-sulfonatocalix[4]arene and positively charged long-tailed guests in neutral (buffered) aqueous solution have been determined in order to find out the best systems and conditions for the assembly of efficient micellar-like aggregates. The aggregation features of the most promising host–guest complexes have been also studied by ITC in neutral aqueous solution. CMC and ΔH_{mic} values of the micellar-like aggregates formed by different supramolecular surfactants highlight the crucial role played by the calixarene scaffold in the formation efficient self-aggregating systems. The effect of the ionic strength has also been studied and is here critically discussed.

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F2 EQ

SPECIATION STUDY OF A BIS-(3-HYDROXY-4-PYRIDINONE) TOWARDS M^{2+}

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This contribution is the result of a speciation study on the complexing ability of a bis-(3-hydroxy-4-pyridinone) ligand ($NTAPr(3,4\text{-}HP)_2$), derivative of nitrilotriacetic acid (NTA), towards divalent metal cations of biological interest, namely Ca^{2+}, Cu^{2+} and Zn^{2+}.
The 3-hydroxy-4-pyridinones are a class of bidentate compounds derivatives of deferiprone and represent good chelating agents for the detoxification of the human body from *hard* metal cations [1]. The synthesis and the acid-base properties of $NTAPr(3,4\text{-}HP)_2$ were already presented [2] and the protonation data confirmed by ^1H NMR spectroscopic measurements at I = 0.15 mol L^{-1} in $NaCl_{(aq)}$ and T = 298.15 K. On the sequence of the study of this ligand as a strong sequestering agent for *hard* metal cations (Al^{3+}, Fe^{3+}) [2], it appeared also relevant to assess its affinity towards Ca^{2+}, Cu^{2+} and Zn^{2+}. Therefore, the complexing ability of the ligand towards this set of metal cations was investigated by means of UV-Vis spectrophotometric titrations at the same experimental conditions of the protonation studies. The speciation models obtained consisted of protonated and simple metal-ligand species; the stability constants refined for the M*L* complex follow the trend: $Cu^{2+} > Zn^{2+} > Ca^{2+}$. Concerning the Zn^{2+}/$NTAPr(3,4\text{-}HP)_2$ complexation, some ^1H NMR spectroscopic measurements at I = 0.15 mol L^{-1} in $NaCl_{(aq)}$ and T = 298.15 K and computational studies were performed to gain information on the metal-ligand coordination. Furthermore, the sequestering ability of the ligand towards the metal cations of interest was investigated by the determination of the $pL_{0.5}$ [3] and pM [4] parameters calculated at different pHs and pH = 7.4, respectively.

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F1 FN

EXTRACTION, ANALYSIS AND ANTIOXIDANT ACTIVITY EVALUATION OF PHENOLIC COMPOUNDS IN DIFFERENT ITALIAN EXTRA-VIRGIN OLIVE OILS

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Extra-Virgin olive oil contains a variety of phenolic molecules that are highly valuable to the quality of the oil with regard to sensory and health characteristics. Its composition greatly varies with genetic, agronomic, and environmental factors. Moreover, differences can be observed based on analysis method employed. For this reason, the objective of this study was to extract and analyze phenolic compounds of EVOO samples collected in different Italian geographic areas. The final aim of the project will be to create a composition data bank with a great number of Italian EVOO samples. Phenolic compounds extraction was assessed according to Ricciutelli et al. [1] with some modifications. Briefly, 1 g of oil dissolved in 1 mL of hexane was extracted with 1 mL of a mixture of methanol:water (60:40, v/v). The extraction was repeated four times and supernatants were combined, washed with hexane and the methanolic solution was evaporated. We determined their total concentration through Folin-Ciocalteau assay. The antioxidant activity was evaluated with the following assays: 2,2'-azinobis-(3-ethylbenzothiazoline-6-sulphonate) (ABTS), 1,1 diphenyl-2-picrylhydrazyl (DPPH), ferric ion reducing antioxidant power (FRAP) and oxygen radical absorption capacity (ORAC). Results showed: TPC values in the range 0.098-0.573 mg gallic acid eq./g of oil and antioxidants activity values in the ranges 2.11-8.94 µmol Trolox eq./g of oil, 0.42-2.41 µmol Trolox eq./g of oil, 0.59-3.19 µmol Trolox eq./g of oil and 1.67-17.99 µmol Trolox eq./g of oil for ABTS, DPPH, FRAP and ORAC assays, respectively. HPLC-PDA/ESI-MS method for the analysis of individual phenolic compounds was developed and validated. The analysis of the extracts highlighted the presence of different phenolic compounds being phenolic acids, tyrosol, oleuropein and its derivatives, luteolin and apigenin.

Acknowledgment

The study was funded by Cariplo Foundation within the "Agroalimentare e Ricerca" (AGER) program. Project AGER2-Rif.2016-0169, "Valorizzazione dei prodotti italiani derivanti dall'oliva attraverso Tecniche Analitiche Innovative"-"VIOLIN". Authors wish to thank Shimadzu Corporation for constantly supporting their research work.

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F2 FN

MULTIVARIATE OPTIMIZATION OF A QUECHERS PROCEDURE FOR THE LC-MS/MS ANALYSIS OF PHYTOESTROGENS IN SOY BURGERS

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In the recent years, several vegetal formulas, presented as meat alternatives, have been introduced in the international market and soy is one of the most common ingredients of such foods. Soy is one of the principal food sources of phytoestrogens, which are a class of natural chemicals, found in plants as secondary metabolites. They present proven interaction with the endocrine system of humans, but the attribution of beneficial or detrimental impact on human health is still controversial [1]. Therefore, it is important to estimate the daily intake of these substances when vegetal meat substitutes are consumed in relevant quantities. In this framework, our efforts were focused on the optimization of the extraction and analysis of five phytoestrogens (daidzein, genistein, formononetin, biochanin A and coumestrol) in soy-based burgers by LC-MS/MS. We chose the QuEChERS technique [2] for sample treatment and developed two different experimental designs to reach the best results in terms of recovery and matrix effect. Several factors are involved in the QuEChERS procedure, which includes an extraction step with a water/acetonitrile mixture, followed by salts-induced phase separation and a final dispersive clean-up. A first screening design (Plackett-Burman) allowed to select the statistically significant variables affecting recovery and matrix effect of the five analytes. Afterwards, response surface methodology was used to model the selected responses as a function of the significant variables. A Box-Behnken design was selected to perform a reasonable number of experiments, but sufficient to obtain the response functions. For daidzein and genistein, which are found in high concentrations, a simple dilution allowed to obtain negligible ion-suppression in the LC-ESI-MS analysis, and quantitative recoveries were obtained avoiding the clean-up step. As for the other analytes, at much lower concentrations, best results were attained using a minimum weight of sample (200 mg extracted with 10 mL of solvent mixture), and performing a clean-up with PSA and Florisil sorbents. High recoveries (90-105%) and low matrix effect (<20%) were obtained for all compounds except for biochanin. This analyte undergoes important ion suppression, but recovery strongly decreases by using the PSA clean-up sorbent. The developed method was applied to the analysis of soy-burgers samples from the Italian market and proved to be fast, simple and reliable.

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F1 FO

DETERMINATION OF ETHYL-GLUCURONIDE IN HAIR BY MEANS PLE-SPE EXTRACTION AND HPLC-MS/MS ANALYSIS

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Alcohol is considered a legal psychotropic substance, whose sale is authorized in most countries of the world, but single nation legislations define minimum purchase and consumption age limits for alcoholic beverages. Every year 139 million DALYs (disability-adjusted life years), 5.1% of the global burden of disease and injury, were attributable to alcohol consumption [1]. In some cases, this consumption becomes abuse, which can lead to a real dependence from this substance. The effects of the alcohol abuse are varied, and can involve a slight state of alteration up to the complete loss of control; its use during work or driving is strictly forbidden [2]. For this reason, the need for restrictive controls by the police is clear, but also the need for analytical methods able to certify the consumption.
While ethanol is the target analyte in blood, ethyl glucuronide (EtG) in the different biological matrices was investigated, since it is the metabolite obtained from the conjugation of ethanol with glucuronic acid. The extraction of EtG from hair is, usually performed by incubating the sample with different solvents [3]. Generally, the detection of EtG in the hair is carried out by means of mass spectrometry; recently it is preferred to work by coupling the detection with liquid chromatography, rather than by gas chromatography [4].
The aim of this work is the development of a rapid, fast and simple analytical method for the determination of EtG in hair, in order to date the consumption of alcohol over time and verify the abstinence of those who are ascertained to be chronic consumers. Therefore, we propose an automated extraction conducted by means of PLE and a rapid SPE clean-up which allows to obtain a sample as much as possible free of matrix effect. EtG concentrations in hair was measured by HPLC-MS/MS in MRM mode. The presented method was tested at two different concentrations 7 pg/mg, 30 pg/mg, respectively the limit value that defines the so-called moderate consumption and the cut-off value in the hair defined by the SoHT guidelines [5].

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F1 GC

CADMIUM UPTAKE AND DIFFUSION IN BIVALVE MOLLUSK SHELLS FROM AQUEOUS MATRICES – AN LA-ICP-MS LINE SCAN AND ELEMENT IMAGING STUDY

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Mollusk shells are formed by a biologically controlled mineralization that leads to the formation of superimposed $CaCO_3$ layers. This process takes place in a confined space between the mantle and the protective organic layer [1].

Intensive shellfish production leads to the formation of large amounts of pre-consumer and post-consumer residues, mainly composed of shells. The improper disposal of this particular material results in a waste of natural resources, but also can raise environmental issues.

The reuse of this material as adsorbent could potentially be a cost-effective approach for the removal of heavy metals in water remediation technologies.

Heavy metals are common pollutants found in natural waters, especially nearby mining sites and metalworking industries. In particular, cadmium represents a contaminant of major interest because of its toxicity even at low concentrations: it substitutes calcium and zinc in biological processes leading to the alteration of cellular metabolism [2].

In this study we investigated the adsorption and diffusion of cadmium through the shell layers using laser ablation (LA-ICP-MS), a well-established technique that provides flexibility to perform spatially resolved analyses at the µm scale and also bulk analyses in short time with minimal sample preparation needed [3].

Line scans and elemental imaging analyses were carried out with an ArF Eximer laser system operating at a wavelength of 193 nm, coupled to an ICP-TOFMS (Tofwerk, Thun, Switzerland) at ETH Zürich.

Both line scans and element images showed that cadmium is adsorbed mainly on the outer layers with little diffusion towards the shell's interior.

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F1 MS

HPLC-ES MS/MS METHOD FOR THE IDENTIFICATION AND QUANTIFICATION IN HUMAN FECES OF GUT MICROBIOTA PRODUCTS: OXO-BILE ACIDS

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Bile acids (BAs) are involved in the transport of lipids in bile, and act as molecular signaling hormones. Via several metabolic pathways, gut microbiota (GM) produces secondary BAs in the intestine from primary BAs synthetized in the liver. Furthermore, GM can produce oxo-BA in the colon through oxidation of BA hydroxy groups. Researchers have demonstrated that these oxo-BA can interact with enzymes and receptors in a similar way to conventional BAs [1]. However, the complete oxo-BA characterization in biological fluids (particularly intestinal content and stool) has not yet been reported.
A new reverse phase HPLC-ESI-MS/MS method has been developed and validated in negative ionization for the targeted analysis of 28 compounds, including primary BAs, secondary BAs, and oxo-derivatives. To ensure a comprehensive method for investigating a wider range of oxo-BAs, non-commercially standards were synthesized, purified, and properly characterized. They have been separated within 40 minutes at 40 °C column temperature, without derivatization. The method is accurate (bias%<15%), precise (CV%<10%), with a limit of quantification (LOQ) <30 ng/mL that is similar for all the studied compounds. The matrix effect does not significantly affect the analysis accuracy, allowing the use of calibration curves in mobile phase, without matrix-matched protocols. The developed method does not require pre-analytical clean-up because of its high detectability and the relatively high concentration of oxo-BAs (in the µmol/g range).
This method was used to analyze oxo-BAs in human fecal samples from healthy subjects. We defined the most representative and assessed their potential involvement in intestinal diseases and their role as potential signaling molecules. We also investigated their passive intestinal absorption in the colon and the potential spillover into the systemic circulation.

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F1 SB

LIFE MARKER DETECTION IN PLANETARY EXPLORATION: A NOVEL BIOSENSOR FOR ATP DETECTION BASED ON CHEMILUMINESCENT DNA SWITCH INTEGRATED WITH AMORPHOUS SILICON PHOTODIODES

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Several studies reported the presence of organic compounds in extraterrestrial environments in order to identify life markers, i.e., molecules (such as organic molecules, amino acids, nucleic acids, polysaccharides) indicators of extant or extinct life [1]. The continuous evolving development of extremely compact systems relying on microfluidics, commonly known as lab-on-chip devices, has gained much attention thanks to their favorable characteristics in terms of reduced size and weight, very low sample and reagent consumption, reduced analysis time and, often, superior achievable performances in terms of limits-of-detection. Lab-on-chip devices are extremely suitable for space missions [2].

Herein we report about the design and optimization of new analytical platform for the detection of bio-organic molecules outside of the Earth. In particular we optimized a DNA switch based on chemiluminescent (CL) detection for the identification of the life bio marker Adenosine triphosphate (ATP). Indeed, CL-based detection allows to ensure high analytical performance without external radiation sources and complex optical systems [3]. The DNA switch will be implemented into a portable device which will be composed by a microfluidic network based on capillary forces for the handling of samples and reagents, a set of functionalized detection sites where DNA nanomachine will be carried out and an array of thin-film hydrogenated amorphous silicon (a-Si:H) photosensors for the detection of the analytical CL signal. The implementation of this functional module will provide a compact and fully-integrated device displaying low power consumption.

Acknowledgements

The project PLEIADES (Planetary Life Explorer with Integrated Analytical Detection and Embedded Sensors) was supported by the Italian Space Agency (ASI) (Accordo n. 2015-037-R.0).

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F2 SB

A COMPETITIVE APTAMER ASSAY FOR GLUTEN DETECTION IN DEEP EUTECTIC SOLVENT

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Deep eutectic solvents (DESs) were firstly reported in 2004 by Abbott, who found that a eutectic solvent was formed when a choline compound and urea were mixed. Ever since, they have been applied in many different fields such as organic synthesis, electrochemistry and bio-catalysis.

DESs are good solvents for a wide range of molecules, including poorly water-soluble molecules. The complex mixture of proteins integrating gluten, responsible for triggering celiac disease, is included in this group. Correct gluten quantification in gluten-free labeled food is still an open topic, since gluten measurements conducted with different extraction procedures do not supply equivalent results. Lately, gluten extraction with deep eutectic solvents has been described [1]. However, the usefulness of this new gluten extraction protocol is subordinated to its compatibility with commonly employed bio-assays based on antibodies as specific receptors. In order to fully exploit the advantage of the gluten extraction protocol using deep eutectic solvents, we selected aptamers in a deep eutectic solvent called Ethaline. Aptamers, which are single-stranded DNA sequences, are selected by an in vitro process called SELEX (systematic evolution of ligands by exponential enrichment) and, until now, most of the aptamer selection processes have been carried out in aqueous media, condition that normally lead to the optimal aptamer-target interaction.

For the first time we report the use of deep eutectic solvents for the SELEX process, illustrating a new and faster way of selecting aptamers targeting poorly water-soluble molecules.

After DES-SELEX, the aptamer with the best affinity was employed to perform a competitive electrochemical assay. In the assay the immunotoxic peptide, 33-mer, was immobilized on the surface of magnetic particles, competing with increasing concentrations of gliadin in presence of the selected aptamer at a fixed concentration. The calibration assay was performed between 1 and 10000 ppb of gliadin. The detection was carried out chronoamperometrically at 0 V after labeling with streptavidin-HRP the aptamer and adding the substrate for 30s. The calibration curve was fitted to a four-parameter logistic equation. This method permitted us to quantify gluten in different food samples.

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F3 SB

RATIONAL CONTROL OF THE ACTIVITY OF A CU^{2+}-DEPENDENT DNAZYME BY RE-ENGINEERING PURELY ENTROPIC DISORDERED DOMAINS

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Here we modulate the catalytic activity of a Cu^{2+}-dependent self-cleavable DNAzyme by rationally introducing different intrinsically disordered regions that, through a purely entropic contribution, control the folding, and thus activity, of the DNAzyme.
To do this, we have designed a triplex-forming DNA sequence that, by recognizing a 11-base DNA strand through the formation of a clamp-like structure, folds into the highly conserved catalytic core of the Cu^{2+}-dependent self-cleavable DNAzyme. The affinity with which the triplex-forming DNA sequence binds to the 11-base DNA strand can be modulated by varying the length, and thus the entropy, of the loop that connects its two recognition portions (Figure 1). This allows to modulate the catalytic activity of the Cu^{2+}-dependent self-cleavable DNAzyme through a simple modulation of the entropy associated to its folding in a very versatile and precise way.

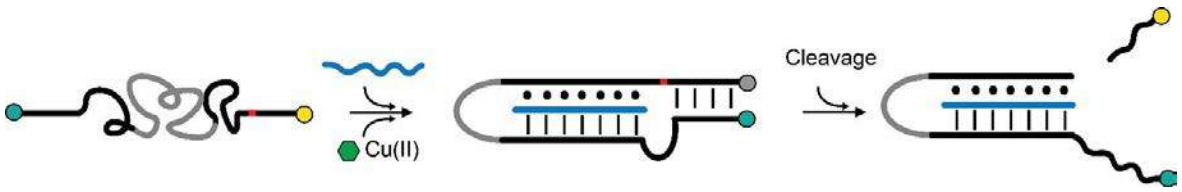

Figure 1. Triplex-forming Cu^{2+}-dependent self-cleavable DNAzyme.

[1] S. Ranallo, D. Sorrentino, F. Ricci, *(in preparation)*.

F4 SB

DNA-BASED QUARTZ CRYSTAL MICROBALANCE ARRAY FOR THE IDENTIFICATION OF AROMA PATTERNS IN FOODS

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DNA has been extensively used in sensors design, fabrication, characterization, and application providing new impulses to bioanalytical research [1],[2]. Currently, gas sensors are addressed by mimicking the olfactory system using olfaction-inspired biomaterials and very few works propose DNA as functional material [3]. In this work, hairpin DNA (hpDNA) conjugated with AuNPs was used as an artificial molecular trap in piezoelectric gas detection. The hpDNA loops having unpaired bases were analyzed for the binding to chemical classes (aldehyde, terpenes, alcohols) of volatile organic compounds (VOCs) and their presence in food. Tetramers, pentamers, and hexamers DNA loops were selected maximizing the recognition properties of the DNA motif between chemical classes. The relative binding affinities of the hpDNA loops against different VOCs belonging to relevant chemical classes were evaluated. It was found that DNA loop size played a very important role in experimental data since the binding affinities improved with size. The ssDNA loops were extended with a double helix stem of four bases (GAAG to 5' end and CTTC to 3' end) and covalently bound to gold nanoparticles (AuNPs) using a thiol spacer attached to 5' end of the hpDNA. hpDNA-AuNP was deposited onto 20 MHz quartz crystal microbalance (QCMs) to realize gas piezoelectric sensors. The gas sensor array has been used to predict the shelf life of carrots; in fact, the good flavor of carrots is one of the main reasons for its acceptance by consumers. The measurements have been carried out on carrots samples cut into rings and kept at four different temperatures: 40°C; 25°C; 4°C; -18°C . The analyses of the aromatic pattern has been carried out on the head-space with the sensor array and GC-MS SPME method. The results, analyzed using principal component analysis (PCA) indicated that the sensors are able to clearly discriminate changes in the evolution of VOCs at the different temperatures of storage.

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F5 SB

DEVELOPMENT OF A REFLECTANCE SMARTPHONE PAPER-BASED CHEMOSENSOR FOR THE EVALUATION OF ANTIOXIDANT ACTIVITY BY *IN SITU* GOLD-NANOPARTICLES SYNTHESIS.

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The antioxidant activity is one of the most important features for the evaluation of quality of extra virgin olive oil (EVOO). Usually, it is determined by microtiter plate-based assays (e.g., ORAC, ABTS, CUPRAC, DPPH), which are time-consuming and require expensive laboratory procedures. Thus, a cheap and easy-to-use device to measure this quality parameter using a point-of-need approach is desirable. We developed a paper-based chemosensor exploiting a colorimetric reaction utilizing *in situ* gold-nanoparticles synthesis [1] to measure the antioxidant activity of EVOO alcoholic extracts. The device, made of black acrylonitrile-butadiene-styrene (ABS) polymer and fabricated using a low-cost 3D printing technology, includes a disposable analytical cartridge, a dark box to avoid interference from ambient light and a holder to connect the dark box to a smartphone. A Samsung S8 smartphone equipped with a BI-CMOS sensor was used as detector, the embedded flash acting as light source. The analytical cartridge contains three reaction chambers (sample, reference standard and blank). All reagents for nanoparticles formation were previously adsorbed on a 1 cm^2 cellulose paper support. Quantitative analysis of color changes was performed using a dedicated software (ImageJ v.1.46). Under the optimized experimental conditions, the intensity of the red color is proportional to the amount of antioxidant species, expressed as equivalent of gallic acid, with a linear range from $1{,}0\times10^{-5}$ M - $1{,}0\times10^{-3}$ M and a limit of detection (LOD) of $3{,}3\times10^{-6}$ M. Our "all in one", point-of-need chemosensor allows to simply quantify antioxidant capacity in a large variety of foods.

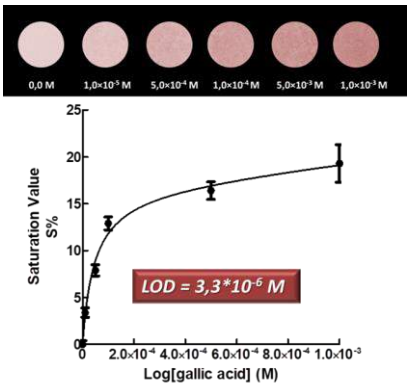

Figure 1. Calibration curve obtained for gallic acid (range $1{,}0\times10^{-5}$ M - $1{,}0\times10^{-3}$ M).

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Acknowledgments: The project was funded by Cariplo Foundation within the "Agroalimentare e Ricerca" (AGER) program. Project AGER2-Rif.2016-0169, "Valorizzazione dei prodotti italiani derivanti dall'oliva attraverso Tecniche Analitiche Innovative (VIOLIN)"

F6 SB

ENVIRONMENTAL AND OPERATIONAL STABILITY OF ORGANIC FIELD EFFECT TRANSISTORS FOR BIOSENSING APPLICATIONS

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Interest towards the use of organic field effect transistors (OFET) for the development of biosensors is constantly growing. In particular, electrolyte gated OFET (EGOFET) devices have emerged as powerful tools for biosensing applications [1]. Early diagnosis and high detection sensitivity for some diseases (e.g. neurodegenerative ones [2]) are particularly important. However, when an OFET biosensor has to be applied in aqueous environments (mimicking for example biological fluids), some critical issues may arise due to the possible lack of environmental long-term and/or operational stability. This holds true for the possible degradation of organic electronic materials [3], such as p-type poly(3-hexylthiophene-2,5-diyl) (P3HT) organic semiconductor, which is frequently employed in these devices. Barrier films are often applied to most organic electronics to impede degradation (due to oxygen and/or water) [3]. This means that an additional step about encapsulation (or lamination) in the device fabrication process has to be included, which increases the costs and the complexity of the preparation.

In this communication, we report some results about the improvement of device stability with different approaches, such as the implementation of inorganic nanophases [4, 5]. Two architectures were investigated, namely OFET- and EGOFET-type. Some additional information gathered through other characterization tools (e.g. X-ray photoelectron spectroscopy) will be also shown.

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F7 SB

POLYDOPAMINE: MOLECULAR IMPRINTING, PLASMONS AND CATALYSIS

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Despite the several important roles in biology, nowadays the vast research outcomes from dopamine studies is due to its chemical reactivity. This self-assembling functional monomer has been adopted for surface coating at nanometric scale as polydopamine (PDA) [1], and reduction potential of catechol moiety has been employed to produce metal nanoparticles *in situ* without other reducing agents or metallic seeds [2]. Recently, we have devoted our study to both coating and redox proprieties of this biocompatible nanomaterial [3-5]. In detail, we have shown that dopamine can be used to create a molecularly imprinted polymer (MIP); a robust and inexpensive alternative to naturally occurring receptors; via dopamine-analyte co-polymerization, which generates cavities complementary to the original molecule in terms of dimension, shape, and noncovalent interactions. We have applied this strategy to describe the first example of epitope-imprinted biosensor for cardiac biomarker troponin T via SPR on PDA-modified gold surface [3]. Moreover, we have reported for the first time that the growth of gold plasmonic nanoparticles (AuNPs) onto optically transparent PDA surface of disposable UV–Vis cuvettes is modulated by polymer thickness [4]. The absorbance displayed by these cuvettes change in intensity in dependence of the filling medium but presents a fixed plasmon wavelength maximum. We have used this peculiar responsiveness to evaluate the total amount of fermenting sugars in beer wort [4]. Finally, we have studied by means of UV-vis spectroscopy the catalytic activity of AuNPs spontaneously grown on PDA by using the reduction of nitrophenol to aminophenol in presence of $NaBH_4$ as catalytic model reaction. We discovered the key role of AuNPs in conferring chemical resistance to the nanocomposite material during the catalytic reaction, and we achieved the effective quantification of this pesticide and fungicide degradation product in human urine [5].

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F1 SS

INVESTIGATION, ISOLATION AND CHARACTERISATION OF NEW PRIONOID PROTEIN AGGREGATES THROUGH HOLLOW FIBER FLOW FIELD FLOW FRACTIONATION AND MULTI ANGLE LIGHT SCATTERING: A TOOL TO FACILITATE THE COMPREHENSION OF INFECTIOUS PROCESSES

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Protein misfolding and aggregation are the cause of a series of human pathologies, from neurodegenerative (Alzheimer's, Parkinson's disease) to non-neuronal (such as type II diabetes), and are mainly linked with the formation of amyloid-like structures, from short segments to fibrils [1]: these conformations can cause accumulation and infer toxicity to cells. In some cases this toxicity can be transmitted to other cells or cultures in a prion-like behavior, by the action of so-called prionoids.
In our work we focused on the investigation of the nature of a toxic factor, partially extracted and isolated from a sample of cerebrospinal fluid taken from a neurological patient [2] which was cytotoxic for monkey epithelial cell cultures. It was also observed that the cytotoxicity could be efficiently transferred and maintained also in cultures of various human cells.
Previous studies showed the absence of viral particles, and of known prions, therefore opening to the idea of abnormally conformed and misfolded protein oligomers (or higher order aggregates) as the toxic agents, while AFM showed that the concentration of protein dimers and low n-oligomer forms was much higher in the cytotoxic fraction than in the control preparation. To assess whether the presence of these species was the actual toxic and self- propagating factor, we employed hollow-fiber flow field flow fractionation, and coupled it to UV and Multi Angle Light Scattering (MALS), in order to fractionate the protein sample into mass- homogeneous fractions and characterize each one in terms of molar mass and abundance. The difference measured between the control and the cytotoxic samples mainly consisted in the latter containing a higher percentage of aggregates, also having a higher molar mass distribution.
The fractions collected were individually tested for cytotoxicity and the later-eluting ones (hence the ones containing the protein aggregates) displayed the same toxicity observed for the unfractionated sample, while the rest was found non-toxic: these preliminary results validate the initial hypothesis and are strongly encouraging of the efficacy of this platform for the investigation of protein-derived toxic pathways.

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POSTERS

P001

GOLD NANOPARTICLES@POLYDOPAMINE FILMS AS INNOVATIVE NANOMATERIALS FOR p-NITROPHENOL DETERMINATION IN URINE

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Gold nanoparticles (AuNPs) are extensively used as efficient, and size-dependent, redox catalysts [1]. The preparation of supported AuNPs for the catalysis of organic reactions is mainly realized by the use of inorganic species such as metal oxides, active carbon, silica spheres and organic polymers [2,3]. The main preparation methods of these active substrates, however, involve impregnation, deposition-precipitation, vapor deposition, co-precipitation, and liquid preparation methods, which require tedious centrifugation and/or filtration steps for the recovery of the substrate after the heterogeneous catalysis [1]. Polydopamine (PDA) is an intriguing self-assembling and adhesive polymer able to form stable nanometric films on almost any surface [4] and has recently displayed to be an extremely efficient and convenient alternative support for metallic nanocatalysts, mainly gold [5]. Moreover, due to the reduction potential of cathecols of PDA (E°=-0.699 V versus normal hydrogen electrode, NHE), Au(III) can be efficiently reduced to Au(0) (E°=0.994 V vs NHE) at the polymer surface, thus allowing gold nanoparticles to grow in situ on any supports without using any reducing agent or metallic seed particles. In this work, for the first time, we investigated and rationalized the catalytic activity of different populations of AuNPs spontaneously grown on PDA by using the reduction of nitrophenol (NP) to aminophenol (AP) in presence of $NaBH_4$ as catalytic model reaction monitored by UV-vis spectroscopy [4]. Furthermore, through the rational variation of the metal ion precursor Au(III), we discovered the key role of AuNPs in conferring chemical resistance to the nanocomposite material (AuNPs@PDA) during the catalytic reaction. Finally, we achieved the effective quantification of this pesticide and fungicide degradation product in human urine, the main bodily fluid of interest for NP monitoring.

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P002

Sputtering-Enabled Intracellular X-Ray Photoelectron Spectroscopy (SEI-XPS): A Versatile Method To Analyze The Biological Fate Of Metal Nanoparticles. Investigation of Ag and Pt cases

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Interactions between nanoparticles (NPs) and cells is a topic of great interest in environmental and health fields. After their internalization the cellular environment can modify NPs chemical composition and structure. Up to now, various techniques are usually employed to characterize NPs upon cellular internalization, including high-resolution optical and electron microscopies and LA-ICP-MS. However, only elemental informations are obtained in this way. An interesting innovation is the combined use of synchrotron-based X-ray Fluorescence (nano-XRF) and XAS, which enables mapping the distribution of metal ions together with the characterization of ion complexes within cells after NP exposure [1]. Nevertheless, synchrotron radiation availability is a significant limit to its routine use. We propose a versatile method, named sputtering-enabled intracellular XPS (SEI-XPS), in which the combination of XPS, argon sputtering and an efficient charge compensation system allow to gain valuable information about the behavior of NPs within cells, directly measuring their internalization, stability/degradation, and oxidation state, with excellent vertical resolution along with semi-quantitative information and without any preparative steps. The proposed approach is easy-to-use and can become a standard technique in nanomedicine and in the rational design of metallic NPs. Two model cases were investigated: Ag NPs and Pt NPs with same size and coating. We observed that, after 48 hours incubation with HeLa cells, intracellular Ag NPs were almost completely dissolved, forming nanoclusters as well as Ag-O, Ag-S, and AgCl complexes. On the other hand, Pt NPs were resistant to the harsh endo-lysosomal environment, and only some surface oxidation was detected [2].

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P003

GG-MH HNT HYBRID MULTIFUNCTIONAL MATERIALS FOR CARTILAGE REPAIR: DEVELOPMENT AND ANALYTICAL CHARACTERIZATION

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The major difficulty in cartilage defects repair is that articular cartilage tissues are subjected to intensive wear, but endowed with a very low turnover in healthy adults. Moreover, complications such as inflammation, infection or implant loosening often occur after cartilage replacement surgery. Therefore, recent efforts are being focused on designing multifunctional materials able to mimic cartilage mechanical performances and support the surrounding material, without undesirable side effects.

In this work, hybrid hydrogels, obtained by ionically crosslinked Gellan Gum (GG), enriched with Manuka honey (MH) and Halloysite nanotubes (HNT) are conceived as artificial cartilage implants, due to their inherent proprieties such as biocompatibility, fluid permeability and lubricating capability. These hydrogels show intriguing mechanical performances, never achieved by other natural hydrogels proposed for cartilage applications [1]. MH is further chosen due to its antimicrobial effectiveness, mainly linked to methylglyoxal (MGO) [2].

XPS, ATR-FTIR and HPLC techniques are exploited to perform a deep chemico-physical characterization of the systems, as well as MGO and cations release. Water uptake, rewet ability and degradation behavior of the hydrogels are also monitored. Mechanical compression and stress-relaxation tests evidence compressive moduli >100kPa for all the prepared samples. Finally, *in vitro* antibacterial effectiveness, against clinical isolates of *S.aureus* and *S.epidermidis,* and cytocompatibility on human mesenchymal stem cells (hMSCs) are extensively investigated.

All the obtained results encourage the employment of the developed hydrogels as promising implantable cartilage substitutes.

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P004

XPS STUDY OF REACTION CENTERS EMBEDDED IN POLYDOPAMINE THIN FILMS

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Surface coating and modification are very important in modern material science since allow a fine tuning of the interface properties conferring new functionalities. For example, fabrication of biosensors or biodevices requires highly biocompatible and functional group reach surfaces. The most commonly used strategies to attain surface functionalization include chemical conjugation, self-assembly monolayers (SAMs), layer-by-layer (LBL) film deposition, and plasma treatment. Besides being time consuming and complicated processes, the application of these techniques relies on specific surface properties. Thiolate SAMs, for example, can only form on noble metal surfaces. In the last decade, mussel inspired polydopamine (PDA), a polymer typically formed by oxygen assisted polymerization of dopamine (DA), is gaining great attention due to its simplicity and material independency in deposition, favorable interactions with living soft matter, and possibility of secondary functionalization. PDA deposition as thin film occurs in mild conditions of temperature and pH and can be carried out in a solution containing proteins without any denaturing effect. More interestingly, the protein remains entrapped within the surface-anchored polymeric structure, enabling a facile and versatile deposition method of the biomacromolecule [1].
In this work, a systematic study by X-Ray Photoelectron Spectroscopy (XPS) has been carried out for getting information about the chemical surface composition of thin polydopamine (PDA) films chemically grown on Si wafer, at pH 8, in presence and absence of bacterial photosynthetic reaction centers (RC). In particular, the focus was on the role of the buffer used in the chemical synthesis of polydopamine and RC/polydopamine modified films. The employment of different buffers, such as Tris and phosphate, proved indeed to affect the film growth quality (i.e. thickness, chemical composition and efficiency of RC trapping). Moreover, the influence of the dopamine monomer (PD) concentration on the same properties has been investigated.

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P005

ELECTRODEPOSITION OF METAL ALLOYS OF TECHNOLOGICAL AND INDUSTRIAL INTEREST

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As part of the Regional POR CREO GADGET - ERDF 2014-2020 Call No.2 project, sequencing studies of precious metal alloys are planned in order to increase their resistance to corrosion and wear. These studies provide for the knowledge and use of the main metal Electrodeposition techniques and of the main electrochemical techniques for the development of galvanic baths. At the same time, morphological characterization, surface analysis and corrosion resistance measurements will be carried out. What is required for conducting the Research is an excellent knowledge of basic electrochemical techniques and surface characterization techniques such as AFM (Atomic Force Microscopy) and SEM (Electronic Scanning Microscopy) in-situ and ex-situ.
Thin films made of various materials are used in many scientific, technological and industrial environments. They are deposited through a variety of physical, chemical and electrochemical techniques. In all these fields, it is essential to measure the thickness, the colour, the morphological and compositional of the deposit because the properties of mechanical strength, corrosion, costs, optics and visual appearance depend on this feature.

P006

SPECTROSCOPIC CHARACTERIZATION OF EXCEPTIONALLY STABLE SILVER NANOPARTICLES SYNTHESIZED BY LASER ABLATION IN ISOPROPYL ALCOHOL

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"Laser ablation synthesis in solution" – LASiS is a straightforward technique to obtain metal nanocolloids in a wide variety of solvents, without chemical reductants or capping agents [1]. LASiS is based on the fine fragmentation of a bulk metal target by a focused, pulsed, ultrafast laser beam. The target is immersed in an optically transparent liquid medium. The presence of a liquid layer brings a number of advantages, in contrast with ablation in air. Firstly, liquids have a greater thermal conductivity in respect to air, thus reducing thermal damages; furthermore, a higher yield can be reached thanks to plasma confinement, liquid motion removing debris from the target surface, and enhanced energy coupling efficiency [2]. When the laser interacts with the target surface, a cavitation bubble is formed: its expansion and collapse allowing nucleation and growth of NPs. The resulting material has controlled size, and is released in the surrounding liquid medium when the bubble explodes. This way, ligand-free NPs are formed. Interestingly, LASiS-generated metal NPs are generally highly stable; however, besides many theoretical and mechanistic studies, the reason for this stability is still an open issue, especially when non-aqueous solvents like isopropanol are taken into account [3]. Explanation of this phenomenon is challenging, because of the lack of literature data on naked metal nanoparticles suspended in organic solvents. Both theoretical considerations and basic experiments helped us in formulating some hypotheses, which were corroborated by a systematic spectroscopic and morphological characterization (by means of UV-Vis, FTIR, XPS, TEM, DLS, Z-potential, etc.). All evidences suggested that the stabilization of our NPs involved the presence of organic polar functional groups generated by the interaction of isopropanol molecules with the pulsed, high-energy laser beam. On the one hand, these moieties prevented any chemical (oxidation) reaction on colloidal nanoparticles; on the other hand, they generated a steric hindrance capable of preventing nanoparticle aggregation and flocculation.

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P007

ELONA-BASED APPROACHES FOR THE ANTIBODY-FREE DETECTION OF TROPONIN T, THE KEY BIOMARKER OF ACUTE MYOCARDIAL INFARCTION

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Currently, cardiac troponins (I or T) are the analytes of choice for the diagnosis of acute myocardial infarction, thanks to their enhanced sensitivity and specificity with respect to traditional cardiac enzymes, such as creatine kinase and myoglobin [1-3]. Many efforts are now devoted to the design and synthesis of innovative and effective biomimetic receptors alternative to classic antibodies (still used in clinical protocols at the triage stage of emergency) for the development of a new generation of portable and ultra-sensitive tests for the early diagnosis of Troponin T and I [4].
In this framework, we are exploring the perspective use of molecularly imprinted polymers (MIPs) [5] and aptamers, both by biosensors-based and bioanalytical strategies. In this work we present the first example of the use of a couple of new aptamers able to bind Troponin T. We first characterized the aptamers by a reference optical transduction, i.e. Surface Plasmon Resonance (SPR), and then explored the development of a new Enzyme Linked OligoNucleotide Assay (ELONA) test for Troponin T detection. The ELISA-like approach gives several advantages in terms of number of processed samples (up to 96/assay) and ease of signal reading [6].
Different detection strategies were investigated, both by direct and indirect detection, giving encouraging results. Moreover, the optical signal may be based on traditional enzymatic reactions with chromogenic substrates or by using nanoplasmonics [7].

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P008

EDX THICKNESS ANALYSIS OF METAL COATINGS USING MONTE CARLO STANDARDS

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The thickness and composition determination of thin films is an important task with regard to their wide usage in daily life and for new generation devices. These two aspects influence the properties of mechanical strength, corrosion, costs, optics and visual appearance of the final products. There are many thickness-measuring techniques but none of them allows fast, inexpensive, non-destructive and high lateral resolution analysis.

In our study we focused our attention to galvanic jewelry industries [1], but the procedure could be easily extended to other fields. In the industrial environment the most used technique for coatings analysis is X-Ray Fluorescence spectroscopy (XRF), which is fast and non-destructive. For a correct XRF thickness analysis, the composition and disposition of all the layers must be known exactly. For this reason, the composition information is in general difficult to obtain. With Energy Dispersive X-ray spectroscopy (EDX) it is possible to get a fast, quantitative and non-destructive analysis of both thickness and composition of the topmost layer (due to the low penetrating behavior of the electron probe), with also higher lateral resolution than XRF. The first layer is generally the most interesting to analyze because is that one in contact with the external environment and, for this reason, the first subjected to corrosion. In addition to that, in the case of jewelry, the finishing is made of precious metals for which is important to monitor these properties for economic and aesthetic purposes.

Commercial XRF systems devoted to the analysis of coatings use only few points for the calibration curve to keep the cost low. This leads to errors exceeding 10 % in the thickness determination of the top layer. This is not always acceptable, especially when the coating consists of precious metals.

EDX is generally known as a composition analysis technique, but with an appropriate calibration curve it is also possible to determine the thickness of a coating. To avoid excessive costs in the standards preparation, a software has been used to simulate standards using Monte Carlo algorithm [2]. Then the K-ratios have been determined to build the calibration curves for the thickness determination.

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P009

PM EFFECTS ON METALLIC SURFACES: DEVELOPMENT OF A NEW ACCELERATED AGEING METHODOLOGY

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Deterioration phenomena occurring on outdoor-exposed cultural heritage have been the subject of several studies, but relatively few works investigated the specific role of Particulate Matter (PM) in the corrosion of metallic artefacts. This topic is really complex and, beside field exposures [1], accelerated ageing tests are also necessary to isolate and understand deterioration mechanisms due to PM. For this reason, the development of a methodology that allows to reproduce and analyze the effect of PM on metals through accelerated ageing in climatic chamber has been started.
On a set of quaternary bronze (G85) specimens, single salts (NaCl, $NaNO_3$, Na_2SO_4, NH_4NO_3 and $(NH_4)_2SO_4$) and a mix of them were deposited to evaluate the effects of each salt and to compare the effects of anions and cations. Two deposition methods were tested: dry (directly depositing the salt on the surface) and drop (depositing the salt as water drop and drying it), simulating the initial chemical activation of the salts by RH% variations or by raindrops, respectively. Then, to better simulate the composition of real PM, a mixture containing representative amounts of soluble salts, a mineral, a black carbon and an organic fraction was formulated and spread on the specimens. All the specimens were placed in a climatic chamber and exposed to cyclic variations of T and RH for a total of three weeks. The ageing cycles were set according to predictions on salt deliquescence/recrystallization performed through the E-AIM software and to the evaluation of regional climatic data. The surface evolution was followed by SEM-EDX, Raman, AT-IR and UV-Vis Spectrofotometry. At the end of the aging cycles, mass loss were determined and corroded metals removed by pickling were analyzed by Atomic Absorption Spectroscopy.
On the basis of preliminary results, the tested procedures for aging the specimens seems to be promising in accelerating and mimicking realistic corrosion phenomena. Actually, under the selected conditions, corrosion products typically found at different time of exposure (from days to years) on outdoor bronzes were able to progressively form and evolve. Moreover, the two deposition modes simulating different condition of chemical activation of PM deposits allow to obtain complementary information.

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P010

NIR SPECTROSCOPY, THERMOGRAVIMETRY AND CHEMOMETRICS TO DIFFERENTIATE BURNED AND UNBURNED ANCIENT HUMAN BONES

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24 samples of human bones, (unburied from four different necropolises, two in Italy, Cavo degli Zucchi and Elia-Velia and two in Sudan, El Geili and Saggai) were analyzed by thermal analysis (thermogravimetry) and NIR spectroscopy. The information obtained through the different techniques were compared in order to highlight differences among samples from the different necropolis. Sudanese and Italian findings differ not only for the origin, but they also underwent different burial rituals. Samples date back to different historical periods: the Italian ones are (pre)Roman while the Sudanese come from the Prehistoric, the Meroitic and the Christian era. The dataset has been investigated by Principal Components Analysis (PCA) [1]. Models were calculated on the individual matrices (NIR spectra and thermograms) and in a multi-block analysis on the super-scores matrix obtained by concatenating the components extracted from the individual models and on the data-block created joining NIR spectra and the three main TG mass losses. The investigation of the scores plot obtained from this latter approach (Figure 1) allowed distinguishing samples on the basis of the funeral rite; cremated samples fall at negative values of PC1 while the un-burnt present positive score-values. Additionally, PC2 seems very suitable for dating samples: the oldest, i.e., the Mesolithic ones (red diamonds) present positive values of PC2, the (pre)Roman ones (cyan downward-pointing triangles) fall around zero and Meroitic and Christian (green squares and blue triangles) samples present negative PC2 scores-values.

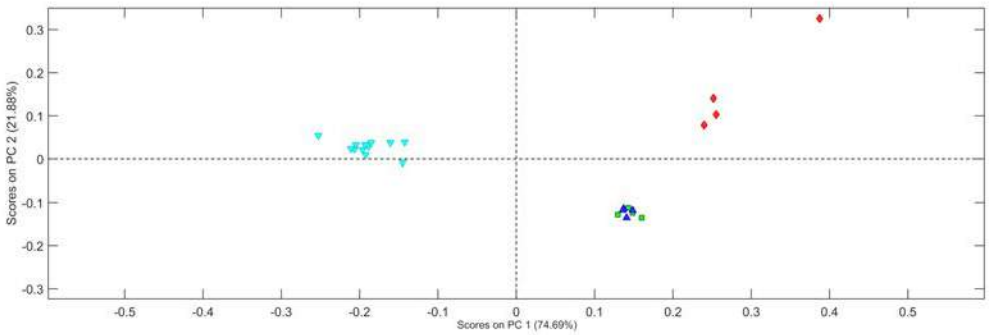

Figure 1 Scores Plot. PCA calculated on NIR spectra, water, total collagen and carbonate mass losses.

Legend: Italian (Pre)Roman-cyan downward-pointing triangles; Sudanese Prehistoric (Mesolithic)-Red diamonds; Sudanese Meroitic-Green squares; Christian-Blue triangles

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P011

Z POTENTIAL FOR THE EVALUATION OF THE WATER SENSITIVITY IN MODERN OIL PAINTINGS

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During surface cleaning by conservators, modern oil can exhibit water and solvent sensitivity, which causes are object of researche [1,2]. There are several empirical approaches that can be used for the evaluation of the water sensitivity, one of the most important is based on the use of swab rolls.
The aim of this work was to identify analytical approaches to measure quantitative parameters that can be related to the water sensitivity of a paint layer. The use of zeta potential measurements of the paint surface (□) was tested for this purpose.
The zeta potential of a solid surface is related to its surface charge. The charge established on the surface of a solid material in contact with water determines the behavior of the material in processes where aqueous systems are in contact with the surface, as water cleaning. Z potential is related to the charge at a solid/liquid interface, and it is a powerful indicator for the surface chemistry and for surface adsorption processes.
The analyses were performed using a SurPASS Electrokinetic Analyzer for surface analysis. The analyzer determines the Z potential of macroscopic solids based on streaming potential and streaming current measurement, and it is also capable to determine the isoelectric pH point (IEP) of a surface by mean of measuring the potential during a microtitration.
The measurements were performed using a liquid phase (KCl solution) pumped at controlled pressure through the measuring cell, creating a flow in contact with the paint surface (0.5 x 2 cm). The investigated paint layers were four Winsor & Newton oil paint layers on Melinex, featuring different water sensitivity [3]. Winsor & Newton Raw Sienna and Zinc White paints were previously demonstrated to be non-water sensitive paints, while Cobalt Blue and Ultramarine Blue were water sensitive paints. The results showed significant differences in the dynamic Z potential and in the isoelectric point of the paint layers containing different pigments.

P012

CHARACTERIZATION OF MATERIALS IN HISTORIC STRINGED MUSICAL INSTRUMENTS BY ANALYTICAL PYROLYSIS GC-MS WITH ON FIBER SILYLATION

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Historic stringed musical instruments are a unique class of cultural heritage objects. Crafted during the 17th-18th centuries, the golden age of violin making in Cremona, Italy, these instruments remain somewhat mysterious. Due to the absence of written historical documents of traditional varnish recipes, their chemical characterization is the only way to recover the lost secret of the Cremonese stringed instrument maker Stradivari and his contemporaries, whose secrets had been lost by 1800 [1].
The analytical characterization, both with non-invasive and minimally invasive techniques, provides information about the material composition, methods of manufacture, and past restorations of the finishes. The composition of the instrument finish (collective term for the treatment of the surface of the wood, which includes preparatory and varnish layers) has been studied by several techniques including analytical pyrolysis. A more comprehensive study of especially the minor organic materials that were used is lacking.
Previous results on samples from an Amati viola and Stainer cello showed the potential of pyrolysis combined with gas chromatography mass spectrometry using a SPME carboxen fiber for the sampling of the pyrolysis products followed by on fiber silylation [2]. In this presentation the same method was applied to a large collection of standards including pure resins like colophony, amber, mastic, sandarac, elemi, and different types of shellac, as well as colorants or additives such as madder, dragon's blood, and aloe and other materials like propolis and beeswax in order to obtain an extensive database to be used for the characterization of these unique historical objects. A set of distinct pyrolysis patterns and products were chosen as specific markers for each standard. The bias and efficacy of the fiber toward certain chemical compounds will be discussed by comparison to traditional solvent-based derivatization. Silylation is quantitative since no partially derivatized compounds are shown. The method was applied to real samples including Bajoni, Guarneri, Gasparo, Maggini, Guadagnini, and Stradivari instruments.

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P013

DEVELOPMENT OF BIOACTIVE NANOCOMPOSITES FOR THE CONSERVATION OF MURAL PAINTINGS

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Biodeterioration is one of the main decay processes of hypogean and outdoor mural paintings. Conservation strategies are usually based on the application of biocidal products (*e.g.*, quaternary ammonium salts) which generally show short-term efficacy.
Recently, in the field of stone conservation combined materials including biocides and consolidants/water repellents have been proposed and promising results have been obtained [1-4].
This research is focused on the development of nanocomposite materials with consolidant properties and marked biocidal activity to be applied on mural paintings affected by biodeterioration. Nanocomposites were prepared by embedding ZnO-nanoparticles (NPs) and TiO_2-NPs at different concentrations in commercially available nanolime suspensions (Nanorestore Plus®). The materials were first analysed with micro-Raman spectroscopy with the purpose of following the curing processes in different conditions of relative humidity (RH) and to get insight into the possible influence of the ZnO- and TiO_2 NPs on the nanolime matrix. The photo-activity of the nanocomposites was evaluated by measuring the decomposition of a target colourant (Rhodamine B).
The micro-Raman data evidenced that high RH conditions favour the carbonatation of $Ca(OH)_2$ and the formation of stable crystalline calcium carbonate (calcite), also in presence of ZnO-NPs, while TiO_2-NPs seem to inhibit such processes. The decomposition rate of Rhodamine B depends on the NPs concentration and is higher for ZnO-NPs as compared with TiO_2-NPs, both upon exposure to light and in the dark.
Based on these results, Nanorestore Plus® and Nanorestore Plus® with ZnO-NPs (50% m/m) were applied to fresco mock-ups. No significant chromatic changes were observed and the photo-activity of the ZnO-NPs was assessed.

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P014

CHARACTERIZATION OF ARABIC/CHRISTIAN MANUSCRIPTS USING A NON-INVASIVE APPROACH

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The correct conservation of paper artworks plays a fundamental role in the field of our cultural heritage. In this contest, the determination of paper composition as well as degradation state is fundamental to determine the suitable restoration and conservation processes for paper artworks. To this aim, several diagnostic techniques are available, both invasive and not. In this study we present the characterization of Arabic Christian manuscripts, belonging to the XIII century, held in Vatican Library (BAV, Vatican City). The paper artworks have been characterized by several techniques using portable instrumentation (colorimetry, X-ray fluorescence spectroscopy (XRF), Infrared Reflectance (IRR), Fourier Transform Infrared Spectroscopy (FT-IR)), directly *in situ* at the restoration laboratories of BAV. Simultaneously, the manuscripts are cleaned in specific points using the dry cleaning sponges, and the removed materials (pollutants and cellulosic degradation products) have been analyzed by destructive techniques as high pressure chromatography (HPLC) [1], and through no destructive techniques as FT-IR in ATR configuration [2]. Sponges, indeed, absorb dust and degradation products during the cleaning of the paper sheets, avoiding damaging on the paper surface itself. Summarizing, in this work, a non-invasive method of sampling has been developed and optimized based on the analysis of residue materials absorbed by cleaning sponges during the dry cleaning of paper. The validation of the chromatographic results has been performed by non-invasive spectroscopic analysis using a portable instrumentation. The composition and degradation state of the analyzed manuscripts have been determined as well as their inks composition. In this paper, some of the most significant results are reported.

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P015

CHASING THE FUGITIVE – THE RED-COLOURED TEXTILES OF PHARAONIC EGYPT

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When the imagination conjures up an image of an Egyptian mummy, it is normally one of a human body wrapped with pallid-coloured linen bandages, made from natural flax fibres, but the reality can be much more colourful. In the first millennium B.C. some mummies were in fact covered by red shrouds, which have fully retained their intense colour over time. In some other cases, damage or the removal of straps or other mummy bindings, can expose other red-coloured textiles, suggesting the original colourful appearance of the bandages.

A collaboration between analytical chemists and archaeologists is in place in order to shed new light on how the use of red shrouds and textiles is embedded in the funerary practices of Pharaonic Egypt. Primarily the team aims to investigate the materials used to obtain these colours, by analysing a set of 15 samples taken from mummy bandages and shrouds from the collections at the Museo Egizio in Torino and at the British Museum in London.

The red colourants have been investigated both by non-invasive and micro-invasive approaches using HPLC-ESI-Q-ToF, SEM-EDX, micro-XRF, FORS and portable fluorimetry.

The discolouration of some of these textiles represents an intriguing aspect [1], as in some cases the red colour is still vivid and well-preserved , whereas in others it appears faded or severely discoloured. Preliminarily results point towards the presence of at least three sources of the red colour: safflower (*Carthamus tinctorus*), madder (*Rubia* sp.) and a red ochre. Further investigations are on-going to confirm these results and relate them to the discolouration process. This information will also be of extreme importance for the display and future preservation of these precious mummies.

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P016

TARGETED FORENSIC SCREENING AND SEMI-QUANTITATION OF DRUGS IN PLASMA USING HIGH-RESOLUTION ACCURATE-MASS DETECTION AND ONLINE SAMPLE PREPARATION

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Background
The opportunity to screen a very large panel of compounds on a single injection of a low volume of sample is of high importance in forensic toxicology; improving the throughput by reducing the runtime of the method plays an important role as well. Moreover, the use of multiple parameters for identification and confirmation provides additional confidence in the outcome of the screening.
Methods
A spectral library and compound database for the screening and semi-quantitation of more than 1500 compounds in plasma and other biological matrices, were developed. For each compound, the database includes the exact mass, isotopic pattern, retention time, and exact masses of its main fragments. A Thermo Scientific™ Transcend™ II TLX-1 system was used with two different analytical approaches, one based on high-performance liquid chromatography (HPLC), and the other based on online sample extraction using Thermo Scientific™ TurboFlow™ technology prior to HPLC separation. Runtimes were 15.5 minutes for the LC-only approach and 16.75 minutes when using TurboFlow. Detection was performed using a Thermo Scientific™ Q Exactive™ Focus Orbitrap™ high-resolution, accurate-mass spectrometer with heated electrospray ionization with polarity switching. Detection was performed by FullMS in data-dependent MS2 acquisition mode with an inclusion list. Full Scan data were acquired with a resolution of 35,000 FWHM at m/z 200, and the MS2 spectra for confirmation were acquired with a resolution of 17,500 FWHM at m/z 200. Thermo Scientific™ TraceFinder™ 4.1 software was used for data processing. A panel of 41 compounds covering different compound classes, retention times, and polarities was selected to evaluate the sensitivity of the online extraction method in plasma.
Results
A database containing compound-related information was created for both methods. For the quantitation method, sensitivity was evaluated for the 41 selected compounds using the TurboFlow approach. Results proved that it is possible not only to perform a screening workflow with identification and confirmation of compounds, but also a quantification with LOD down to 0.5 ng/mL.
Conclusions
The implemented method proved that the Q Exactive Focus high-resolution accurate-mass spectrometer is suitable for both target screening with multi-parameter confirmation. Moreover, the same approach was successfully applied to the quantification of 41 compounds in plasma with a simplified sample pre-treatment.

P017

PROPOSAL OF A COLOURIMETRIC TOOL FOR PROVIDING ACRYLAMIDE CONTENT IN FOOD PRODUCTS

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Acrylamide is a toxic compound considered as thermal marker of food, and deriving from Maillard reaction during cooking process. A recent European Regulation established mitigation measures and benchmark levels for the reduction of its presence in many products encouraging the use of colourimetric scales providing a statistical correlation between colour intensity and measured acrylamide level.
This study was focused on the determination of acrylamide in pizza prepared by different flours and in baked potato samples cooked at different conditions. Portions of cooked product characterized by different colours were sampled to create a colour scale. Acrylamide level was measured by liquid chromatography coupled to mass spectrometry, correlating its content with colour indices measured by means of image analysis.
Results concerning pizza showed that the type of flour affects acrylamide formation, thus permitting to optimize a recipe for reducing its content in the final product. As for potato samples, it could be noticed that similar colours, even obtained under different cooking conditions, were characterized by similar acrylamide levels, allowing to build a colour gradation suitable to obtain information on acrylamide content from colour analysis.
A statistical evaluation of the data demonstrated that, despite the intensity and the modality of the thermal treatment, the final colour of the product is connected to acrylamide amount. This allowed to build a colourimetric indicator suitable to predict acrylamide content by a simple colour analysis providing the RGB values. The obtained scale represents a useful and extremely practical tool for industrial, commercial and domestic use, since it permits to monitor the level of toxicity of a food product without the need of time-consuming, expensive and requiring high-expertise such instrumental analyses.

P018

TETRADESMUS OBLIQUUS MICROALGAE AS A SOURCE OF BIOACTIVE PEPTIDES: PURIFICATION AND IDENTIFICATION BY MULTIDIMENSIONAL LIQUID CHROMATOGRAPHY - MASS SPECTROMETRY

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The research in the field of food bioactive peptides has greatly increased in the last decades. Besides the classical matrices (e.g. fish, milk, etc.), more recently, particular attention is being paid to microalgae, which are one of the most promising sources for new food and functional food products. Their chemical composition depends on environmental factors, and generally it is 40–70% proteins, 12–30% carbohydrates, 4–20% lipids, 8–14% carotene, and vitamins.
In the literature, only a few researches have studied novel bioactive peptides in microalagae, just reporting the identification of their amino acid sequence. However, none of these works was focused on the analytical aspect of sample preparation, and peptide separation was not achieved and simple filtration of protein hydrolysates was performed, instead.
In our work [1], a peptidomic platform was developed for the extraction, separation and identification of bioactive peptides in protein hydrolysates of *Tetradesmus obliquus* microalgae. Indeed, extraction of proteins from recalcitrant tissues is still a challenge due to their strong cell walls and high levels of non-protein interfering compounds. Therefore, seven different protein extraction protocols, based on mechanical and chemical methods, were tested in order to produce high-quality protein extracts. Proteins obtained by the best protocol, i.e., milling the recalcitrant tissue with glass beads, were subjected to enzymatic digestion with Alcalase®, and subsequently the hydrolysate was purified by two-dimensional semi-preparative reversed phase (RP) liquid chromatography (LC). Fractions were assayed for antioxidant and antihypertensive activities and only the most active ones were finally analysed by RP nanoLC-tandem mass spectrometry. Around 500 peptide sequences were identified in these fractions. The identified peptides were subjected to an in silico analysis by PeptideRanker algorithm in order to assign a score of bioactivity probability. Twenty-five sequenced peptides were found with potential antioxidant and angiotensin-converting-enzyme (ACE)-inhibitory activities. Four of these peptides, namely WPRGYFL, GPDRPKFLGPF, WYGPDRPKFL, SDWDRF, were selected for synthesis and in-vitro tested for the specific bioactivity, exhibiting good values of antioxidant and ACE-inhibitory activity.
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P019

TOWARDS A MISPE FOR ROXARSONE: MOLECULARLY IMPRINTED POLYMERS BASED ON TAILOR-MADE MONOMERS FOR THE RECOGNITION OF ORGANO-ARSENIC COMPOUNDS

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Roxarsone (4-hydroxy-3-nitrophenylarsonic acid) is an organo-arsenical feed additive for swine and poultry, which increases weight and serves as an anti-microbial agent. Although the use of arsenic-containing feed additive can promote the development of animal husbandry, concerns have been raised on the presence of arsenical residua in animal husbandry-derived foods for human nutrition. Moreover, livestock excreta containing organic arsenic compounds can be discharged in the environment, causing further pollution issues.

With the aim of developing a molecularly imprinted solid phase extraction selective for roxarsone, we prepared stoichiometrically imprinted polymers against this target contaminant.

Five different MIPs were synthesized using tailor-made functional monomers, based on urea or squaramide structures as molecular recognition elements, with the goal to bind stoichiometrically roxarsone in polar environments. Prepolymerisation studies of template–monomer complexation by ^{1}H-NMR experiments showed that squaramide monomers give K_{eq} values higher than ureas, even if both kinds of monomers could generate MIPs with good binding properties toward roxarsone.

After the synthesis of imprinted polymers, equilibrium rebinding experiments performed in environments of different polarity showed that roxarsone is well recognized in water and methanol. Moreover, the imprinted polymer showed a fair selectivity towards possible interfering substances like acetarsone (N-acetyl-4-hydroxy-m-arsanilic acid) and nitarsone (4-nitrobenzenearsonic acid). Preliminary results on the feasibility of a MISPE for roxarsone in aqueous matrix will be presented.

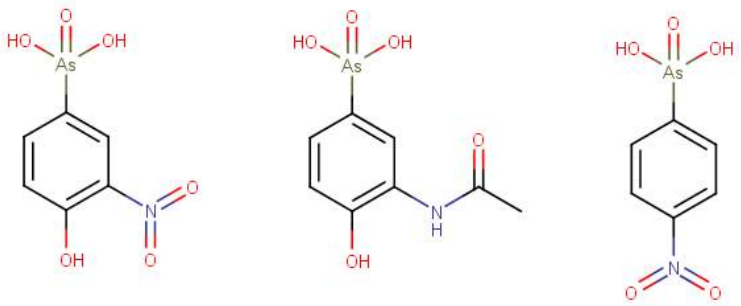

Figure 1. From left to right: roxarsone, acetarsone and nitarsone

P020

SYNTHESIS AND CHARACTERIZATION OF AN IRON (II) CITRATE NEUTRAL COMPLEX TO EVALUATE ITS USE AS A FOOD SUPPLEMENT TO OFFSET IRON DEFICIENCIES

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Iron is an indispensable mineral for the human organism and most individuals do not need an iron supplement, as it is usually sufficient to have adequate intake of the foods that contain it (liver, meat, fish and dry legumes). Moreover, it is known that the presence of vitamin C, citric acid, sugars (especially fructose) and amino acids, facilitates the absorption of iron.[1] However, in particular situations, iron supplements are a valuable aid to prevent the emergence of deficiency frameworks and the possibility that these evolve to sideropenic anemia.[2] One of the first attempts at integration of iron in the past is the preparation of the "nailed apple" (ordinary carpenter's nails were put into a sour apple, the nailed apple was left to rest overnight and the day after the apple could be eaten after removing the nails). Starting from these premises, a chemical reaction was developed for obtaining a neutral complex of iron citrate (II) from iron filings and citric acid, in aqueous solution. The obtained compound showed a 1:1 stoichiometry between the iron (II) and the citrate ion showing the amount of iron equal to 22.2% (w/w). To highlight the stability of the oxidation state II for iron, an important factor for its potential bio-assimilation, on the complex obtained, the colorimetric dosage with ortho-phenanthroline was carried out. Furthermore, the compound was subjected to crystallographic, thermogravimetric, spectrophotometric and total organic carbon (TOC) analyses. Finally, for an understanding of the type of coordination of the iron, an analysis of the infrared spectrometry was also carried out, which confirmed the coordination between iron and citrate after synthesis. In the future, further studies will be conducted on the compound obtained (yield of 75% (w/w)) for a more detailed characterization regarding its assimilation in the human organism, in order to realize a food supplement to compensate for iron deficiencies.

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P021

DISCRIMINATION OF OLIVE TREE VARIETIES INFECTED BY *XYLELLA FASTIDIOSA* USING VOLATILES BY HS-SPME-GC-MS COMBINED WITH MULTIVARIATE STATISTICAL ANALYSIS

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Xylella fastidiosa is a Gram-negative, plant-pathogenic bacterium that causes diseases in different plant species [1]. It is noted that the VOCs emitted by plants are a very complex mixture of several hundreds of components that play an important role in trophic relations in diverse ecosystems and provide important cues for insects in their search for hosts. Moreover, these compounds may work out as direct and indirect plant defense and to attract insects for pollination [2]. For this reason, HS-SPME-GC-MS technique was proposed to highlight VOCs composition differences between twigs coming from healthy and *Xf* infected olive trees. Four different fibers (PDMS, Carboxen-PDMS, DVB-Carboxen-PDMS, and PDMS-DVB StableFlex) were tested and GC-MS conditions were evaluated in order to optimize the number of VOCs detected by the proposed method. Finally, differences between samples healthy and *Xf* infected were evidenced by means of a chemometric analysis (PCA and ANOVA-test). More than one hundred different volatile compounds, comprising acids, esters, alcohols, methyl esters, other esters, aldehydes, hydrocarbons, terpene derivates, amides, aromatics, furanes and ketones, were identified in the analyzed samples. PCA analysis has allowed to highlight differences between the two olive tree cultivars and the important discrimination among healthy and *Xf* infected trees. PCA and ANOVA have also evidenced the involvement in the in the defensive mechanism paths of the olive tree and/or in the infective action of *Xf* thought the formation of new methyl esters, a decrease of ketones and aldehydes and an increase of hydrocarbons that can be considered disease markers. The proposed approach has been used to set-up a quick, easy and solvent-free screening method to evaluate the presence of *Xf* in olive trees.

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***Acknowledgement**: This work was financially supported by the Apulia Region, Research Programme "Sperimentazione Finalizzata alla Prevenzione e al Contenimento del Complesso del Disseccamento Rapido dell'olivo (CODIRO)" – Project EZIOCONTROL.*

P022

SIMULTANEOUS DETERMINATION OF 12 RED DYES IN MEAT PRODUCTS BY A SIMPLE EXTRACTION FOLLOWED BY HPLC-UV-DIODE ARRAY DETECTION

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Control of the presence of food additives is very important to ensure meat quality and safety. Among food additives, the analysis of both natural and synthetic food dyes represents a great challenge, since very frequently single or mixtures of several dyes are used particularly in meats and meat products to obtain attractive colors of such commodities. The use of these color additives is regulated because they can occasionally produce allergy, asthma and other health disorders. In particular, the addition in food of six red food dyes is admitted by European Legislation, and regarding meat products only cochineal, carminic acid, carmines (E120), Ponceau 4R, cochineal Red A (E124) and Allura Red AC (E129) are allowed with precise restrictions (European Commission Regulation 2011/1129/EC). Furthermore, the presence of several non-permitted red dyes, including some carcinogens, has been found in some types of spices used in the production of meat products (European Commission Decision 2004/92/EC). It is very difficult to find in the literature studies focused on the quantification of food coloring levels in meats. This was confirmed by an External Scientific Report of the European Commission [1], which concluded that regarding the monitoring of food dyes in foodstuffs some gaps in standard methods, post-market surveys, and other important legislative aspects subsist. For these reasons, in the present study an accurate method has been developed combining a simple and rapid extraction of 12 food dyes in meat and meat products followed by HPLC-UV-diode array detection. The chromatographic separation for the simultaneous identification and quantification of banned and not banned red dyes (Amaranth, Ponceau 4R, Carmine, 32 Ponceau SX, Ponceau 3R, Allura Red AC, Carmoisine, Erythrosine, Sudan I, Sudan II, Sudan III and Sudan IV) in meat products has been accomplished by a C18 RP column eluted with an optimized step-change gradient, based on a mobile phase consisting of a sodium acetate solution and acetonitrile, which has guaranteed a very good selectivity towards endogenous interfering substances. The method validation, performed by an in-house model according to the Decision 2002/657/EC and Regulation 2017/625/EC, provided excellent results in terms of linearity ($r^2 > 0.997$), expanded measurement uncertainty (below 15%), recovery values (in the range 86.4% - 105.0%), repeatability (CV% < 18%) and sensitivity, demonstrating the conformity of the proposed method with the European directives.

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P023

STUDY OF LANTHANIDES DISTRIBUTION PATTERN IN DIFFERENT SOIL MIXTURE

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Today, it is growing the interest by consumers for food products with a clear geographical identity. Moreover, the possibility of tracing the origin of foodstuff is assuming an increasingly important role at the legislative level, as a tool that may allow to prove on product authenticity and to control adulteration. Recent works have been demonstrated the potentiality of lanthanides as geographical markers due their coherent and predictable chemical behaviour. Furthermore, have been demonstrated that the normalization of the lanthanides distribution allow to appreciate their relative enrichments in soil-plant-fruit systems[1,2]. Therefore, the study of the distribution pattern of these compounds together the Heavy/Light lanthanides ratio seems to be a promising system to establish univocal traceability systems. In order to evaluate the robustness of the analytical strategy developed, we have chosen to determine the relative abundances of lanthanide in different soil mixture testing the behaviour of the original pattern and Heavy/Light lanthanides ratios and their ability to reproduce soils mixing to verify the analytical performances in terms of reliability.

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P024

RARE EARTH ELEMENTS ANALYSIS FOR GARLIC ASSESSMENT: THE CASE STUDY OF RED VARIETY CULTIVATED IN ITALY

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Traceability of the food origin is important for label protection. Food ingredient fraud and economically ingredient adulteration are emerging risks, but a comprehensive compilation of information about known problematic ingredients and detection methods does not currently exist.
In spite of the increasing attention of consumers for the origin of food and high reputation of products with a distinct geographical identity, a relatively small number of investigations regarding traceability of garlic (*Allium sativus L*.) can be found in the scientific literature [1-3]. The above studies proved the fingerprint ability of the organo-sulfur compounds of garlic and other metabolome components, including organic acids, sugars, fatty acids and amino acids.
This research project proposes an alternative method to evaluate the geographic origin of garlic by determining the rare earth elements (REEs) within the soil and corresponding food [4]**.** Starting from the assumption that the REEs present in the soils and substrates are uptaken by plant roots, we hypothesize that different geological substrates give a combination of REEs that characterize the traceability of the garlic. This study will focus on the red garlic variety cultivated in four different areas of Italy: Sulmona, Castelliri, Proceno and Nubia. The production territories are featured by alluvial river-side soils (Sulmona and Castelliri) and predominantly clay soils (Nubia and Proceno). The specific objective was to find a response in the isotopic ratios (normalized) pattern of rare earths in soil and in garlic samples taken as a function of different lithologies (or geographic origin). First results were reported and discussed.

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P025

BIOACTIVE MOLECULES FROM TOMATO FRUITS AND BY-PRODUCTS

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Tomato (*Lycopersicon esculentum*, L.) is one of the most important worldwide agricultural crops and its fruits are among the main ingredients in the Mediterranean diet. The tomatine is a 1:10 mixture of two glycoalkaloids, α-tomatine and dehydrotomatine, synthesized by tomato plants and green tomatoes as a defense against fungi and bacteria [1]. α-Tomatine is reported to have potential health promoting effects in cells, animals, and humans [2].
Quantification of α-tomatine and dehydrotomatine was performed by reverse phase liquid chromatography, coupled with electrospray ionization tandem mass spectrometry, RP-HPLC-ESI-MS/MS. The glycoalkaloids were evaluated in industrial varieties of vine-ripened tomatoes at different ripening stages, and in commercial varieties of post-harvest ripened fruits, stored at different temperatures conditions. Data showed that the tomatine concentration decreases as function of the maturity stage, either in vine- and post-harvest ripened tomatoes. An increase of the tomatine content was observed for long storing periods, after mold occurrence. The content of the two glycoalkaloids was also analyzed in green tomatoes thermally treated, simulating industrial processing conditions (boiling at 100 °C), and compared with industrial prototype products. Thermal treatment does not seem to affect the total tomatine content. Finally, a particular attention was devoted to the determination of tomatine content in plant leaves (at different vegetation stages) and locular gel from fruits, as by-products from agricultural production and industrial processing, respectively.
Selected samples were also characterized as regards antioxidant properties, via Folin-Ciocalteu assay, and Trolox Equivalent Antioxidant Capacity assay (TEAC) as ABTS and DPPH radicals scavengers. Selected polyphenols were also quantified via HPLC-ESI-MS/MS methods. The results showed that chlorogenic acid and caffeic acid were the main hydroxycinnamic acids, while rutin was the most abundant flavonoid.
On the basis of these results, spontaneously hypertensive rats (SHR) were daily fed with locular gel obtained from tomatoes (Camone variety), to evaluate its efficiency as potential nutraceutical product with antihypertensive activity.

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P026

RELEASE OF HYDROCARBONS FROM FRESH CHEESE PACKAGING

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Fresh cheese and dairy products are usually sold in packaging made of polymeric materials. "Food packaging system" is made of three components: food, packaging and environment. These could interact each other: chemical, physical and biological phenomena are often leading to a mass transfer between them. In fact, packaging are able to release undesirable substances in food, modifying its characteristics and organoleptic properties.
"Materials and objects on contact whit aliments" (MOCA), are materials and commodities that are in prospect to be in contact with food such as cooking tools, cutlery, recipients, food cans, food transforming machinery, packaging materials, etc...
The regulation (EC) No. 1935/2004 and further reviews is dedicated explicitly to the management and regulation of food packaging material in the EU.
Despite legislation, some compounds are not specified or included in ordinance: many states in EU decided to establish their own law.
This study focuses on determination of organic volatile substances released from plastic material packaging in fresh cheese and dairy products. Different products with mainly packaging of polyethylene (PE) and nylon, polystyrene (PS), polystyrene (PS) coupled with polyethylene (PE) and polypropylene (PP) were analyzed. The analyses were made by P&T-GC-MS with cryogenic trap.
The presence of hydrocarbons in the packaging and food was found through qualitative analysis. The study showed BTX traces in many samples, probably due to an external contamination. Moreover, isododecane and styrene were the mainly compounds present. Isododecane is probably used as a diluent for the radical initiator for the polymerization while styrene is the polystyrene monomer. For this reason, quantitative analysis of these compounds was performed. Quantitative analysis showed high amount of isododecane and styrene in the packaging. The different concentrations found in the samples were related to different conditions, such as: 1. the brand, 2. the shop where the product was bought 3. shelf life and residence time before using products. However, in general, the MOCA regulation limit value (60 mg/kg of contaminants in the food) were not exceeded.
This study highlighted the importance of monitoring the presence of organic volatile compounds since they could be source of human health-related risk during the assumption of the food product.

P027

BIOGENIC AMINES IN TYPICAL ITALIAN CHEESES AND CORRELATION OF THEIR CONTENT TO THE MAIN PROCESSING AND NUTRITIONAL CHARACTERISTICS

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The presence of biogenic amines in fermented food is today well ascertained. Biogenic amines can affect food quality and can pose risk health effects. Within this work four typical Italian cheeses were analysed to determine the biogenic amine content by ion chromatography (IC) with integrated amperometric detection (IPAD). The performance of the method was assessed in terms of linearity, detection and quantitation limits. Matrix effect and recovery of the method were studied before cheeses analysis.
Cheeses, supplied from different providers (open-air street markets/supermarkets) with different intrinsic hygienic practices, were subjected to common/incorrect habits of consumers (home grating, out-of-fridge storage) and analysed with the IC-IPAD method for the determination of biogenic amines. Biogenic amines were present, as a sum, in the range 19-44 mg/kg, well below the limit currently available from EU. Home-manipulation involves cheese recontamination. The content of biogenic amines was finally correlated through multivariate statistical analysis (principal component analysis, PCA) to the main processing parameters -recognized to affect biogenic amine formation- and with nutritional properties of the cheeses. Main correlations were found among cadaverine, putrescine and spermidine. An interesting correlation of these biogenic amines with fats, supported by an additional PCA assisted by literature data, was also identified.

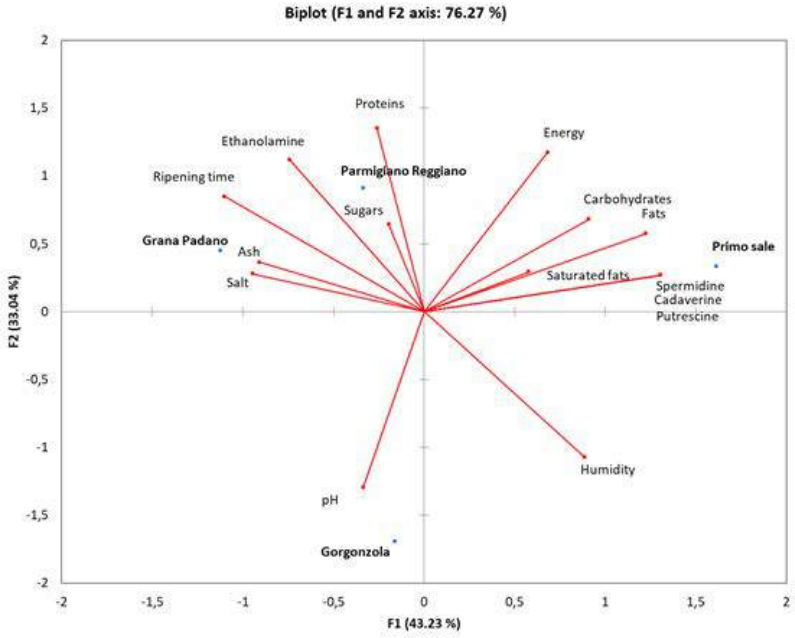

Figure 1. Biplot graph of the objects (cheeses) and of the loadings (red lines: BAs content, pH, humidity, ripening time, ash, salts, fats, carbohydrates, proteins) after PCA.

P028

ANALYSIS OF MILK AND NONDAIRY BEVERAGES: METHOD VALIDATION FOR DETERMINATION OF MERCURY BY HYDRIDE GENERATION ATOMIC FLUORESCENCE SPECTROSCOPY AND OF MAJOR AND TRACE ELEMENT BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY

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Milk contains a variety of nutrients and is long associated with a number of health benefits. It is rich in high-quality proteins and important vitamins and minerals, including calcium, phosphorus and B vitamins. Recently, however, some people have started to avoid milk due to health problems, such as dietary restrictions, allergies and intolerances, and ethical issues regarding the use of animals. As a result, various types of non-standard dairy milk and non-dairy milk beverages are now available (goat milk, donkey milk, soy milk, rice milk, almond milk, oat milk etc.).
Environmental pollution, and manufacturing and packaging processes can alter the concentration of the metals present in milk and in non-dairy milk beverages. Together with essential macro-elements, it is therefore unfortunately possible to find trace of toxic elements. Only for lead, with Commission Regulation No. 1881/2006 [1], the European Union established a maximum level in raw milk, heat-treated milk, milk for the manufacture of milk-based products and in infant formulae and follow-on formulae; although, in some EU countries, national action levels have been set for arsenic and cadmium, as well.
The aim of this study is to optimize and validate a method for the determination of a total content of 41 elements (Al, As, B, Ba, Be, Bi, Ca, Cd, Ce, Co, Cr, Cs, Cu, Fe, Ga, Hg, K, La, Li, Mg, Mn, Mo, Na, Nb, Ni, P, Pb, Rb, Sb, Se, Si, Sn, Sr, Te, Ti, Tl, U, V, W, Zn and Zr) in milk and drinks alternative to milk. Liquid and powder samples (0.5 g) are subjected to HNO_3:H_2O_2 (2:1) digestion in open polypropylene tubes heated in a water bath (80 °C) and subsequently analysed for Hg by hydride generation atomic fluorescence spectroscopy and for major and trace elements by inductively coupled plasma mass spectrometry. Particular attention was paid to quality control and measurement uncertainty assessment. In fact, good quality measurements are always required to control and monitor food and beverages quality, in manufacturing processes, trade and in research. The validated method offers satisfactory detection limits and provides a precise and accurate method (trueness and recovery percentages 80–105%; coefficient of variation <10%; and relative repeatability <12%) with high sample throughput. The proposed method was successfully applied to analyze the set of milk, non-standard dairy milk, and non-dairy milk beverages collected randomly from local markets in the city of Rome.

[1] Commission Regulation (EC) No. 1881/2006 of 19 December 2006 setting maximum levels for certain contaminants in foodstuffs.

P029

Core-shell columns in the HPLC determination of antibacterial drugs in food and feed

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Fast separations of antibacterial drugs in food and feed with high efficiency and resolution are desiderable in official control analysis for the laboratories with an high samples throughput. In addition, less solvent consumption and waste production are important targets for the green chemistry. Analytical columns packed with core-shell particles were made of a solid core surrounded by a thin porous shell. This particular structure allows to reduce the eddy diffusion and mass transfert contributions, two main causes of peak broadening in HPLC, as described in Van Deemter Equation. The core-shell columns offer short chromatographic separation with resolution and efficiency comparable to sub-2 µm totally porous particles with the advantage of a low back pressure (≤ 400 µm). This allows the use of these columns on conventional HPLC system without any up-grade on the instrumentation. In the present study, columns packed with core-shell particles were used for the separation of sulphonamides, tetracyclines and penicillins in meat, milk, eggs and feed.
As first application, two analytical methods for the determination of sulphonamides (SAs) in meat (13 SAs) and feed (10 SAs), developed using columns packed with totally porous particles (1,2), have been modified employing core-shell columns with the reduction of analysis time from 40-45 to 13 minutes. Since no change was made to the sample clean-up, the optimized methods do not require a complete re-validation.
Furthermore, good results in terms of resolution and efficiency were obtained, in only 13 minutes, by a C18 core-shell (2,6 µm) for the analysis of 7 tetracyclines in milk and eggs and 13 SAs in the milk. Finally, an UPLC-ESI-MS/MS method was developed for the analysis of penicillins in the milk at the Regulation 37/2010 limits and, in the feed, at the cross-contamination levels. A good separation of 7 penicillins was obtained in 6 minutes by a C18 core-shell (1,7 µm) using a eluition gradient. While for the feed sample is enough a simple extraction and dilution with water, milk sample was furtherly purified by a C18-SPE clean-up phase. For each penicillin, the most intense m/z ion transition was used as quantifier and the second most intense for identification.

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P030

A NEW RAPID AND GREENER METHOD FOR EXTRACTION OF CANNABINOIDS FROM FLOWERS OF ***CANNABIS SATIVA:*** COMPARISON BETWEEN THREE VARIETIES OF HEMP

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Cannabis (Linneus, 1753) or hemp is a genus of angiosperm plants that has been of medicinal interest for centuries. In the recent years the interest in this plant has grown enormously for possible uses in the medical field.[1] Among the different species of *Cannabis*, the most studied is the *sativa* species. Many different pharmacological properties have been associated with cannabis use, including increased heart rate, decrease of body temperature, ataxia and a loss of time-space perception.[2] *Cannabis sativa* is rich in essential fatty acids (ω3 and ω6) and is also a precious source of vitamins, but the cannabinoids (psycho-active components biochemically classified as terpenophenols) have been recognized as the active constituents for most clinical activities.[3] The most known cannabinoids are CBD (cannabidiol) and THC (Δ^9-tetrahydrocannabinol). Nowadays, according to global trends, "green" products and technologies are needed to replace conventional ones. Therefore, in this study, we used a greener method for extraction, the Naviglio Extractor (NE) or rapid solid-liquid dynamic extractor (RSLDE) that is an innovative solid-liquid extraction technology that allows to exhaust in a short time, compared to other extraction techniques currently used, the solid matrices containing extractable substances by using an organic or inorganic solvent and in their mixtures,[4] obtaining extracts that can also be used in therapeutic and food field. Moreover, hemp extracts obtained with this method were subjected to chromatographic analysis by HPLC, which allowed the identification and quantification of the cannabinoids. In particular, the quantities of cannabidiolic acid (CBCA), CBD and THC present in three different varieties of *C. sativa*: Finola, Futura and KC Virtus were compared.

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P033

NUTRACEUTICAL PROPERTIES OF EXTRAVIRGIN OLIVE OIL: OLEOCANTHAL CHARACTERIZATION BY LIQUID CHROMATOGRAPHY-ELECTROSPRAY IONIZATION FOURIER-TRANSFORM MASS SPECTROMETRY

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Several epidemiological studies about the existing correlation between the regular consumption of extra virgin olive oil in Mediterranean diet and the decrease of cardiovascular, metabolic and cancer diseases have stimulated a great deal of interest towards olive oil bioactive polyphenols belonging to the class of secoiridoids. Among them, oleocanthal (OC) stands out for its anti-inflammatory properties, comparable to those of a well-known drug like ibuprofen [1][2], and for being the main responsible of olive oil pungency. The biosynthesis of OC occurs during the crushing of olive fruits via either the hydrolysis, catalyzed by a methylesterase enzyme, of a methyl ester embedded into the structure of another relevant secoiridoid, the ligstroside aglycone, or the decarboxylation of a less abundant secoiridoid, the demethyl-oleuropein aglycone, catalysed by a decarboxylase enzyme [3]. In accordance to NMR investigations, both pathways should lead to an open dialdheydic form of OC, most likely in equilibrium with the corresponding enolic form [4][5]. In the context of a more general investigation on olive oil secoiridoids, a method based on reverse phase liquid chromatography coupled to electrospray ionization and Fourier-transform mass spectrometry (RPLC-ESI-FTMS) has been developed in our laboratory to separate those forms of oleocanthal and characterize their molecular structure with the aid of tandem mass spectrometry data. In the present communication the results obtained from the systematic application of the described approach to a set of Italian extra-virgin olive oil, produced in different Italian regions from mono-cultivar or blended olive drupes, will be described. The occurrence of oxidized by-products of OC will be discussed as a possible marker of processes (e.g. periodical exposure to air or prolonged storage) that can negatively affect the quality and the nutraceutical properties of olive oil.

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P034

ANALYSIS OF VOLATILE ORGANIC COMPOUNDS OF HONEY PRODUCED IN TRIESTE KARST AREA BY HS-SPME-GC-MS, EVALUATION OF AN ELECTRONIC NOSE DISCRIMINATION POTENTIAL AND CORRELATION WITH VOCs PRODUCED BY LOCAL BEE HOST PLANTS

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Honey composition is closely associated with the botanical origin and geographic area of production because the soil and climate determine the bee flora. Volatile compounds, which primarily account for food aroma and flavor, are present in honey at very low concentrations as complex mixtures of different chemical classes, including monoterpenes, norisoprenoids, sesquiterpenes, benzenoids, alcohols, esters, ketones and aldehydes. The volatile compounds present in honey usually come from flower nectar and may be considered markers of bee-visited plants [1]. In scientific literature the analysis of volatile organic compounds of honey is usually focused on finding correlation between VOCs and the mono-floral origin [2].

In the Trieste Karst area several honey producers are present. Aiming to enhance the site-specific characteristics of local products they collect honey according to blooming mixtures from May to October to obtain specific multi-floral honeys. The aim of this study is the qualitative chemical characterization of Trieste Karst honey volatile organic compounds by HS-SPME-GC-MS. Moreover, more than fifteen local bee host plant flowers have been collected for VOC profile characterization by use of the same analytical method aiming to find possible correlations between the honey and plant profiles.

The honey VOC profiles have been also analyzed by a 32 sensors array electronic nose to correlate the sensor signals to the chemical characterization and evaluate the e-nose discrimination potential for the local products.

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P035

MULTIDIMENSIONAL LIQUID-GAS CHROMATOGRAPHY COUPLED TO A SIMULTANEOUS ISOTOPE RATIO AND QUADRUPOLE MASS SPECTROMETRY FOR OLIVE OIL TRIGLYCERIDES ANALYSIS

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Isotope Ratio Mass Spectrometry (IRMS) is a specialized technique used to provide information about the geographic, chemical, and biological origins of substances. The ability to determine the source of an organic substance stems from the relative isotopic abundances of the elements which comprise the material. Usually a separation is performed prior to isotope ratio analysis using LC or GC techniques. However, for complex samples a single chromatographic step could not be effective for the complete purification of target components. Multidimensional chromatographic approaches could enhance the purification power of specific fractions before the detection. LC-GC is a powerful technique when a pre-separation step is required aiming to remove non-volatile components and/or to reduce the complexity of a sample. The TAGs analysis is often used for the detection of the adulteration of olive oil. The profile is characteristic for each kind of oil, as it depends on the fatty acid composition and on the biosynthesis rules, so that it can be used to check for the presence of extraneous oils. However, the quality of extra-virgin olive oil greatly depends also by the plant cultivar and geographical origin. Applied to olive oil triglycerides, the RP-LC step provides the pre-separation of the fractions based on the partition number (PN) depending on the total carbon number subtracting two for each double bond. The resulting fractions show a greatly reduced complexity avoiding coelution problems respect to direct GC analysis. The present research deals with the development of an LC-GC-MS/IRMS prototype characterized by the improved resolution of the heart-cut mode. Two different chromatographic mechanisms were employed with simultaneous qMS and IRMS detection. Fast GC was applied for the separation of each fraction transferred before the IRMS/qMS step (after the LC pre-separation), providing quali/quantitative and isotopic ratio information ($\delta^{13}C$). Different origin and cultivar olive oils were analyzed and the results are here presented.

P036

AUTHENTICATION OF TRUFFLES AND PRODUCTS CONTAINING TRUFFLE BY MEANS OF MDGC-C-IRMS / qMS WITH A LOW-BLEED IONIC LIQUID SECONDARY COLUMN

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Gas chromatography coupled to combustion-isotope ratio mass spectrometry (GC-C-IRMS), exploiting the $^{13}C/^{12}C$ ratio abundance of the key flavourings compounds in foods, has been a recognized technique for authenticity and traceability purposes, however a number of issues have greatly limited its widespread use, so far.

Truffles are among the most expensive foods available in the market, usually used as flavouring additives for their distinctive aroma. The most valuable species is Tuber magnatum Pico, better known as "Alba white truffle", in which bis(methylthio)methane is the key aroma compound. Given the high economical value of genuine white truffles, analytical approaches are required, able to discriminate between natural or synthetic truffle aroma.

In the present research, a high-efficiency HS-SPME MDGC-C-IRMS with simultaneous quadrupole MS detection, has been applied for the evaluation of bis(methylthio)methane, resolving the coelution occurring with other components. With the aim to minimize the effect of column bleeding on δ 13 C measurement, a medium polarity ionic liquid-based stationary phase was preferred to a polyethylene glycol one, as secondary column. Twenty-four genuine white truffles harvested in Italy were analysed, attaining $\delta^{13}C$ values between -42.6 ‰ and -33.9 ‰, with a maximum standard deviation lower than 0.7 ‰ . Two commercial intact truffles and 14 commercial samples of pasta, sauce, olive oil, cream, honey and fresh cheese flavoured with truffle aroma were analysed, and the results from $\delta^{13}C$ measurement were evaluated in comparison with those of genuine "white truffle" range and commercial synthetic bis(methylthio)methane standard.

P037

AN ANALYTICAL STRATEGY FOR MALDI–MS-BASED UNTARGETED METABOLOMICS OF VITREOUS HUMOR TO ESTIMATE POST-MORTEM INTERVAL

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Over the last years, the vitreous humor (VH) has gained a key role in forensic science to identify several causes of death and, more importantly, to estimate the time since death (Post-Mortem Interval; PMI). [1] VH is easy to collect even when an autopsy is not required, it is anatomically isolated and well protected from the external space, therefore is well-preserved from exogenous contamination and degradation. Moreover, chemical changes occur at a slow rate, expanding its applicability to a wider range of time since death (up to 144 hours). [2] The search for new ''analytes'' on postmortem changing parameters is an important task in forensic science, however new parameters should be taking in account the nature of the studied process and the presence of several influencing factors, including physical process (body cooling, hypostasis), metabolic process (e.g. concentration of metabolites, activity of enzymes) and autolysis (loss of selective membrane permeability, diffusion, morphological changes).
In this report we present an analytical strategy for MALDI MS-based untargeted metabolomics study on VH looking for statistically significant parameters correlated to death time estimation. The incubation of VH at physiological pH and controlled temperature mimed post mortem conditions to evaluate metabolic variations and maybe correlate them with the PMI.

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P038

AN USER-FRIENDLY R SHINY APP FOR THE INTERPRETATION OF CHRONIC ALCOHOL ABUSE BIOMARKERS

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The quantitative determination of chronic alcohol abuse biomarkers is consistently used throughout the world to assess chronic excessive alcohol consumption. Direct ethanol metabolites, including ethyl glucuronide (EtG) and fatty acid ethyl esters (FAEE), are highly specific and sensitive, in particular when they are quantified in the keratin matrix, typically scalp hair. In particular, the conjoined determination of direct biomarkers currently represents the most accredited strategy for proving chronic alcohol abuse. Current practice involves comparing the analytical results with cut-off values recognized by regulatory authorities and scientific societies, for both administrative and legal purposes. However, the involvement of cut-off values might result in an arbitrary interpretation by the experts, especially when the measured EtG and FAEEs values are close to the cut-off values and/or contradictory. Consequently, combining the results from FAEEs and EtG analysis by means of several Multivariate Data Analysis (MDA) techniques and Likelihood Ratio (LR) approaches represents a valuable approach to decrease the number of misleading conclusions caused by biased data interpretation procedures. The main aim of this study was to develop an open-source user-friendly R Shiny application[1], capable of calculating MDA classification scores, plots and LR results, in order to assist the forensic experts and, eventually, laymen to interpret the results from both the indirect and (mainly) the direct ethanol metabolites. Data from clinical and toxicological analyses were used as training (reference) set for building the MDA (e.g. Logistic Regression, Linear Discriminant Analysis, etc.) and LR models (i.e. uni- and multivariate) in the developed R Shiny application, developed in the open-source R Studio environment. Analyses were commissioned by Local Committees for Driving Licences and Alcohol Abuse Treatment Services located in Piedmont (northern Italy), and performed at the Regional Antidoping and Toxicology Center "A. Bertinaria" (Orbassano, Italy). Data are also available in [2]. The developed R Shiny application represents a useful and open-source tool to perform a robust and not arbitrary interpretation of chronic alcohol abuse biomarkers. Futhermore, it allows analysts and practitioners to test on their own data the several MDA and LR models that are implemented in the application.

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P039

Development of a innovative analytical procedure for Organic Gunshot Residues (OGSR) investigation

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The objective of this study was to develop an analytical method, based on High Performance Liquid Chromatography hyphenated to Mass Spectrometry (HPLC-MS/MS), able to identify alternative solutions to the critical issues in gunshot residues investigation and, in particular, in the analysis of the organic gunshot residues (OGSR).
A large number of different analytical approaches has been reported for the evaluation of powder composition present in the charge and, in particular, for the sampling of the gunshot residues from the hands and clothing [1-2]. These applications still didn't solve critical points related to these components that may be very challenging in such situations involving lead-less bullet.
In order to optimize the analytic method, shooting experiments were performed to evaluate transfer of OGSR using different cartdriges fired by the same shotguns, so as to find features particles of the ammunition used. In particular, for targeting the major number of stabilizers, the main goals of the present study were to find the best conditions for the chromatographic separation and the best parameters of the Mass spectrometer. Specifically there were compared two different types of sources (ESI, APCI), exploiting the high sensibility and analytical strength of the Orbitrap mass analyser. In fact, the LC-Orbtrap technology is a powerful tool for the analysis of OGSR thanks to its analytical performance in terms of resolutions, mass accuracy, space charge capaticity and linear dynamic range.
The achieved results have shown that, using the results derived from the analysis of OGSR, in addition to other traditional techniques, could help in interpretation of the analytical results in order to understanding the dynamics of a crime, giving a confirmation of the hypothesis of offence.

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P040

Electrodeposited Prussian blue on carbon black modified disposable electrodes for direct enzyme-free H_2O_2 sensing in a Parkinson's disease *in vitro* model

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Reactive Oxygen Species (ROS) are reduced forms of oxygen such as superoxide anion, hydroxyl radical or hydrogen peroxide. These molecules have a critical role in physiological processes like cellular signalling, immunological activity. However, an overproduction may cause the so-called oxidative stress (OS) which is able to cause damage to lipids, proteins or DNA. These alterations promote pathophysiological conditions such as diabetes, cancer, Alzheimer's and Parkinson's disease. Carbon Black (CB) is a carbon nanomaterial widely used as reinforcing material and as filler in the preparation of rubber and plastic compounds and composites. CB dispersions after sonication, in appropriate solvents, appears as carbon nanoparticles. The 'nano CB' exhibit excellent conductivity, unique electrochemical properties and cost-effectiveness (about 1 euro/kg). For these reasons, in the last years several works have been reported on the CB dispersion for electrode modification [1–3] In this work, we present the combination of Carbon Black (CB) and electrodeposited Prussian Blue (PB) covered with a Nafion layer on Screen-Printed electrodes (CB/PB-SPE) used for non-enzymatic H_2O_2 sensing in Neuroblastoma cell line SH-SY5Y. These cells were challenged with 6-hidroxidopamine (6-OHDA) for modelling Parkinson's disease. The electrodes surface was investigated using Scanning Electron Microscopy (SEM) and electrochemically characterized, in terms of electroactivity and stability. Electrochemical sensing of H_2O_2 was carried out at very low potentials (-50mV), allowing interference-free detection of H_2O_2 in the selected cell culture. The H_2O_2 concentration was successfully monitored in an experimental model of Parkinson's disease. These results pave the way to a method for the continuous monitoring of H_2O_2 in culture medium for future studies of the role of H_2O_2 in Parkinson's disease.

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P041

EFFECT OF MOBILE IONS IN THE ELECTRON TRANSFER PROCESS IN ENZYME-BASED AMPEROMETRIC SENSORS

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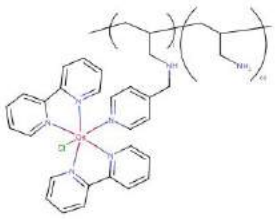
Polyallylamine is a weak polyelectrolyte widely used in materials science because of its ductility as working probe. Its interaction with polyelectrolytes of opposite charge allows to create multilayer polyelectrolytes (PEML) forming highly stable interfaces. The ionic strength of the solutions is critical in determining the properties of the PEMLs [1]. Cations and small anions (called mobiles), both univalent and multivalent, can form ionic pairs with charged sites on the polyelectrolyte chains to reduce their intra-chain electrostatic repulsions, thus allowing weaker interactions such as Van der Waals and/or hydrogen bonds, promoting the formation of ball-like conformations. In the last years, divalent ions (SO_4^{2-}, HPO_4^{2-}) have been applied in the construction of multilayer polyallylamine systems [2]. Although these systems have been characterized by diverse techniques, little has been studied on the electron transfer processes in modified polyallylamine with species able to carry out charge transport to the electrode in an efficient form [2]. No results are reported in literature about the incorporation of negative charged complex species, such as proteins, into the PEML. In this work is presented the use of polyallylamine modified with a polypyridine complex of osmium (fig. 1) which has been assembled in the presence of sulfate, phosphate, oxalate or citric ions, using as counter charged layer the Glucose Oxidase enzyme. Characterization of such system was carried out by electrochemical techniques and quartz crystal microbalance. The results show that the catalytic signal obtained in presence of glucose is different depending on the mobile ion used. Phosphate ions proved to be the best in the construction of polyelectrolyte. These results allow to hypothesize the use of this platform to create enzymatic biosensors with high reliability and reproducibility.



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P042

SENSING PLATFORM APPLIED TO OLIVE OILS ANALYSES: SCREEN PRINTED ELECTRODES MODIFIED WITH NANOMATERIALS AND GREEN IONIC LIQUIDS

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The analysis of olive oil represents an important tool in the agri-food field, because of the frequent scam and fraud in extra virgin olive oils (EVOO). For the determination of the quality and origin of Italian EVOOs many analytical methods have been proposed, regarding triglycerides or antioxidant content and/or DNA profiling [1,2]. None of them has provided a simple and fast procedure suitable to identify cultivar and/or geographic origin of the EVOOs. Therefore, the individuation of olive oil adulteration remains nowadays a nodal problem for Researchers in the field.
Our sensing proposal only represents a small tile in the diversified mosaic of this fundamental argument. In particular, the amperometric biosensor previously described [3] has been further implemented with TiO_2 nanoparticles, to ensure better electrochemical responses. After analyzing commercial and/or artisanal EVOOs, a laboratory method for olive oil extraction has been developed, to obtain more reliable results coming from certainly comparable oil samples. The developed extraction method resulted reliable, reproducible and safe. The oil samples to be analyzed were obtained from olives of sure and undisputed cultivar and geographic origin, collected in the Lazio region of Italy during the 2016 campaign.
The sensor platform (GC/MWCNT/TiO_2/[Ch][Phe) has been applied to the oil samples, after enzymatic triglycerides hydrolysis causing the release of antioxidant compounds, responsible for the electrochemical signals. A good differentiation of oils cultivar was achieved.
The same platform has been used to quantify the total hydrosoluble antioxidant component on edible oils. It is known [4] that these compounds abundant in olive oil are almost absent in seed oils. The hydrosoluble antioxidants analysis could be a good tool to identify adulterations in EVOOs. The platform results have been compared with antioxidants determination performed by a spectrophotometric instrumentation that allows quick measurement of acidity, peroxide index and polyphenol amount.

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P043

ELECTROCHEMICAL PRINTED AND MINIATURISED SENSORS TO EVALUATE THE STATE OF CONSERVATION OF CONCRETE-BASED SAMPLES

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In the production of 20th Century buildings and artworks, several modern materials have been employed, including acryl and vinyl paints, plastics, synthetic textiles, and reinforced concrete. Among them, the use of concrete has boosted several buildings sectors mainly due also to its low costs. Concrete is an extraordinarily versatile construction material exploited in utilitarian, ornamental, and monumental structures from the last century. However, the artworks in concrete are subjected to several deterioration mechanisms including carbonation, freeze-thaw deterioration, corrosion of reinforcement, alkali silicate reaction, erosion of surface matrix, and superficial sulfate reaction. It is now essential to develop sustainable strategies and tools to help communities to better characterize, understand and conserve their 20th Century heritage, through ageing process monitoring. This is especially true for 20th century cultural heritage, where the use of modern materials could enhance deterioration mechanisms more than ancient cultural heritage. Herein, we present a miniaturized potentiometric sensor combined with portable instrument to monitor easily and on-site the state of conservation of concrete. To accomplish this issue, several samples of reinforced concrete were realized using same weight of Portland cement and river sand with an iron rebar. To simulate carbonation process the concrete's pH is lowered to the value of 8-9 adding calcium bicarbonate. Other reinforced concrete samples are de-protected adding calcium chloride accelerating the oxidation of rebar. To monitor the aging, the sensor has been put in contact with the concrete surface, working as counter and reference electrodes, while the steel present in the concrete as working electrode, exploiting an agarose gel-based electrolyte. With a measurement less of 30 s, we demonstrate that the sensor is capable to evaluate the ageing process before to see evident corrosion of the sample.

Acknowledgements
INNOCONCRETE project within Executive Programme on Scientific and Technological Cooperation between Italian Republic and the Kingdom of Sweden for the years 2018-2020.

P044

ELECTROCHEMICAL SENSOR FOR NADH DETECTION BASED ON ELECTROCHEMICALLY EXFOLIATED GRAPHENE OXIDE

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We describe the use of nanosheets of Electrochemically exfoliated graphene oxide (EGO)[1] for electrochemical sensing of β-nicotinamide adenine dinucleotide (NADH), a coenzyme involved in electrochemical redox reactions of all living cells.

Thanks to the versatile chemistry of EGO, we could activate an efficient electrocatalytic oxidation of NADH. This was achieved by tuning the density of oxidized functional groups on the surface of the nanosheets while keeping, at the same time, a good electrical conductivity of the nanosheets.[2] The high tunability of the functionalization degree and electrical conductivity render EGO a promising material for electrochemical detection.

The surface chemistry of EGO was then improved even more by functionalization of the carboxylic groups of EGO with organic molecules, namely dopamine or caffeic acid, bearing terminal alcoholic moieties. The functionalization was performed using both a chemical and an electrochemical approach, yielding, in both cases, better sensibility, reproducibility and lower NADH detection limit as compared to non-functionalized EGO. The analytical performance of pristine EGO, EGO functionalized with dopamine and caffeic acid was studied using electrochemical, spectroscopic and UV-Vis spectroelectrochemical analysis, and compared with the performance of standard commercial electrodes. The good sensibility and the low limit of detection of this new sensor could be exploited in future applications to develop enzymatic biosensor based on NADH – dependent enzymes.

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P045

AMPEROMETRIC DETECTION OF HISTAMINE WITH A DIAMINE OXIDASE – POLY[(TAT)Ru(TpyCOOH)]$^{2+}$- BASED SENSOR

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Histamine is a biogenic amine mainly deriving from histidine decarboxylation by positive decarboxylase bacteria. This biogenic amine is well-known due its toxic effects on human health; a high quantity of histamine in foodstuffs can be a result of poor quality of the raw materials, contamination and/or inappropriate sanitary conditions during the production and storage processes. So, histamine detection is important in the context of quality control and food safety respectively for the evaluation of the foodstuffs freshness and quality and to minimize health risks.
Here, we report the assembly of a biosensor based on diamine oxidase (from porcine kidney) immobilized on a polymer film obtained by the electropolymerization of the metal complex [(TAT)Ru(TpyCOOH)]$^{2+}$ (TAT = 4'-(2,2':5,2''-terthien-3'-ethynyl)-2,2':6,2''-terpyridine; TpyCOOH = 4,4',4''-tricarboxylate-2,2':6,2''–terpyridine)[1].
The choice to use a metal-polymer matrix as a modified agent for the electrode surface is due to high conductivity of this type of materials and its electrocatalytic ability. Furthermore, this type of surface allows to immobilize the enzyme avoiding denaturing or misfolding processes.
Diamine oxidase from porcine kidney is a commercial and quite inexpensive enzyme which catalyzes the oxidation reaction of different biogenic amines but preferentially of histamine, its main substrate.
This biosensor demonstrated to be an interesting analytical instrument with a good linearity, sensibility and selectivity for the determination of histamine and, to the best of our knowledge, it is one of the first second-generation biosensor based on diamine oxidase.

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P046

CHARACTERIZATION AND APPLICATION OF ELECTROCHEMICAL SENSORS BASED ON CONDUCTING POLYMER NANOCOMPOSITES

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In the last years, most of the work was devoted to synthesize new sensing nanocomposites to improve a sensor performance in terms of sensitivity, selectivity and biocompatibility. Of those synthesized nanomaterials, conducting polymers composites have been widely used in the construction of sensor surfaces. Several conducting polymers *i.e.* polythiophene, polyaniline, polymethylene blue, polyanthranilic acid, polypyrrole, and poly(o-phenylenediamine) display advantages due to their charge transport properties and electrochemical redox efficiency, which are attributed to the delocalization of π-electrons over the polymeric backbone [1, 2].

For a greater enhancement of the electrochemical sensor performance, various platforms have been developed based on electrode surface modification with nanomaterials [3]. The synergy of multifunctional materials, recognition elements, and electrochemical methods is improving the selectivity, stability and reproducibility, thus promoting the development of new sensors.

Conductive polymers such as polyaniline and polyanthranilic acid were used to obtain a nano/micropatterned surface at graphite screen-printed electrodes (GSPEs) with applications in the biosensors field. The obtained thin films were electrochemically characterized by cyclic voltammetry and electrochemical impedance spectroscopy using different redox probes. Different architectures were obtained by electrodepositing noble metal nanoparticles (AuNPs, PtNPs) at the modified electrodes and the performance of the hybrid composites was assessed. In addition, scanning electron microscopy was used as a surface characterization method of the nanostructured surfaces. Applications of the developed polymer-based sensors will also be presented, with emphasis on quantification of food and water contaminants.

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P047

A VERSATILE AND SENSITIVE VERSATILE POINT-OF-CARE TEST FOR THE RAPID DIAGNOSIS OF VISCERAL LEISHMANIASIS

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Visceral leishmaniasis (VL) is a zoonotic infectious disease with severe impact on humans and animals. Infection is transmitted by phlebotomine sand-flies and several domestic and wild mammals act as reservoirs for the infection, among which domestic dogs are considered the main reservoir for human infection. The prompt detection of infected hosts is crucial for the prevention and control of the spread of the disease and of transmission to humans. Canine VL (CVL) can be diagnosed by combining clinical and epidemiological parameters with parasitological, serological, or molecular methods. Serology is preferred and the detection of anti-leishmanial antibodies is commonly realized by the immunofluorescent antibody test (IFAT), which is considered as the reference method in dogs, though data on its diagnostic sensitivity and specificity are controversial. Enzyme-linked immunosorbent assays (ELISAs) exist for CVL diagnosis that also provide very sensitive and specific quantitative results. However, the rapid and cost-effective detection of infected dogs is a key point in the control of infection and infection transmission. The lateral-flow immunoassay (LFIA) is the most popular diagnostic tool for rapid onsite assays. Its main advantage is represented by its perfect match with ASSURED criteria required for point-of-care testing (Affordable, Sensitive, Specific, User-friendly, Rapid/Robust, Equipment-free and Deliverable to end users).

This study describes a rapid and portable diagnostic tool for VL diagnosis based on the LFIA technology. The specific recognition element is represented by a recombinant chimeric antigen, comprising three Leishmania antigens, which has been shown to be highly specific for CVL. The signal reporter is constituted by staphylococcal protein A labelled with gold nanoparticles that are used as colored probes for the visual interpretation of the qualitative result. A total of 167 canine sera were involved in the study collected from an endemic (37 samples) and non-endemic (130) regions. Canine sera were characterized by reference methods (IFAT and ELISA). The LFIA shows excellent diagnostic sensitivity (98.4%,), specificity (98.9%) and agreement with serological reference methods for diagnosing CVL. The long-term stability of the LFIA device was confirmed for 6 months storage at room temperature and 4°C and the qualitative response was not affected by limited thermal stress. The use of the broad-specific protein A enables the versatile application of the LFIA to VL diagnosis in in other mammals (9 feline sera and two fox sera were tested and provided agreeing results compared to the reference methods), thus assuring the opportunity of efficiently controlling the spreading of the infection.

P048

SCREEN PRINTED ELECTRODES MODIFIED WITH BIOCHAR: TOWARDS A NOVEL ELECTROCHEMICAL PLATFORM

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The beer brewing process is one of the most polluting industrial processes, generating a huge amount of wastewater effluent and solid wastes (i.e. spent grain and yeast). Among them, spent grain can constitute as much as 85 % of a brewery's total by-products. As a consequence, there is a great interest to find innovative ways to prevent spent grain from going to waste. At this regard, Sperandio et al. developed a process for the production of biochar (charcoal) from dried spent grain through a thermochemical process of pyro-gasification [1]. Biochar is considered a good agricultural soil improver, with high content of carbon and nitrogen, able to promote water and nutrient retention, thus reducing the need of water and chemical fertilizers. In the present study, we presented an innovative way to use biochar from spent grain for the realization of screen printed electrodes, prepared with the modification of SPEs by drop casting with a stable dispersion of biochar(Biochar/SPE sensor), have been reported. This study was conducted using different electroactive species, such as ferricyanide, benzoquinone, epinephrine, ascorbic and uric acid, in order to understand the electrochemical behaviour of the modified electrode. The results were compared with those of commercial screen-printed electrodes confirming that modification allowed to obtain a sensor with improved electrochemical behaviour in terms of resolution, peak-to-peak separation, current intensity, and the resistance of charge transfer. A tyrosinase biosensors (Ty/Biochar/SPE) has been developed using the Biochar/SPE for the determination of epinephrine. The detection has been performed by measuring the current due to the reduction of the corresponding quinone at low potential, equal to -0.310 V for epinephrine. The experimental conditions for the tyrosinase immobilization and the analytical parameters, such as applied potential and pH of buffer have been studied and optimized. Under these conditions, the electrochemical biosensors have been characterized. A linear working range of epinephrine was obtained from 0.05 up to 0.5 mM. The detection limit is 2×10^{-4} mM for developed biosensors. The biosensors construction was highly reproducible.

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P049

Disposable paper-based sensor for rapid free chlorine detection

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In the last decades, the scientific community has focused the attention in the development of portable, cost-effective, user-friendly, and ready-to-use devices for fast on-site measurements. To seek more sustainable solutions, paper has been recently selected as support for printed sensors, exploiting its features such as porosity, cheapness, and easy availability, used to load the reagent and to filter the sample, delivering a lab on a chip on paper [1].
For the detection of free chlorine, colorimetric, spectrophotometric, and electrochemical devices have been developed. Free chlorine is defined as the sum of hypochlorite ion and hypochlorous acid, produced from chlorine compounds hydrolysis. They are the most widespread chemicals used for the disinfection of swimming pool and drinking water, as well as in domestic and industrial fields [2].
Actually, the only paper-based available devices are based on colorimetric detection (strip-test), however this detection is highly affected by operator eyes sensitivity.
Herein, we propose the first electrochemical reagent-free, easy-to-use paper-based sensor for chlorine quantification, combining the advantages of paper with the sensitivity of the electrochemical detection. In detail, the detection has been carried out indirectly, exploiting the reaction between the analyte and the iodide, as previously reported by W. Matuszewski and T. Marek using bulk platinum electrodes [3]. To deliver a sensitive measurement, several working parameters have been optimized, such as the nanomaterial used to modify the working electrode, the applied potential, the buffer concentration, etc. Satisfactory results (sensitivity equal to 32 ± 3 nA/ppm) have been obtained with filter paper-based sensor modified with 6 µL of gold nanoparticles, loading few microliters of the needed reagents onto the hydrophilic area. The preliminary results achieved demonstrated that this paper-based sensor can be a suitable sensing tool for free chlorine detection in water samples.

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P050

FLUORESCENT DNA-BASED IMMUNOASSAY FOR THE DETECTION OF SMALL MOLECULES

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The development of rapid, cost-effective and single step methods for the detection of small molecules is crucial for improving quality and efficiency of many applications ranging from life science to environmental analysis. Unfortunately, current methodologies still require multiple complex, time-consuming washing and incubation steps, which limit their applicability. In this work we present a competitive DNA-based platform that makes use of both programmable DNA-switches and antibodies to detect small target molecules. The strategy exploits both the advantages of proximity-based methods and structure-switching DNA-probes. The platform is modular and versatile and it can potentially be applied for the detection of any small target molecule that can be conjugated to a nucleic acid sequence. Here the rational design of programmable DNA-switches is discussed, and the sensitive, rapid and single-step detection of different environmentally relevant small target molecules is demonstrated.

P051

Analytical and Energetic Applications Using a Yeast-DMFC Device and Glucose as Fuel

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First results, using a DMFC-yeast system for glucose determination, are reported in the present communication. Measurements were carried out by using the apparatus illustrated in Fig. 1. A 50 mL glass flasks, suitably closed with a glass stopper and containing weighted amount of glucose, glycine and yeast in 30 mL of aqueous solution, using a magnetic stirrer, to maintain the yeasts in suspension, was kept in an incubator (Fig. 1) at a fixed temperature of 25 ± 1 °C, for 24 hours. At the end of this time, 2 mL of solution was taken from the flask with a graduate syringe, equipped with small filter, and placed in a (DMFC) Direct Methanol (or Ethanol) Catalytic Fuel Cell, H-TEC Model F111, (50 x 50 x 40 mm). For potentiostatic measurement format, a Palmsens mod. EmStat potentiostat was used, connected to the fuel cell and a PC. The current was recorded until the steady state, at which the supplied current value was read.

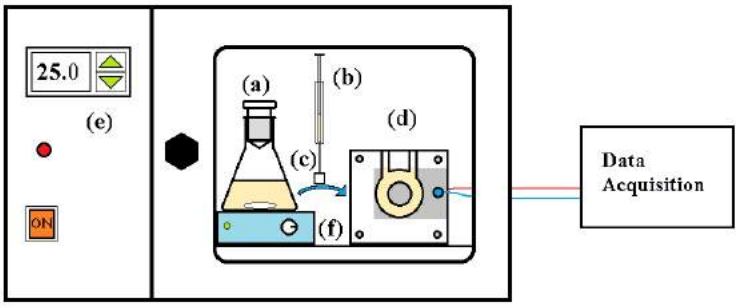

Figure 1 Experimental Apparatus: a) flask containing glucose in glycine aqueous solution and yeast; b) graduated syringe; c) small filter; d) catalytic fuel cell; e) thermostatic apparatus; f) magnetic stirrer.

First of all we have experimentally verified that a glucose solution, inserted in the DMFC cell, does not give any significant signal; but, if the glucose solution was put in contact with yeast cells (Saccharomyces cerevisiae), it can be observed the source of an e.m.f. between the DMFC cathode and anode of the fuel cell, from which electrical current can be generated. In the first results obtained with the present research, it was optimised, by operating in isotonic glycine solution and at room temperature, the quantity of yeast and the time necessary for the best production of ethanol and to maximize e.m.f. under the chosen operating conditions. Finally we recorded the cell response to the increasing glucose concentration in solution, using the optimized conditions and obtained a calibration curve. Lastly, the fuel cell power (as Watts) was measured. Actually further research are running by varying the operating conditions with especially regard to the operating temperature. Infact this research was on purpose carried out at 25 °C, precisely in order to check whether the system can operate even at room temperature, but it is indeed foreseeable that, by carefully increasing the thermostating temperature of the system, it will be possible to shorten the measurement times and increase the sensitivity. First results encouraged this perspective.

P052

A COMPETITIVE AMPEROMETRIC MAGNETO-IMMUNOSENSING STRATEGY FOR HE4 OVARIAN CANCER BIOMARKER DETECTION

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Human epididymis protein 4 (HE4) has been recently identified as relevant and promising biomarker for ovarian cancer (OC) [1], which is characterized by one of the highest mortality rate between gynaecologic malignancy. Nowadays analytical techniques are moving towards the development of immunosensors for more simple, fast, high-throughput and point-of-care accurate analysis of disease markers to meet the requirement of medical diagnosis and biomedical research applications [2]. In this context, the aim of the present work is the development of an innovative strategy in immunosensing for the determination of HE4 protein based on a competitive immunoassay performed on the surface of HE4-functionalized magnetic beads (MBs), followed by amperometric reading on glassy carbon screen printed electrodes. Before optimization of the experimental protocol, the effectiveness of MBs functionalization, the immunoreactivity of the immobilized HE4 towards anti-HE4 antibodies as well as the extent of aspecific interactions were assessed. For the preliminary experiments, commercial anti-antibody conjugated with phosphatase alkaline (ALP) was used, however for the final protocol the conjugation of the anti-HE4 antibodies with ALP enzyme will be considered with the aim of developing a fast and easy-to-use diagnostic tool.

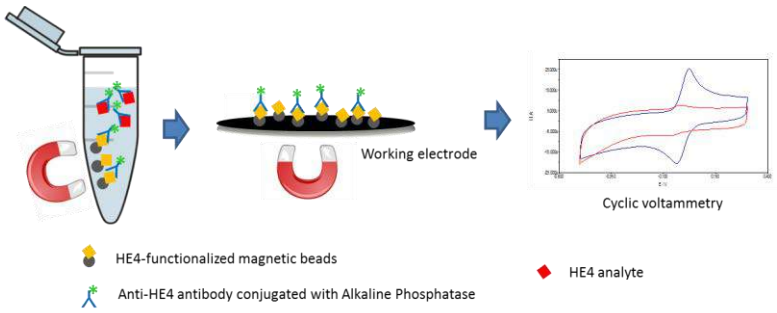

Figure 1. Competitive magnetic beads-based immunosensing strategy

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P053

DEVELOPMENT OF AN ORIGAMI-LIKE REAGENT-FREE ELECTROCHEMICAL BIOSENSOR FOR ON-SITE DETECTION OF SULFUR MUSTARD

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Sulfur mustard (SM) is one among the most alarming chemical weapons, which represents still nowadays a critical threat. SM can be found as remnants of past wars in several contaminated sites, and the risk of its employment within the current scenario of ongoing wars and terrorist attacks is not negligible. Since a chemical attack is typically carried out by spreading SM into air, suitable detection methods are needed for the early detection of the airborne SM. Reference methods used for SM detection, such as mass spectroscopy and chromatography, allow revealing its presence in the environment at a trace level with high reliability, but they are not suitable for the on-site and fast monitoring of SM. With the aim to answer to these needs, herein we report the development of a paper-based miniaturised electrochemical biosensor for SM detection. The advantages of paper, such as versatility and the cost-effectiveness, make it an attractive support for the development of sensors. In this work, the use of filter paper allowed us to realise a ready/easy-to-use origami-like biosensor, based on the inhibition activity of SM toward choline oxidase. The enzyme and its substrate choline were preloaded onto the sensor, exploiting the absorptive properties of filter paper to entrap the biocomponents and thus resulting in a reagent-free biosensor. The inhibition extent was determined by amperometric monitoring of the enzymatic by-product H_2O_2, as reported in a previous work[1]. The sensor consisted in a screen-printed electrode (SPE) printed onto filter paper by using a graphite ink, which was modified with a carbon black/prussian blue composite in order to exploit its electrocatalytic properties toward H_2O_2 detection[2]. The origami-like sensor was obtained by overlaying two filter paper layers, i.e. the SPE and a paper pad, containing the preloaded reagents. The resulting origami-like biosensor was applied for the SM detection both in liquid phase and in aerosolised phase, to simulate the biosensor application for SM revealing in contaminated waters as well as for the detection of airborne SM. LODs of 1 mM and 20 mg/m^3 were obtained, respectively. This biosensor can represent a useful analytical tool for the early and in-field detection of SM, allowing for the real-time alarming of the military corps and civilians.

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P054

ALIZARINE RED S-BASE RECEPTOR FOR SIMULTANOUES DETERMINATION OF Fe(III) AND Al(III)

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A very cheap, disposable, differential sensor for the detection of Fe(III) and Al(III) is presented.

The selected solid support is an extremely cheap cellulose based sheet, the CC, the "*Colour Catcher®*", a product of the detergents market, distributed, in Italy, by *Grey* a partner of the Henkel company, which exhibits strong anion exchange properties. As response unit, we selected Alizarine Red S, an old and well known ligand for hard metal ions detection. The properties of this ligand for signalling metal ions was already applied successfully in the case of a device based on a triacetyl cellulose based film. Here, Alizarine Red S is anchored on CC, and the resulting optoprobe is called Aliz-CC@, where the operational concentration of active site was fixed equal c_{Aliz}=0.02 mmol/g. The stability and the reproducibility of the device were tested and the product was selected as possible differential sensor.

As an example in Figure 1 the colours of the Aliz-CC@ in water without any metal, and after contact with Al(III) and Fe(III) solutions, are shown.

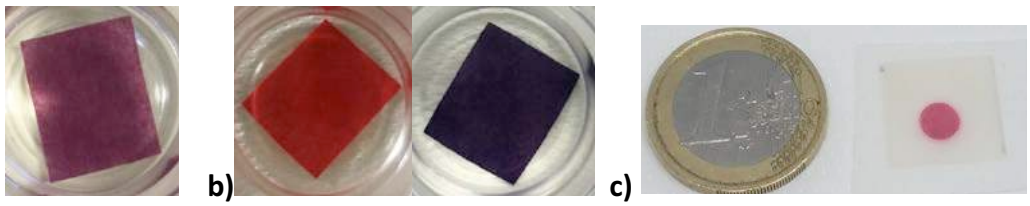

Figure 1. a) Aliz-CC@ in water, b) after contact with Al(III), Fe(III) solutions respectively, c) the same on cellulose acetate supported spots.

The Aliz-CC@ properties towards each metal ion was studied through sorption isotherms and kinetics experiments, based on the vis spectra of the solid phase. Under very mild stirring conditions, at pH 5.5 for acetate buffer, the sorption of Al(III), Fe(III) through formation, in both cases, of 1:1 complex is quantitative after one hour.

To detect the two cations, if simultaneously present in a solution, PLS (Partial Least Square Regression) has been used. A training set of different solutions with known amounts of the two metal ions was analysed to build a calibration model. A test set of independent experiments was employed to validate the model. A certificated sample (Sewage Sludge ERM®-CC136a) was also analysed as external set of data for validation. LOQs values around 1 10^{-3}mmol/g were found that correspond to operative LOQs around 10^{-7} M, if V_{sol}= 500 mL and $w_{Aliz\text{-}CC@}$ = 0.03g

Aliz-CC@ is a promising solid support to realise disposable devices. Further investigations are in progress to optimize its applicability, as shown for instance in Figure 1 c, where Aliz-CC@ spots are supported on acetate cellulose sheets.

P055

ENVIROMENTAL SENSOR FOR HEAVY METAL BASED ON ION IMPRINTED POLYMER

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Imprinting is the formation process of specific recognition cavities in a synthetic material. Thus, e.g. imprinted polymers allow specific recognition of analytes. These materials are versatile, scalable and cost-effective approach to create synthetic receptors. Precisely, ion imprinted polymers (IIPs) owing their unique selectivity and specificity have been successfully used for metal detection in environmental applications [1,2]. Firstly, monomers were selected according to their functionalities and their metal binding capacity. Afterwards, bulk IIP were prepared by controlled free radical polymerization in aqueous and in presence of the metal ion. Subsequently, the metal is removed from the IIP, which creates specific metal recognition sites. Then, the resulting IIP particles are immobilized on screen printed electrodes using carbodiimide crosslinker chemistry. IIP formulations were optimized by changing the functional monomer composition and choosing the best monomers that increase the sensor sensitivity towards the metal analyte. Characterisation of these materials was performed via dynamic light scattering, scanning electron microscopy (SEM) and X-Ray Fluorescence, respectively. Electrochemical determination of $Cu^{2+,}$ Co^{2+} and Pb^{2+} was achieved in water samples using differential pulse voltammetry (DPV).

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P056

STUDY OF PROCESS MARKERS DERIVING FROM DRYING TREATMENT OF PASTA USING A PEPTIDE BASED GAS SENSOR

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Pasta is a sample food made from water and durum wheat semolina. As increased in popularity of this food, studies endeavored to analyze the attributes that contribute to increase the quality. Pasta drying is of the most commonly studied aspect of pasta making because are a high capital investment and a most important aspect for determination of the quality of this product. The volatile compounds, responsible for the odor, can be informative about the raw material quality and their processing. In fact, the effect of the drying temperature on the pasta samples, unless controlled, can cause the formation of compounds that can derive from the Maillard reaction [2]. The aim of the work was to develop a methodology based on ZnO-peptide based QCMs array of gas sensors for monitoring of the drying process and relative formation of different compounds. The samples of pasta analyzed were commercial and of different price. Samples have been ground and analyzed with the gas sensor array and a GC-MS SPME method. The results obtained have been studied with the multivariate analysis, principal component analysis (PCA) and Partial least squares regression (PLS). Some molecules as Nonanal, Hexanal, Lactamide, and furans proved to be crucial in the differentiation of the commercial samples tested. These compounds could be used as pasta quality markers, alternatively to already recognized marker Furosine, or as process markers to keep the drying treatment under control. The gas sensor array was able to discriminate samples with different heat treatment markers.

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P057

A POCT FLUORESCENCE-BASED INTEGRATED PLATFORM AGAINST LIFE-THREATENING INFECTIONS

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Fluorescence-based immunoassays for sepsis biomarkers have been implemented on multichannel optical chips. The optical chip was designed in order to be used in a fluorescence module, which will be integrated in an innovative technological prototype for early, fast and reliable medical diagnosis of sepsis developed within the European Project Hemospec.

The fluorescence module makes use of a diffractive optical element (DOE) able to generate 13 parallel lines (each one in correspondence of each microchannel of the chip) when it is illuminated by a laser source. An array of 13 colored glass absorbing filters, faced on the sensitive part of a CCD camera, guarantees the parallel acquisition of the data. Each filter rejects the unwanted scattered excitation light and at the same time guides internally the collected fluorescence signal, coming from each microfluidic channel, by total internal reflection. The initial development of an in-Lab version of the fluorescent prototype on a small optical breadboard was accomplished after characterization and optimization of the custom DOE and of the absorption filters. A filter holder (Figure 1) was also designed in order to minimize any undesirable contributions such as stray light and cross-talks. A dedicated software for measurement, data elaboration and device management was created. All the hardware components and the software modules were optimized in order to be integrated in the final Hemospec fluorescence module, which was implemented and used for the detection of C-reactive protein (CRP) and suPAR (soluble urokinase-type plasminogen activator receptor) by the optimized immunoassays. Results will be presented on the detection of CRP and suPAR in spiked commercial plasma samples and in real plasma samples from patients.

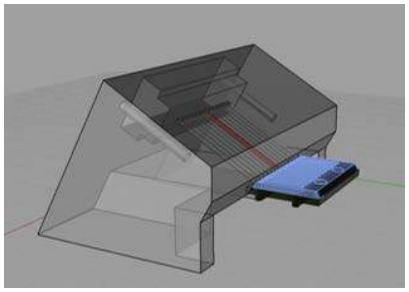

Figure 1. The filter holder faced to the microfluidic chip.

Acknowledgments. This research was supported by the European Community within the framework of the project Hemospec (FP7 - 611682).

P058

IMMOBILIZATION OF CARBONIC ANHYDRASE ON AuNPs DEPOSITED ONTO SILANIZED GLASS SUBSTRATE FOR HEAVY METALS DETECTION

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In recent years the increasing sensibility to environmental pollution problems has promoted the development of environmental "diagnostic" tools for early warning detection of pollution. The measurement of alteration in the structure or function of a biological macromolecule can represent an effective tool for detecting the presence of bioavailable pollutants and for screening the toxicity of environmental samples.
Nowadays, optical devices sensitive to both inorganic and organic pollutants are subject of study and research in view of their application in those sites where a continuous monitoring is required in the biomedical or environmental or industrial field.
Aim of this work was the realization of an optical biosensor based on enzyme inhibition for the detection of pollutants in environmental samples. The dynamic monitoring of the presence of chemical pollutants (responsible for the enzymatic inhibition) could be carried out by means of an optical investigation in the visible spectral range by monitoring the variation of the plasmonic peak typical of gold nanoparticles immobilized onto glass substrates [1,2]. A study about the development of metal (gold) nanoparticles chemically anchored by means of appropriate surface treatments onto glass substrates is reported.
In particular, glass substrates have been modified through different chemical silanization [3] strategies to optimize the adhesion of colloidal gold nanoparticles suitable to generate a plasmonic transducer for biosensing application. An optimized stabilization process through the use of heat treatment and deposition of polydopamine (PDA), is presented. This system will be used as platform for enzyme (carbonic anhydrase) immobilization. All preparation steps have been monitored by UV-Vis absorption spectroscopy and X-ray photoelectron spectroscopy (XPS). Preliminary results on detection of heavy metals are reported.

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P059

A novel easy to use and portable detection tool: a Lab-on-a-tip device for copper detection

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Sensing technologies have been highly boosted by the use of new technologies and smart materials, i.e. 3D printings and nanomaterials. In this way cost-effectiveness, functionality, sustainability and disposability have been improved, allowing the development of portable and easy-to-use sensing platforms for analytic purposes. Among the analytical methods, i.e. colorimetry, fluorimetry, chromatography, mass-spectroscopy and electrochemistry, the last one deserves a primary role as it is i) blind towards colored/turbid solutions, ii) easily delivered, iii) disposable, and iv) affordable. Moreover, the increasing use of filter paper to realize reagent-free platforms, helps electroanalytical tools in satisfying the ASSURED criteria established by WHO [1].
Here, we propose the development of a novel concept in de-centralized electroanalysis. A pipette tip has been adapted as the electrochemical cell to perform measurements, and it has been customized in order to introduce a three-configured μ-wire-electrodes. The extremely high portability of this lab-on-a-tip electrochemical sensor has been improved by its reagent-free approach: a small piece of cigarette filter has been inserted at the bottom of the tip, allowing both to load the media/reagents necessary for the assay (i.e HCl) and to purify complex matrices, preventing gross impurities, i.e. soil in river water, from interfering with the measurements. In order to demonstrate this novel approach, copper has been selected as the model analyte to be detected in river waters.
First the lab-on-a-tip has been characterized by cyclic voltammetry experiments, in a ferrocyanide/ferricyanide ($Fe(CN)_6^{4-}/Fe(CN)_6^{3-}$) solution, without the filter. After, they have been optimized some important features of the filter: the releasing properties of the preloaded reagent and the dipping time in this reagent.
Finally, copper has been detected by linear-sweep anodic stripping voltammetry, with a linear response in the range comprised between 50 and 300 ppb, a detection limit of 6.3 ppb and a regression equation $-0.097 + 0.01\ x$ (R^2=0.982).
The effectiveness of the platform has been confirmed by testing 50, 100, and 150 ppb Cu-spiked river water sample, with recovery value comprised between 92 and 103%.

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P060

NANOATRAZINE OPTICAL DETECTION FOR SMART AGRICULTURE

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The increasing democratic pressure, climate change, industrial globalization and the intensive use of resources of last decades represent nowadays a few main global challenges, being factors that generate a huge impact on the environment and people's health. Among human practices, agriculture is one of the main cause of environmental pollution since farming activities have been oriented toward the indiscriminate use of resources as land and water, high-tech machinery, and chemicals as pesticides and fertilizers, with the aim of producing ever higher food volumes. For these reasons, consumer demand for more sustainable agricultural practices and waste minimisation has become imperative in modern agrifood sector. In this context, smart agriculture entails the exploitation of different multifarious approaches based on more energy efficient and environmentally friendly cross-cutting technologies, including among others i) the use of nanomaterials to increase the dispersion and wettability of agricultural formulations, and ii) advanced diagnostic tools for the analysis of ground/drinking water to assess water matrices pollution level [1]. In this scenario, we presented the development of a whole-cell optical biosensor based on the green photosynthetic algae *Chlamydomonas reinhardtii* for the detection of nanoatrazine. This nanoherbicide is constituted of poly(ε-caprolactone) nanocapsules loaded with atrazine, a forefront nanoformulated herbicide with a high effective post-emergence herbicidal activity [2, 3]. The impact of nanoatrazine on algae growth, photosynthetic activity, and pigment content was investigated to highlight the effect of this nanoherbicide on specific interactions with the D1 plastoquinone binding niche of the photosystem II, as already exploited in the case of atrazine detection. Then, the experimental set up was optimised for nanoatrazine detection by following the variable fluorescence parameter $1\text{-}V_J$ calculated from the algae fluorescence response described by the Kautsky curve [4]. Thus, cell cultures at mid-point of exponential growth phase were immobilised on glass substrate with 0.1 % alginate/200 mM calcium chloride and incubated for 15 min with standard solutions of nanoatrazine in a concentration range from 0.5 to 200 nM. The obtained results evidenced that $1\text{-}V_J$ parameter decreased proportionally to the increase of nanoherbicide concentrations, allowing the construction of a calibration curve, using a linear regression described by the equation $y = 0.5200(\pm0.0005) - 0.0014(\pm0.0007)\ x$ ($R^2 = 0.9795$). A detection limit of 14 pM was obtained for I_{50} value (calculated as $2.6 \times \sigma \times I_{50}/100 - 2.6 \times \sigma$). Interference studies were achieved in the presence of 0.5 ppm copper (Cu^{2+}) and 10 ppb arsenic (AsIII), at safety limits provided by World Health Organization (WHO) in drinking water, indicating that the interfering species were not able to affect nanoatrazine analysis at the exploited concentrations. Matrix effect and recovery studies were also performed exploiting tap water as real matrix, highlighting a slight matrix-dependence and satisfactory recovery values of 103±16 % and 95.5±8.5 % for 75 and 125 nM of nanoatrazine. This study

demonstrated the suitability of the presented biosensor for its application in pollution level control of matrices of environmental and human health interest as tap water, due to agricultural practices.

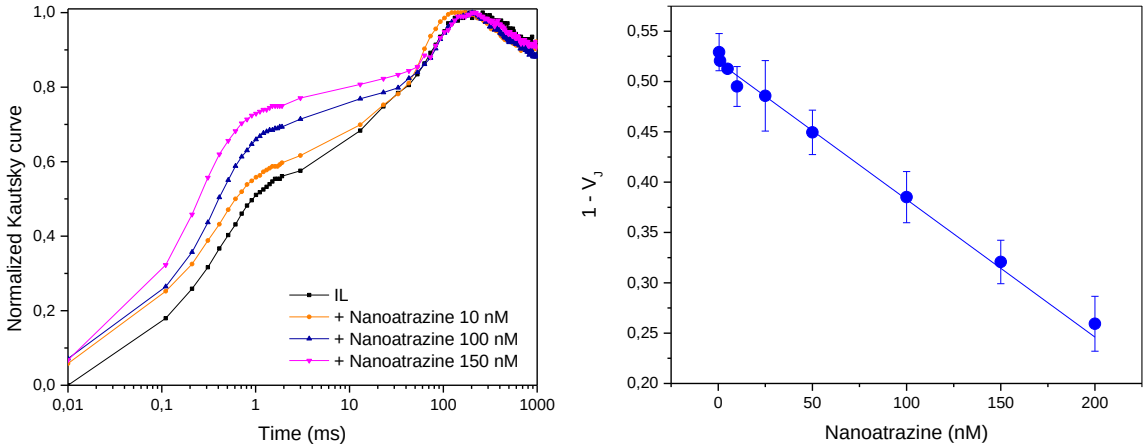

Figure 1. Left: Kautsky curves of *C. reinhardtii* in the presence of increasing concentrations of nanoatrazine (10, 100, and 150 nM as examples, incubation time 15 min). Right: Calibration curve with linear fit (n = 3).

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P061

HUMIC ACIDS PYROLYZED ONTO SILICA MICROPARTICLES FOR SPE OF BENZOTRIAZOLES AND BENZOTHIAZOLES FROM ENVIRONMENTAL WATERS

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This work describes the analytical application of a new carbon-based sorbent for solid-phase extraction (SPE). The material was obtained by pyrolysis (600°C, 1 h) of humic acids (HAs) onto silica microparticles (20 wt% HAs), which provided a silica-supported, mixed-mode carbonaceous phase consisting of aromatic structures bearing oxygenated functionalities. The material (HA-C@silica) was tested for fixed-bed SPE of 2 benzotriazoles and 3 benzothiazoles from natural waters, namely 1-H-benzotriazole, 5-methyl-benzotriazole, benzothiazole, 2-hydroxybenzothiazole, and methylthiobenzothiazole. These compounds are included in the list of emerging contaminants [1] and, at present, trigger limits have been fixed in surface water for benzotriazole and 5-methyl-benzotriazole (EQS-AA: 19 and 20 µg/L, respectively). The environmental concentration levels almost range from few to some tens micrograms per liter, and the few analytical methods currently available for their determination involve an enrichment step, mainly performed by SPE using co-polymers as mixed-mode phases [1]. In this study, SPE tests using HA-C@silica were performed in tap and raw river water samples (50-250 mL) spiked with each compound in the concentration range 1-50 µg/L. Quantitative adsorption was gained using 200 mg sorbent, working at the sample native pH, with a loading flow rate around 5 mL/min. After extraction, the analytes were simultaneously desorbed (1 mL/min) by 4 mL methanol, reduced to small volume (0.25 mL) under N_2 flow before HPLC-HESI-MS/MS analysis [2]. Recovery was satisfactory for all compounds, ranging from 70 to 127% in tap water and 70-114% in river water, with RSD values generally below 16% (n=3). The developed procedure provided enrichment factors up to 1000, thus allowing quantitation of benzotriazoles at concentrations far below the EQS-AA limits. The batch-to-batch reproducibility, evaluated by recovery tests on three independent preparations, was good (RSD < 12%). HA-C@silica proved to be an appealing sorbent for pre-concentration of these polar aromatics, it is easily produced by a common lab instrumentation starting from low-cost materials, and the preparation does not involve toxic/harmful chemicals. Due to its peculiar features, HA-C@silica is expected to give good performance in pre-concentration of other organic contaminants from environmental or biological matrices.

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P062

CHARACTERIZATION AND CHEMICAL PROFILING OF GREEN TEA SAMPLES USING CAPILLARY ELECTROPHORESIS COMBINED WITH CHEMOMETRICS

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Green tea (GT) is made from the leaves of *Camellia Sinensis* and is the most popular beverage in Asia because of its attractive aroma, taste and health promoting effects. The catechins content is associated to the biological value of tea and it could be used as chemical descriptor and potential indicator of the geographical origin [1]. Besides catechins, xanthines and in particular caffeine are important components of GT, due to their stimulating effects.
Cyclodextrin-modified micellar electrokinetic chromatography (CD-MEKC) was applied to the characterization of GT samples by evaluation of the quantitative profile of catechins and xanthines. The CD-MEKC method showed to be suitable for the simultaneous analysis of these compounds, presenting good performances in terms of selectivity, analysis time and possibility of chiral analysis. The enantioselective analysis made it possible to provide information on sample stability and manufacturing processes.
Data analysis was performed by different multivariate exploratory and discriminant techniques to differentiate GT samples according to geographical origin, which is an important factor in order to determine quality and reputation of a commercial GT product. In general, with exception of (-)-epicatechin gallate, the amount of all the compounds was found to be higher in Chinese GT samples compared to those from Japan.
The use of excitation–emission matrix fluorescence spectroscopy coupled with chemometric tools was proposed as alternative analytical approach.

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P063

STUDY OF THE ADSORPTION EQUILIBRIA OF A PHARMACEUTICAL RELEVANT PEPTIDE IN RP-LC THROUGH ADVANCED NUMERICAL MEANS

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Due to their biologic activity, many peptides are used in cosmetic, nutraceutical and pharmaceutical fields [1]. Usually, peptides are obtained by means of solid phase synthesis which, unfortunately, doesn't lead only to the main target molecule but to very complex mixtures [2]. The purification process is the bottleneck in the synthetic production of peptides, so it has to be optimized. Moreover, to purify industrial quantities of peptides, it is necessary to implement separation processes in a continuous manner, and this is feasible only knowing the optimal separation conditions in batch method. RP-LC is one of the most employed techniques for isolating the peptide of interest from the impurities and by-products deriving from synthesis [3].
In this work, a crude (=not purified) mixture of one octapeptide has been considered. Some preliminary gradient tests have been conducted to find out the best conditions for the separation of the peptide and the main impurity. Different mixtures of two mobile phases (0.02% TFA in MilliQ and 0.02% TFA in ACN) have been used during elution. Afterwards, the chromatographic profiles have been obtained also in isocratic conditions at different mobile phase compositions, chosen depending on gradient experiments. The shape of the profiles suggests that the adsorption isotherm is a convex upward type.
Using inverse method, an advanced numerical method which is particularly suitable when only small amounts of sample are available, experimental peaks have been fitted with different isotherm models; Langmuir isotherm gave the best results. The Langmuir isotherm parameters have been estimated for each fraction of organic modifier. It is known that the retention factor of a peptide, and therefore the isotherm parameters, are heavily affected by the organic solvent percentage [4]. This dependence has been evaluated; it has been found out that *b* (=adsorption equilibrium constant) follows an exponential trend and decreases if the organic modifier fraction increases.

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P064

COMPUTER-ASSISTED DEVELOPMENT OF RP-HPLC METHODS FOR THE ANALYSIS OF PLANT BIOACTIVE COMPOUNDS

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High performance liquid chromatography in reversed phase separation mode, generally coupled to mass spectrometry (RP-HPLC-MS), is the technique of choice for the identification and quantification of phenolic compounds in plants and plant-derived food products. The optimization of the HPLC methods is generally carried out by conventional trial-and-error approaches, requiring the screening of a variety of experimental conditions, which include column temperature, pH and composition of the mobile phases, and shape and duration of the gradient elution program.
This communication describes and discusses the results of our studies conducted for the computer-assisted development of RP-HPLC methods for the separation, identification and quantification of phenolic compounds extracted from plant tissues and plant-derived cosmetic and food product. The study has been conducted by a Design of Experiments (DoE) approach that allow the simultaneous optimization of gradient time (t_G), column temperature (T) and binary eluent composition on the basis of retention times and peak areas of the analytes of interest, obtained in twelve different experiments. These experiments consist in the linear gradient separations of the investigated samples performed at two different gradient times and column temperatures, using the aqueous component of the mobile phase at three different pH values.
The presentation describes the use of the above experimental data to construct 3-D resolution maps, which evaluate the influence of column temperature, mobile phase pH and composition, and gradient duration on the retention and resolution of a variety of analytes. In our study, 3-D resolution maps have been constructed using either mixtures of standard phenolic compounds or samples of these compounds extracted from plants tissues or plant-derived products. The goal of our study was to model the variations that can help for the better selection of the mobile phase composition and gradient elution mode, in order to improve peak resolution and to reduce the analysis time, using a limited number of experiments and, consequently, reduced amounts of expensive and environmentally harmful chemicals. Excellent correlation between simulated and experimental separations of phenolic compounds are demonstrated. The application of the above DoE approach to the separation, identification and quantification of phenolic compounds occurring in a variety of plants and plant-derived cosmetic, food, and dietary supplement are illustrated and discussed.

P065

EXTRACTION AND CLEAN-UP OF STEROID HORMONES FROM AQUEOUS PROTEIC MATRICES: A PRELIMINARY STUDY

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Steroid hormones are essential for various biological functions, however, at elevated levels they could have negative effects on human health, such as some hormone-dependent cancers. In clinical settings, determination of steroids levels is essential to diagnostic endocrine disorders. Historically, immunoassays have been used for analysis of steroids in biological fluids, but now chromatographic are preferred. The complexity of biological matrices and the low concentration of steroids in biological fluids (ng/mL levels) demand pre-concentration and clean-up before the chromatographic analysis. The aim of this work is the development of simple, fast and sensitive methods for the determination in biological matrices (plasma and urine) of four classes of steroid hormones: oestrogens, progestins, androgens and corticosteroids. Two different sorbent materials were tested for simultaneous clean-up and pre-concentration of these analytes: thermally condensed humic acids onto silica (HA-C@silica) and restricted access carbon nanotubes (RACNTs) [1,2]. A preliminary test (5 mL of 20 g/L Bovine Serum Albumin -BSA- aqueous solution in 10 mM phosphate buffer) performed on RACNTs and HA-C@silica (50 mg, 1 mL tubes) highlighted their abilities to exclude proteins, probably due to the electrostatic repulsion. Based on such findings, RACNTs and HA-C@silica are selected as sorbent materials for column solid-phase extraction of 15 steroids (estrone, 17β-estradiol, 17α-ethinyl estradiol, progesterone, hydroxyprogesterone, medroxyprogesterone acetate, testosterone, cortisone, hydrocortisone, prednisone, prednisolone, betamethasone, dexamethasone, triamcinolone acetonide, fluocinolone acetonide acetate) from BSA aqueous solutions in 10 mM phosphate buffer (1-5 mL) spiked in the range 0.125-1 µg/mL for each hormone. All analytes are eluted by methanol/acetonitrile and analysed by HPLC-UV. Further tests are ongoing, in order to evaluate the applicability of those materials in samples at lower concentration and in actual biological matrices.

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P066

DEVELOPMENT AND VALIDATION OF A MULTI-RESIDUE EXTRACTION METHOD FOR THE DETERMINATION OF ORGANIC MICROPOLLUTANTS IN SURFACE WATER

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The water pollution assessment to evaluate environmental quality standard on compliance with European Directive 2013/39/EU needs complex analytical approaches to satisfy legislation requirements about quantification of a wide range of pollutants, with different physicochemical properties and concentration levels (trace or ultra-trace). To accomplish this task, a multi-residue method for screening, quantification and confirmation of multi-class pollutants in surface water has been developed. It is based on an integrated approach where solid phase extraction (SPE), gas chromatography–mass spectrometry (GC–MS), gas chromatography–tandem mass spectrometry (GC–MS/MS) and liquid chromatography–tandem mass spectrometry (LC–MS/MS) are simultaneously employed. Target compounds, including several groups of emerging and persistent contaminants (as defined in the 2000/60/EC European Water Framework Directive) and, specifically, polycyclic aromatic hydrocarbons (PAH), phthalate, alkylphenols, polybrominated biphenyl ethers (PBDE), chlorophenols and chloroalkanes were investigated. The multi-residual method was validated according to DLG n°19/2010 with regards to two different concentration levels. According to the *Environmental Quality Standard (*EQS) they are defined as (i) the maximum concentration of a substance in natural water that does not affect the quality of water and (ii) the *limit of quantification* (LOQ), which must be lower than 1/3 of EQS.
Recovery rates of SPE were from 62 to 105%. Precision of method, calculated as relative standard deviation (RSD), was below 27% for most of tested compounds. In conclusion, this method allows for rapid and reliable determination of different classes of organic micropollutants present at trace and ultra-trace levels in complex water matrices, such as surface water.

P067

OPTIMIZATION AND VALIDATION OF A SPE-HPLC-PDA METHOD USING QUANTITATIVE STRUCTURE-RETENTION RELATIONSHIP BASED ON MAPPING THE HYDROPATHY FOR SIMULTANEOUS DETERMINATION OF DRUGS

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Optimization of the extraction of the analytes of interest from biological matrix is an important step in the development of an analytical method, because it will effect the overall sensitivity and selectivity of the method. Sample preparation will not only lead to highly concentrate extracts, but can remove potentially interferents, resulting in enhanced selectivity and a more reproducible method. Despite all these advantages, sample preparation is still regarded as time-consuming, laborious work, and there is much interest in simplifying this step. In an attempt to give rational interpretation to this concept, Molecular Dynamics simulations may be considered a useful technique which is able to describe the relationship between chemical properties and motion behaviour of an small molecule. So that, it may be used to encode and infer, through mathematical models, the chromatographic response parameters and descriptors of the analyte molecular structure. In the present work we analyzed the hydrophobicity and hydrophilicity properties of several non steroidal anti-inflammatory drugs (NSAIDs) by investigating the structural changes of the dynamic hydrogen bond network. In particular, the hydration of each analyte can be studied by investigating changes in the structure of the dynamic hydrogen bond network formed by the surrounding water molecules. This computational approach is innovated because takes into account the properties due to the dynamics of water molecules of hydratation, providing non-trivial information in a compact way. For each analytes, the method provides four theoretical indices that may be useful to describe the chemical-physical features: hydrophilicity, hydrophobicity, the distribution of negative and positive charge. The indices allow us to gather insight on the retention time and the percentage of recovery, inferring from the interactions between analyte and solid phase materials, and observe the similarity and dissimilarity of the adsorbent phases used. Five different sorbents are compared for recovery of (NSAIDs) using in SPE from human plasma samples.

The use of chemometric approaches allows to obtain the combination of the variables which provides the best recovery with a limited number of experiments. Finally we have developed and validated an HPLC-PDA method for simultaneous determination of this NSAIDs in biological fluids and applied in their routine analysis.

P068

IOHEXOL A NON-RADIOLABELED CONTRAST MEDIUM IN HUMAN PLASMA MEASURED BY ULTRA HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY (UHPLC) WITH DAD DETECTION

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Kidney function is an important determinant of mortality in patients with cirrhosis both before and after liver transplantation. Serum creatinine concentration has routinely provided the best performing endogenous marker of glomerular rate (GFR). However, neither the measurement of serum creatinine concentration nor the estimation of GFR is accurate in patients with cirrhosis. Iohexol or 5-[acetyl(2,3-dihydroxypropyl)amino]-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-1,3-benzenedicarboxamide, (Figure 1), is a non-ionic, iodinated, water soluble contrast medium of low osmolality, considered free from side effects in dogs [1]. Following intravenous injection, iohelol does not bind to plasma proteins and enters the urine through glomerular filtration undergoing no tubular secretion or reabsorption. Hence, it is a suitable marker for glomerular filtration rate determination [2].
In this study, a ultra high-performance liquid chromatographic (UHPLC) method using photodiode array detection and isocratic conditions was developed for the analysis of plasma iohexol concentrations.
Iohexol concentration in biological fluids were analyzed on a Poroshell C_{18} column under isocratic conditions.

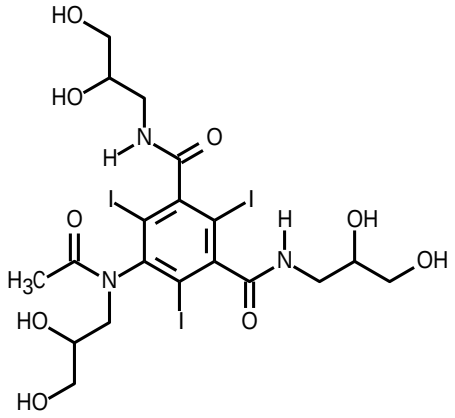

Figure 1. Chemical structure of iohexol.

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P069

SELECTIVITY OF SOLID PHASE MICROEXTRACTION FIBERS TOWARDS POLYCYCLIC AROMATIC HYDROCARBONS IN AIRBORNE PARTICULATE

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In this work the solid phase microextraction (SPME) procedure was investigate for the analysis of polycyclic aromatic hydrocarbons in atmospheric aerosol, as an environmental friendly alternative to the common approaches, reducing the laboratory generated waste and time for sample preparation [1].
Two SPME fibers with different polarity were investigated: a semi-polar polydimethylsiloxane/divinylbenzene (PDMS/DVB 65 µm) and a polar in polyacrylate (PA 85 µm). The extracted samples were analysed by Gas Chromatography with MS detection (GC/MS). The obtained results were compared in terms of the extraction yield of ten PAHs of environmental interest and selectivity towards C_{17} - C_{32} n-alkanes, as the most abundant interferences in ambient PM samples from urban sites.

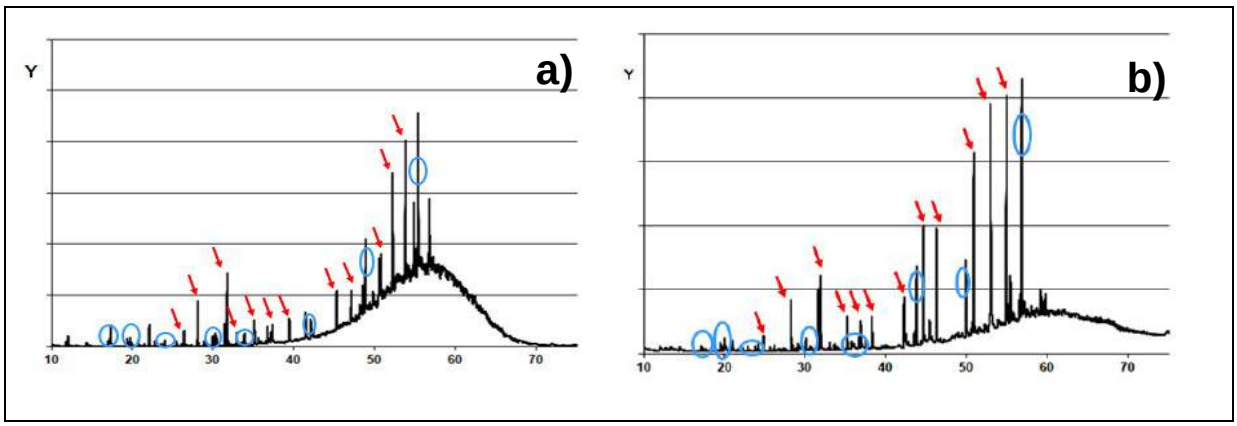

Figure 1. GC/MS signals of the same PM sample extracted with PDMS/DVB (a) and Polyacrylate (b) SPME fibers spiked with n-alkanes(red arrows) and PAHs (blue cyrcles) (0,25 ng μL^{-1}).

In comparison with the PDMS/DVB fiber, the Polyacrylate fiber selectively decreases the extraction for n-alkanes, so reducing strong interference from unresolved complex mixture of hydrocarbons, keeping still constant the general yield of PAHs. Therefore, PA seems a good candidate for purification processes of PM complex mixtures.

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P070

NEW ASCORBIC ACID-BASED SPECTROPHOTOMETRIC METHOD FOR MEASUREMENT OF THE OXIDATIVE POTENTIAL OF ATMOSPHERIC AEROSOL

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There is increasing evidence that the adverse effects of PM exposure to human health is mediated by inflammatory responses originated from PM-induced oxidative activity, leading to the generation of reactive oxygen species (ROS).
This work investigates the ascorbic acid (AA) method (OP_{AA}), that uses AA as a simplified model of the respiratory tract lining fluids (RTLF): redox active species present in PM catalyse ascorbate oxidation with subsequently ROS formation (Fig.1).
OP is measured as the rate of the ascorbate depletion, that is followed by spectrophotometric determination of the AA concentration (ε_{AA} = 14500 M^{-1} cm^{-1}) absorption at 265 nm [1].

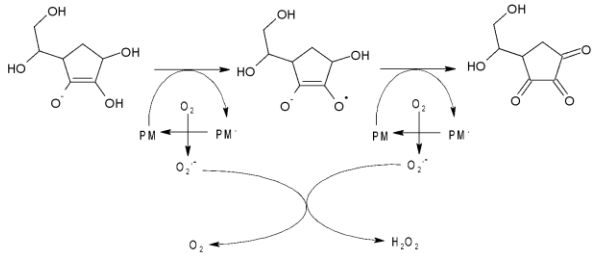

Figure 1. Scheme of AA oxidation with subsequently ROS formation.

In this study an alternative method is proposed based on the investigation of the production rate of the reaction products, such as hydrogen peroxide. For this purpose, a colorimetric method using 4-Nitrophenyl Boronic Acid (4-NPBA) as a selective probe for H_2O_2 is used [2].
H_2O_2 stoichiometrically converts 4-NPBA into 4-nitrophenol, which can be quantified by the spectrophotometric measurement of the absorption at 405 nm ($\varepsilon_{4\text{-NPBAPE}}$ = 19400 M^{-1} cm^{-1}).
In conclusion, a good agreement was found with complementary data obtained by following AA depletion and H_2O_2 production: the sum of the two species is approximately the same (~80%) as the initial concentration of AA added in the UV cuvette (100 µmol).

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P071

Zwitterionic teicoplanin chiral stationary phases on 2.0 µm and 2.7 µm superficially porous particles: chromatographic evaluation and comparison with teicoplanin on 1.9 µm fully porous particles.

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During the last years, the research in the enantioselective Ultra High Performance Chromatography (eUHPC) is going to push the limits of high efficient and ultrafast analyses. In this work, new UHPC-Chiral Stationary Phases (CSPs) were prepared by covalently bonding the teicoplanin selector (TE_A2-2) on Halo 2.0µm and 2.7µm Superficially Porous silica Particles (SPP) [1]. An innovative bonding protocol allowed to obtain a zwitterionic teicoplanin based CSP, which was used to produce the already known UHPC-FPP-Titan-Tzwitt 1.9 CSP based on Fully Porous monodispersed silica Particles (FPP) [2]. Columns with an internal diameter of 4.6 mm and different length (20, 50 and 100 mm) were packed with the three CSPs and characterized in terms of permeability, efficiency and thermodynamic under HILIC conditions. The kinetic performance were evaluated through the use of van Deemter curves. The column packed with sub-2mm CSP exhibited extremely high efficiencies on both achiral (>310,000 theoretical plates/meter, N/m; h_r: 1.61) and chiral compounds (>290,000 N/m; h_r: 1.72) under HILIC conditions. Aiming to explore the Ultra-High speed – Ultra-High Performance chromatography three 2-cm long columns were packed with the SPP-Halo 2.0 and on the FPP-Titan 1.9 and different racemic samples were injected at different flow-rate (1.0 – 8.0 mL/min) showing very high efficiency in the seconds time scale. The fastest baseline resolution (Rs: 2.0) was obtained on the SPP-Halo 2.0, injecting Haloxyfop at 8.0 mL/min, in only 3 seconds.

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P072

DEVELOPMENT OF A MICROEXTRACTION BY PACKED SORBENT-PROGRAMMED TEMPERATURE VAPORIZATION-GAS CHROMATOGRAPHY-TRIPLE QUADRUPOLE MASS SPECTROMETRY METHOD FOR PHTHALATE MONOESTERS ASSAY IN HUMAN URINE

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Phthalates esters are industrial compounds used for a variety of products such as personal care products, medical devices, pharmaceutical and packing materials. Due to the large use phthalates have become ubiquitous environmental contaminants. They are not chemically bounded to the products and for this they are easily released into the environment. These compounds are hazardous to human health, they are considered as endocrine distruptors and show activity on the reproductive system. They have also carcinogenic effects and adverse effects on liver and kidney. Phthalates esters are rapidly metabolized through hydrolysis to their respective phthalates monoesters, which are excreted through urine in their free or glucuronide-conjugated forms. To monitor the exposure to phthalates esters their urinary metabolites are generally used as biomarker [1].
The goal of the present work was the development of a fast and simple method based on alkyl chloroformate derivatization followed by microextraction by packed sorbent-programmed temperature vaporization-gas chromatography-triple quadrupole mass spectrometry (MEPS-PTV-GC-QqQ-MS) analysis [2] for the determination of monomethyl phthalate, monoethyl phyhalate, monoisobutyl phthalate, monobutyl phthalate, monocyclohexyl phthalate, monoethylhexyl phthalate, monoisononyl phthalate, monooctyl phthalate and monobenzyl phthalate in human urine. The signals were recorded in selected reaction monitoring (SRM) acquisition mode that allows the achievement of high specificity by selecting appropriate precursor–product ion couples. The derivatization reaction was directly carried out in urine with propyl chloroformate in order to obtain a fast and simple protocol. The extraction ability of five MEPS cartridges and seven elution solvents were evaluated in univariate mode, while the variables affecting the MEPS analysis, the PTV system and the derivatization reaction were optimized by the multivariate approach of "Experimental design" (DoE).

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P073

NON-mAb PROTEIN PURIFICATION BY MEANS OF SPLIT-INTEIN MEDIATED AFFINITY CHROMATOGRAPHY

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The purification of biomolecules is a very challenging process due to the presence of a very complex mixture of other cell culture components. In order to achieve high protein yield and purity, a so-called affinity chromatography step is widely used [1].
In this study, affinity chromatography has been performed through the use of split-inteins. The stationary phase resin is functionalized with a N-intein affinity tag, while the Protein of Interest (POI) has a C-intein tag. The capture of the POI from the crude lysate occurs due to the high affinity between these two tags [2]. The subsequent cleavage causes the release of the purified protein. After the elution, a regeneration step is required in order to get rid of the C-intein tag (see Figure 1).
This stationary affinity phase was tested and characterized.
During the first purification processes, proteins pre-purified by IMAC (Immobilized Metal Affinity Chromatography) as well as cell lysate were utilized. Then the results were compared and the purification protocol has been optimized for the crude lysate.
Afterwards, using a model based optimization [3], both a batch capture process and a two-column CaptureSMB process were simulated in order to predict the best conditions in terms of productivity and column capacity utilization.

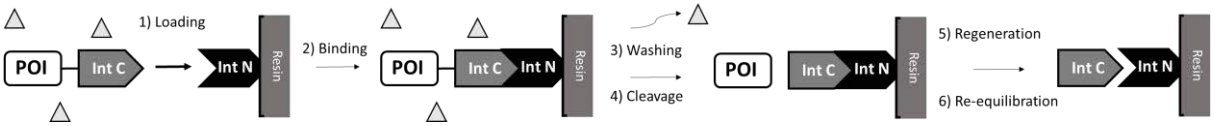

Figure 1. N-intein resin cycle: 1) Loading of the unpurified product, 2) binding of the POI to the resin, 3) removal of other components, 4) release of POI, 5) cleaning of the resin, 6) re-equilibration to the initial conditions.

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P074

ORTHOGONAL CHARACTERISATION OF NANOVESICLES THROUGH DIFFERENTIAL AND DENSITY GRADIENT CENTRIFUGATION HYPHENATED TO FLOW FIELD FLOW FRACTIONATION: DIFFERENCES IN SIZE, COMPOSITION AND RELATIVE ABUNDANCE OF DIFFERENT SPECIES IN EXOSOMAL SUBPOPULATIONS

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The ability of separating and enriching biologically relevant nanoparticles, such as exosomes, is crucial to better investigate specific molecular and signaling patterns: a soft separation step such as flow field-flow fractionation (F4), coupled with a multidetection platform, can add another dimension and provide uncorrelated information to the existing characterisation techniques and give insight to unravel such complex dynamics [1].
Our work was focused on HF5 (miniaturized, hollow-fiber F4), capable to achieve high performance and low dilution at the same time,[2] and its hyphenation to centrifugation techniques, which usually are the main steps of vesicles isolation from cell medium. We worked with samples obtained from culture medium of murine myoblasts (C_2C_{12} cell line), known to release different subsets of membrane-derived vesicles [3].
The first study involved two fractions obtained through differential ultracentrifugation (UC). The medium indeed is previously concentrated starting from whole medium through a series of UC steps, to obtain subpopulations of nano(exosomes) and microvesicles. Through an HF5 method employing UV and Laser Scattering as detectors, we characterised these subpopulations in terms of size, abundance and DNA/protein content; moreover, we showed that UC provides enrichment rather than separation and that microvesicles tend to hyper-aggregate and partially release nucleic matter. The quali-quantitative information we obtained from the fractographic profiles was improved with respect to NTA estimation.
In the second part of our study, we worked with C_2C_{12}-derived fractions obtained from Density Gradient Centrifugation (DGC); this technique is based on a fully orthogonal principle -since F4 does not separate by density- and allowed us to obtain uncorrelated information for each of the four fractions processed. The "second dimension" achieved with HF5 showed good promise in sorting particles with both different size and content, and allowed to identify the presence of fibrilloid nucleic matter.
This analytical bidimensional approach proved to be effective for the characterization of highly complex biological samples and could provide purified fractions for further biological characterization.

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P075

PHENOLS BIOCONVERSION BY IMMOBILIZED LACCASE IN A FLOW REACTOR

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Olive mill wastewater (OMW) is a serious environmental concern in the Mediterranean basin countries because of its high organic load (sugars, tannins, pectins, lipid and phenolic substances). Particularly, phenolic compounds are responsible of phytotoxic and antibacterial activity of OMW, which resist to biological degradation [1]. In addition, phenols exert a toxic effect on animal and human health.
Therefore, OMW must be treated to remove the phenolic fraction, before being discharged in receiving water bodies or used for irrigation purposes. The enzymatic treatment, compared to conventional methods and advanced oxidation processes (AOP), presents lower costs, higher selectivity and the possibility to operate over a wide concentrations range [2].
Oxidative enzymes like laccases (EC 1.10.3.2) are highly attractive for the treatment or removal of environmental and industrial pollutants due to their high efficiency, high selectivity and because they are an "eco-friendly" enzymes [3].
The aim of this research is to evaluate the efficiency of a laccase-bioreactor in the removal of the phenols from model aqueous solutions. A high-redox potential laccase from *Trametes versicolor* has been immobilized on a silica-chitosan support.
In the proposed method, the preparation of the support was carried out binding chitosan on microparticolate silica gel through the action of calcium ions which coordinate silanol and hydroxyl groups of chitosan. Laccase was first oxidized by periodate and then put in contact with the support for the immobilization. In this way, the immobilization via carbohydrates moiety did not cause inactivation of the enzyme. The coupled enzyme was then packed in a column and used in a flow system as immobilized enzyme reactor (IMER).
A preliminary study has been carried out for the optimization of pH and flow rate for the phenol-removal process.
Michaelis–Menten constants (apparent (V'max, K'm) and the inherent (V_{max}, K_m)) were determined by Lineweaver–Burk method in order to evaluate the influence of the substrate nature on the kinetic parameters of the system.

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P076

MAKING ORDER OF DNA NANODEVICES THROUGH DISORDER

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Proteins employ intrinsically disordered domains to gain control over their activity through purely entropic contribution. This discovery has recently challenged the original dogma that disorder plays against functional activity and that proteins require well-folded domains to function properly [1]. The possibility to mimic naturally occurring mechanisms to design and control synthetic molecular devices has led to tremendous advances in the fields of nanotechnology. In this vein, we report here a convenient and versatile approach to control the activity and response behaviour of synthetic nanodevices by rationally designing intrinsically disordered domains. We demonstrate that, similarly to intrinsically disordered proteins, such approach allows to finely modulate the affinity of a wide range of synthetic receptors through a purely entropic contribution in a highly versatile way without requiring any complex thermodynamic designing approach (Fig.1).

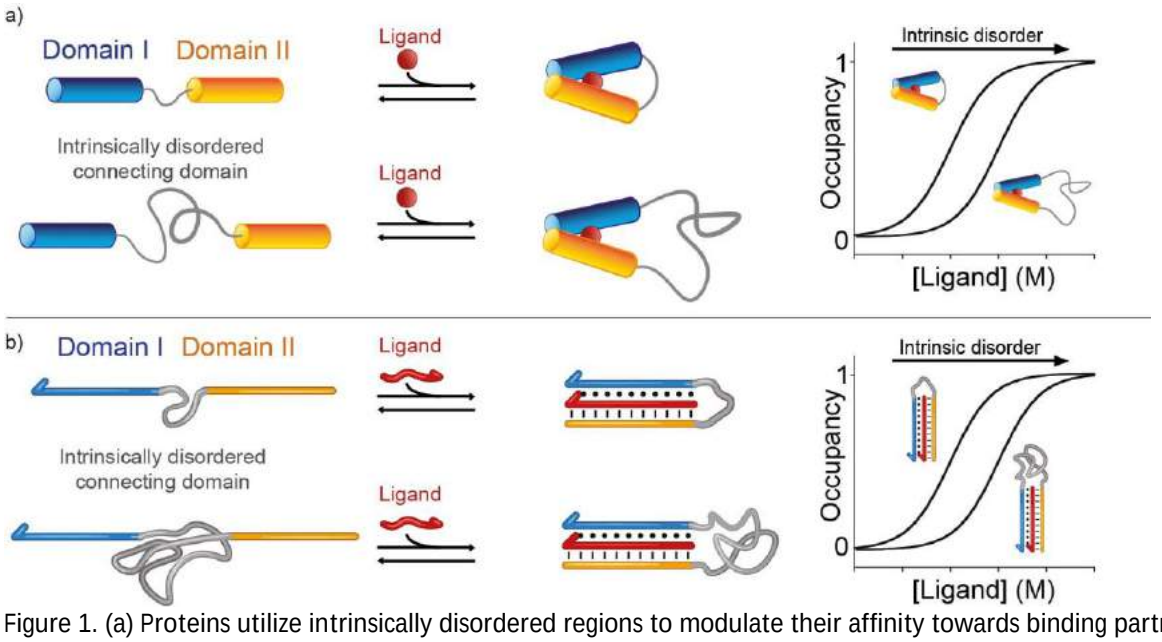

Figure 1. (a) Proteins utilize intrinsically disordered regions to modulate their affinity towards binding partners. (b) The same principle can be re-engineered into a synthetic DNA- Nanodevice.

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P077

A COLORIMETRIC APPROACH TO EASILY MEASURE GOD ENZYME ACTIVITY

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Glucose oxidase (GOD) is a dimeric enzyme which catalyzes the oxidation of β-D-glucose to gluconic lactone, concomitant with the reduction of oxygen to hydrogen peroxide. This enzyme, given the high number of turnover and high stability, is an excellent candidate as marker in ELISA. Although this potential it is poorly exploited. In fact, a typical glucose oxidase measurement requires the saturation of the reaction buffer with oxygen, the presence of peroxidase (POD), as additional enzyme, and a chromogenic substrate (i.e. ABTS, o-dianisidine). In this way, the hydrogen peroxide produced by GOD is used by the second enzyme to convert the substrate to its oxidized form, presenting a strong absorption at an established wavelength. The reactions involved are the following:

$$\text{D-glucose} + GOD_{ox} + H_2O \rightarrow GOD_{red} + \text{gluconic lactone}$$

$$GOD_{red} + O_2 \rightarrow H_2O_2 + GOD_{ox}$$

$$H_2O_2 + \text{dye-}H_2\ (\text{colorless}) \xrightarrow{POD} \text{dye (colored)} + 2\,H_2O$$

In this work a more simple approach to measure GOD activity, avoiding the use of an additional enzyme and the tedious saturation with oxygen of the reaction buffer, is presented. The strategy involves two sequential reactions:

$$GOD_{red} + PMS_{ox} \rightarrow GOD_{ox} + PMS_{red}$$

$$PMS_{red} + 2\,Fe(CN)_{6ox}\ (\text{colored}) \rightarrow PMS_{ox}\ (\text{which cycles } \textit{via} \text{ the reaction}) + 2\,Fe(CN)_{6red}\ (\text{colorless})$$

After optimization of PMS_{ox} and $Fe(CN)_{6ox}$ concentrations, we tested different amount of GOD and for each amount a linear decrease of the absorbance (at 420 nm) was recorded for a fixed interval time (15 min). The absorbance variations ($Abs_{t=0} - Abs_{t=15}$) were used to construct a calibration curve for glucose oxidase. Under these experimental conditions we are able to detect 30 mU/mL, as the low concentration. The next step will be the use of GOD enzyme as marker in an ELISA assay, exploiting this binary redox configuration.

P078

STRATEGIES TO IMPROVE THE SENSITIVITY OF AN ELIME ASSAY FOR THE DETECTION OF *CAMPYLOBACTER*

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Campylobacter is an important cause of acute bacterial diseases in humans worldwide. Many bacterial species in the genus of *Campylobacter* are considered harmful and may cause several infectious diseases, but most infections (about 90%) are caused by C. *jejuni* and C. *coli* species.
Conventional bacterial testing methods rely on specific microbiological media to isolate and enumerate viable bacterial cells in food. These traditional methods are very sensitive and inexpensive, but require several days to generate results because they rely on the ability of microorganisms to multiply to produce visible colonies. Biosensors potentially provide a powerful tools to detect *Campylobacter* spp. with the advantages of rapidity, sensitivity and specificity.
In this work strategies to improve the sensitivity of an ELIME (Enzyme-Linked Immuno Magnetic Electrochemical) assay to detect *Campylobacter* are presented. The system is based on the use of Magnetic beads (MBs), coupled to a strip of eight-magnetized screen-printed electrodes which support a sandwich immunological chain.
Compared to the ELIME assay already developed last year [1], the sensitivity has been improved by preparing pure broth-cultures of *C. jejuni and coli* (used as calibrators) in Bolton Broth (BBH), a specific medium for *Campylobacter* growth. In fact, we found in literature that the composition of the culture medium influence the antigen expression [2] and then the successive interaction with the antibody, used as bio-recognition element in our assay. Different antibodies were screened as a function of the growth medium and of cellular treatment (i.e. whole cells inactivated with NaN_3 or heat killed cells), in order to select the best conditions for the ELIME assay. The assay was designed so that the two sequential incubations for the immuno-recognition events (the first between *Campylobacter* and the capture antibody on MBs surface, and the second one between *Campylobacter* and the detection antibody conjugated with AP or HRP) occur in a single step of 1 h.

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P079

RULES TO PREPARE PEPTIDE-IMPRINTED NANOGELS WITH HIGH-AFFINITY BINDING SUITABLE FOR SENSING AND ASSAYS BY PRECIPITATION POLYMERIZATION

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Molecular imprinting is a technique for preparing polymeric scaffolds (Molecularly Imprinted Polymers, MIPs) that function as synthetic receptors and show affinity and selectivity towards a target analyte [1]. The most attractive characteristic of MIPs is the possibility to tailor the binding selectivity so to gain recognition levels on the par of biological receptors. When MIPs are downsized to the nanoscale (nanoMIPs), they show an increase in the number of accessible imprinted binding cavities per material weight and an enhanced molecular recognition ability, leading to faster binding kinetics, higher affinity and selectivity [2,3], thus strengthening the resemblance to antibodies and natural receptors.
Being the recognition properties of the nanoMIPs strictly correlated to the effective formation of the imprints in the chosen synthetic conditions, a deeper comprehension of the polymerization at the nanoscale is required.
In order to fill this lack, we studied the best conditions to form imprints at the nanoscale when the synthesis occurs by a precipitation polymerization protocol by means of an one-pot synthesis *via* free radical initiation in aqueous solution, using as target analyte the peptide of Troponin I, clinical marker of cardiac failure. By exploring a range of monomers combinations, polyacrylamide-based MIP nanogels having homogeneous nano-dimensions and a low number of binding sites per nanoparticle were synthesized.
To this purpose, we evaluated the influence of the monomer composition and the total monomers to template molar ratio on the hydrodynamic sizes and on the recognition properties, respectively, defining the conditions to tune the nanoMIP dimensions (from 60 to >600 nm) and to improve the efficacy of the imprinting process.
In the light of the achieved results, the present work contributes to define the best conditions to obtain imprinted peptides at the nanoscale and impact on the production of synthetic recognition materials suitable for sensing and assays.

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P080

QUANTITATIVE ANALYSES OF PROTEIN PROFILING TO STUDY THE DUAL PROTECTIVE/DAMAGING EFFECT OF 4-HYDROXYNONENAL (HNE) ON THE INTESTINAL BARRIER

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4-Hydroxy-*trans*-2-nonenal (HNE) is a molecule derived from lipid peroxidation of PUFAs and is involved in some damaging and beneficial effects, depending on the aldehyde concentration. Hence HNE is a multifactorial molecule and its molecular mechanisms have been so far studied using targeted approaches such as qPCR and Western blot analyses. As an example, in cardiomyocytes, HNE is protective against ischemia at concentration lower than 20 μM and the effect is due to a Nrf2/ARE pathway evidenced by monitoring an increase of antioxidant enzymes by PCR/WB [4].
In order to better understand the cellular mechanisms modulated by HNE and to identify novel targets, aim of the present work was to use an untargeted approach based on label free quantitative proteomic approaches [2], to investigate the cellular pathways modulated by HNE.
Extracted proteins from CaCo-2 cells treated with HNE at different physiopathological concentrations (0.1 – 100 μM) were digested by proteolytic enzymes. The peptide mixture was analysed in triplicate by a high resolution mass spectrometer coupled with a nano liquid chromatography system (Orbitrap Fusion™ Tribrid™ Mass Spectrometer). The raw data were analysed by quantitative and statistical software and Gene Ontology and pathways analyses tools (MaxQuant, Perseus, Proteome Discoverer, Cytoscape).
This quantitative approach allowed the description of differentially expressed proteins and in depth characterization of differentially regulated pathways during the HNE treatment versus controls. The involved pathways were in depth analysed, focusing on the ones connected with Nrf2, oxidation metabolism, cell proliferation and inflammation to describe the HNE effect on intestinal barrier. Cellular pathways involved in toxic response were detected at higher concentrations.
In conclusion quantitative analyses of protein profiling was found as suitable tool to investigate the molecular pathways modulated by HNE at different concentrations which well explain its dual action. Protein targets and pathways involved in the cellular response at low dose of HNE will be considered for the design of novel bioactive compounds.

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P081

QUALITY BY DESIGN-DRIVEN OPTIMIZATION OF DRIED BLOOD SPOT EXTRACTION FOR A BIOANALYTICAL LC–MS METHOD

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Dried Blood Spot (DBS) extraction satisfies several prerequisites for an effective sample preparation technique such as easy storage, shipment and logistics. Indeed, the DBS has been reported to be stable under ambient conditions and do not need any freezing; it is thereby cheap and hardly affected by biohazard contaminations. Moreover, this technique can be automated and thus included among high throughput extraction methods. Other evident advantages are the low sample consumption and microsampling, especially for the pharmaceutical and newborn clinical fields. In bioanalysis, liquid chromatography coupled to mass spectrometry in the multiple reaction monitoring mode (LC-MRM/MS) has been established as the technique of choice for the quantification of pharmaceuticals in biological matrices [1]. Both adequate selectivity by detecting compound-specific mass transitions and short analysis time can be achieved by LC-MS techniques. The development of analytical methods based on the recent principles of Quality by Design (QbD) has been gaining popularity due to enhanced understanding of the effects of critical method parameters, greater flexibility and enhanced method performance. In this study, QbD was applied for investigating in a systematic way the effect of the different parameters involved in the extraction efficiency from DBS of protease inhibitors. This approach made it possible to identify the design space, a multidimensional region where the specified quality of the extraction was obtained with a chosen probability. The extent of DBS possibilities was widely exploited by QbD, which allowed a rational development and an in-depth understanding of the extraction method.

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P082

MULTI-OMICS PROFILING OF PANCREATIC CANCER STEM-LIKE CELLS

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Pancreatic ductal adenocarcinoma (PDAC), one of the most aggressive solid tumors of the pancreas, is characterized by a remarkable resistance that also depends on the presence of the so-called pancreatic cancer stem-like cells (PCSCs) [1]. It is evident that, to make an impact on pancreatic cancer, it is necessary to eradicate CSCs with targeted therapies and, for this reason, a complete molecular characterization of CSC biology is fundamental.
In this work MIAPaCa-2, PaCa3 and Panc-1 CSCs and parental cells were cultivated and subjected to metabolomics and proteomic analyses. Different protocols have been evaluated to improve the identification of metabolites from adherent pancreatic cancer cells and suspended CSCs. In particular, different extraction approaches based on methanol:water, and methanol:chloroform; as well as different derivatization protocols based on Ethyl chloroformate, N,O-bis(trimethylsilyl) trifluoroacetamide and Methoxamine, have been evaluated and compared.
The results obtained indicate that CSCs are characterized by downregulation of succinate, fumarate, and malate and by upregulation of glutamate, in comparison to the parental cell lines. A reduction of Krebs cycle intermediates and an increase of a Krebs cycle-related metabolite may suggest a switch to a less oxidative metabolism. The results of the proteomic analyses are still in the collection phase. Preliminary data suggest that a total of 121, 188 and 186 proteins are modulated in Panc-1, PaCa-3 and MIA PaCa-2 CSCs as compared to the parental cells with p-value ≤ 0.05 and fold change ≥ 1.5, respectively.
Altogether the findings obtained may clarify some critical aspects of the metabolic network signature of PDAC and may suggest metabolites and proteins from which biomarkers and therapeutic targets can be identified. Further analysis of biological replicates and validation of results are required to confirm our preliminary data.

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P083

TIME MONITORING OF ENDURANCE ATHLETES' URINARY STEROIDAL PROFILE

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In 2014, the World Anti-Doping Agency (WADA) introduced the Steroidal Module of the Athlete Biological Passport [1]. In a previous work [2], we highlighted the performance's improvement that arose from using a multivariate approach - based on identical biomarkers - with respect to the univariate method currently in use. In the present study, we investigated the effect of physical training and fatigue on the athletes' urinary steroidal profile (USP). Two male endurance athletes (i.e., a marathone- and a mountain runners) were monitored during the time period preceding the competition. From two to three samples per day were collected – in the morning, in the evening and after the training - and analyzed by means of GC-MS; a total of 18 endogenous androgenic anabolic steroids (EAAS) were quantified. A PCA model was built using all the "reference samples" (those collected in non-training days). The after-training samples were used to test the model and the diagnostic Hotelling's T^2 vs Q residuals plot was employed to investigate the presence of outliers. The profiles associated to strong physical efforts (long distances and high intensity trainings) resulted statistically different from the reference model. In conclusion, the physical effort represents a bias factor in the USP evaluation that should be considered to avoid the occurrence of false positive anti-doping screening testing.

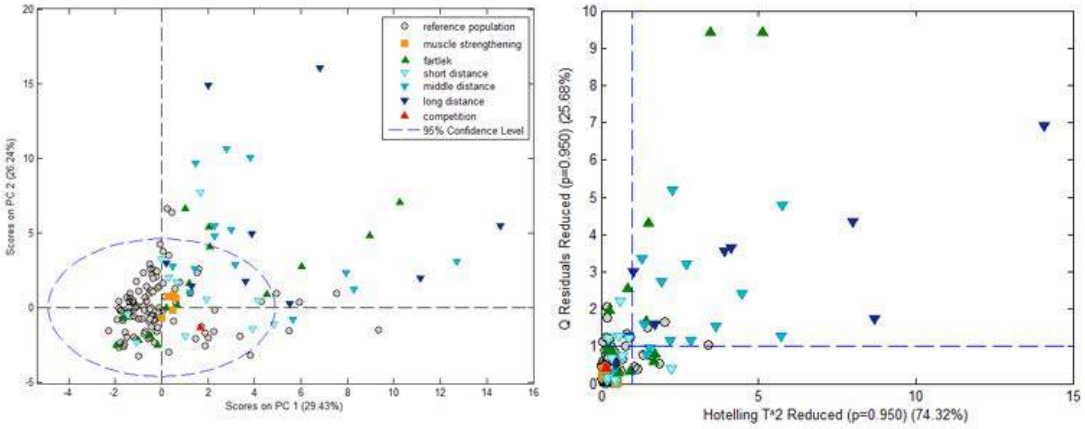

Figure 1. Scores plot (left) and Hotelling's plot (right) of the marathoner's dataset

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P084

SILVER NANOPARTICLES: A POSSIBLE VERSATILE COLORIMETRIC LABEL IN LATERAL FLOW IMMUNOASSAY

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In the last decades, huge efforts have been made to develop portable, affordable and user-friendly systems for point-of-need testing. Among these systems, the Lateral Flow ImmunoAssay (LFIA), also known as immunochromatographic strip test, is one of the most successful analytical format for point-of-need analysis, because it requires unskilled personnel and no infrastructure to be performed [1].
In a typical LFIA, the sample and a suitable label flow by capillary forces along an analytical porous membrane that contains immobilized reagents with molecular recognition properties, placed in specific area called Test line and Control line. The occurring of immunoreactions leads to the development of detectable bands in correspondence of these lines, due to the accumulation of the label in such zones.
Labels hold a very important task in LFIA because without them it would not be possible to detect the formed immunocomplexes on Test and Control lines. Moreover, the choice of the labels and the corresponding detection method directly affects the LFIA performances.
Historically, the LFIA was specifically design to allow the naked-eye detectability of the signals; therefore, the first LFIA labels had to ensure this kind of detection.
Gold nanoparticles (GNPs) have become the most extensively used labelling system for LFIA, because of their simple preparation, easy conjugation to antibodies, high extinction coefficients and strong surface plasmon resonance (SPR) band in the visible spectroscopy region (around 520 nanometers).
These formidable peculiarities have partly limited the study and the use of other colorimetric labels in LFIA. However, other noble metal nanoparticles, such as silver, are of considerable interest thanks to their optical properties, as well.
Silver nanostructures have received much focus recently due to their unique SPR properties and significant application prospects including biosensing and chemosensing [2].
In this communication, the possible use of silver nanostructure as label in LFIA will be discussed underling the major advantages and drawbacks.

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P085

DETERMINATION OF PROSTAGLANDINE-LIKE MARKERS FOR OXIDATIVE STRESS IN HUMAN URINE BY SPE-UHPLC-MS/MS

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Oxidative stress is caused by an imbalance between exposure to free radicals, like Reactive Oxygen Species (ROS) and antioxidant defenses and enzymes;
Oxidative modifications of highly reactive cysteine residues in several target proteins such as tyrosine phosphatase and thioredoxin-related proteins control the functions of relevant molecules, and thereby play an important role in signal transmission. Advanced glycation endproducts (AGEs) gradually accumulate with aging and are involved in the development of diabetic complications, Alzheimer's disease, and arteriosclerosis. Therefore, it should be easy to understand how important the estimating of oxidative stress level is.
Several molecules have been proposed as markers for the evaluation of oxidative stress: the challenge is the determination and quantification of specific markers, represented in many of the cases by derivate molecules from their oxidative pathway [1].
Isoprostanes are prostaglandin (PG) –like substances that are produced in vivo independently of cyclooxygenase (COX) enzymes, primarily by free radical- induced peroxidation of arachidonic acid, thus being a direct indicator of oxidative stress levels [2]. We focused on the measurement of two different analytes, 8-iso-prostaglandine-F2α and 5iPF2α-IV. On the other hand, it is common knowledge that the use of urine samples is fundamental in the recognition of substances derived from metabolic pathways [3].
The aim of this study was to provide an accurate and reliable method to evaluate the oxidative stress levels in human subjects. In this work, an analytical method for the determination of Isoprostanes was carried out by using an UHPLC-MS/MS system with a SPE clean up procedure for urine matrix. The presented method was developed and validated on the target analytes in order to achieve the best performances in term of sensitivity and repeatability in order to assess the oxidative stress level for further studies on the relationship between nutrition and health [4].

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P086

NOVEL CARBON NITRIDE NANOPARTICLES AS CUSTOMIZABLE FLUORESCENT PROBES FOR IMMUNO-ANALYTICAL ASSAYS

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Among the immuno-analytical assays, the homogenous FRET-based tests are promising as a diagnostic tool due to the intrinsic advantages of working in solution, their simplicity, specificity and sensitivity. Carbon nitride nanoparticles (CNNPs) have been employed as fluorescent probes owing to their unique properties such as low cost synthesis, high hydrosolubility and good quantum yield.[1] This work examines the properties of novel CNNPs, synthesized from thermal condensation of urea and lysine, as convenient probes for developing fluorescence quenching immunoassays. CNNPs have never been reported in this kind of applications, at the moment. The CNNPs properties were widely investigated, their structure was characterized by means of IR spectroscopy and TEM microscopy, their UV-vis absorption and fluorescence features were also studied in deep. In the model quenching test set up, the CNNP emits in the visible range (420-460 nm) when excited under UV irradiation (a). Gold nanoparticles (GNPs) are employed for their efficiency in quenching the CNNPs photoluminescence (PL) by a resonant energy transfer when these are kept at a convenient distance, i.e. the distance achieved by the antibody-antigen complex formation. In order to achieve a specific recognition-related signal, the CNNP and the GNP are conjugated with an antigen and with the corresponding antibody, respectively. In the absence of the analyte (antigen), the decrease of PL in the presence of the GNP-antibody conjugate is due to the FRET specific effect (b), while in the presence of the analyte the PL emission increases proportionally to its concentration (c). The PL yield and the availability of surface functional groups on the CNNPs were optimized varying the synthesis parameters. A successful bio-conjugation of the exposed groups with model antigens was then achieved. The synthesis approach here reported is versatile and allows to design nanoparticles with different desired surface functionalities, suitable as novel probes in effective 'positive readout' immuno-analytical tests.

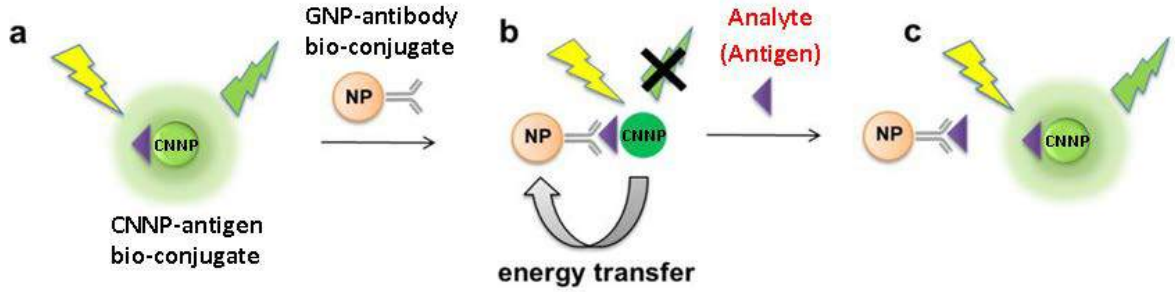

Figure 1. CNNPs employed as fluorescent probes in a model immuno-analytical FRET-based quenching test.

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P087

DEVELOPMENT OF AN ANALYTICAL STRATEGY FOR THE METAPROTEOMIC INVESTIGATION OF ATMOSPHERIC BIOAEROSOL

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Metaproteomic analysis of air particulate matter provides information about the properties of bioaerosols in the atmosphere and their influence on climate and public health [1].
In this work, a method for the extraction and analysis of proteins in airborne particulate matter from quartz microfiber filters was developed. Filters were reduced to fine pieces. Different protein extraction procedures were tested using 50 mmol L-1 tris-HCl (pH 8.8) with protease inhibitors and added with a) 1% sodium dodecyl sulfate (SDS), ethylenediaminetetraacetic acid (EDTA) and 1,4-dithiothreitol; b) 192 mmol L-1 glycine, 0.1 % SDS; glass beads with c) 1% SDS; d) 1% sodium deoxycholate; e) 0.5 % sodium dodecanoate. The optimization was performed spiking the filter with BSA at different concentrations. Protocols a-d required a precipitation step to remove SDS and EDTA and resulted not compatible with protein trace analysis. As size exclusion chromatography was previously applied to glass fibre filters [2], a filter aided sample preparation protocol was tested, but it was not suitable due to the presence of carbon in the extract. Protocols d and e exploited detergents compatible with protein digestion and can be precipitated by acidification [3].
The developed method is based on shotgun proteomics: proteins were digested by trypsin, separated by nanoHPLC and analysed by high resolution tandem mass spectrometry and bioinformatics.
The final method was tested for extraction of proteins from spores of ubiquitous bacteria species and used for the metaproteomics characterization of filters from environmental sampling (composting plants, waste-water treatment plants, livestock holdings and farms).

Acknowledgments:
This work was funded by INAIL within the project BRIC ID23.

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P088

HIGH-THROUGHPUT SCREENING OF HEMOGLOBINOPATHIES

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The coupling of thermogravimetry and chemometrics proved to be an innovative and accurate method to screen for thalassemia [1].
Thermal behavior of blood has been studied to improve bioanalytical investigations in hematology and to develop an alternative diagnostic tool able to provide a high- throughput prediction of hemoglobinopaties.
In this study, the TGA followed by multivariate statistical analysis was used to investigate blood samples in order to develop classification models with high predictive capacity for the screening of β-Thalassemia and Sickle Cell Disorders (SCD), the most widespread among all hemoglobinopathies, characterized by complex and heterogeneous clinical and hematological pictures. To this aim, a pattern recognition algorithm based on a discriminant method, Partial Least Squares – Discriminant Analysis (PLS-DA), was employed.
Whole blood samples from healthy individuals and anemic patients (thalassemic and sickle cells) were analyzed by thermobalance and the resulting TG curves were studied by Principal Component Analysis (PCA) so as to highlight a possible correlation among the thermal profiles of the three populations according to a different amount of water content and corpuscular fraction. Moreover, with the aim of associate the thermal profiles to diseases, the collected data set was used to build and validate two PLS-DA models of prediction: the first, to identify sickle cells patients and healthy donors and a second model to identify the hemoglobinopathies (thalassemia and sickle cells anemia). To optimize the models, as several variability sources can hinder their performance, different kinds of TG curves pre-treatments were tested.
The optimized and validated models permitted to recognize healthy, thalassemic and sickle cells individuals proving their high prediction capability in the early diagnosis of patients with different clinical pictures. Achieved results suggest the possibility to use the TGA/Chemometrics approach as high-throughput screening method for the hemoglobinopathies detection.

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P089

EVALUATION OF AN ELIME ASSAY TO REVEAL THE PRESENCE OF HEPATITITIS A IN DRINKING WATER

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Water-borne viral diseases pose high risks for public health worldwide. Urban wastewaters contain large number of pathogenic viruses, and full removal of virus particles cannot be guaranteed by conventional wastewater treatments. Presently, water quality indicators rely on bacterial fecal indicators, which do not provide adequate information about the presence of pathogenic viruses. Current legislation for microbial contamination in food products and for hygiene in primary production (EC 2073/2005, EC 853/2004, EC 852/2004) does not include any specific provision on enteric viruses in waters used in food production environments or for irrigation purposes. The currently available tests for virus detection, based on molecular biology, are expensive and labor intensive, thus limited to laboratories with suitable equipment and well-trained personnel. Nevertheless, the protection of water networks against pathogenic viruses is crucial. In this work, a cost effective and rapid system for Hepatitis A virus (HAV) monitoring in different freshwater bodies is designed. An electrochemical sandwich Enzyme Linked Immuno Magnetic assays (ELIME) is proposed [1]. The system is based on the use of Goat Anti-Mouse IgG magnetic beads as solid support for the immunochemical chain, and screen-printed electrodes as a sensing platform. This rapid, sensitive and low-cost analysis method involves the use of a portable instrument, able to perform measurements directly in the field. Using these ELIME assays, a quantitative determination of HAV can be achieved with a detection limit of 0.4 genome copies /mL. The proposed system was successfully applied to detect HAV in drinking water. Results obtained on spiked samples were compared to those obtained by the standardized qRT-PCR analysis (ISO 15216-1) commonly applied to assess HAV presence in water samples.

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P090

PHARMACOKINETICS OF GEMCITABINE HYDROCHLORIDE AND IRINOTECAN HYDROCHLORIDE ALONE AND IN COMBINATION IN RAT PLASMA BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-DIODE ARRAY DETECTOR

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This communication reports an easy and quick HPLC-PDA method for the simultaneous analysis of Irinotecan Hydrochloride and Gemcitabine Hydrochloride in rat plasma samples both after single drug administration and drugs association. Gemcitabine Hydrochloride is commonly administered to treat non-small cell lung cancer (NSCLC), pancreatic adenocarcinoma, and in combination with paclitaxel for the treatment of breast cancer in the metastatic phase. Additionally Irinotecan Hydrochloride was used to treat colorectal cancer (CRC), gynecological cancers, carcinomas, non-small cell and small cell lung cancer. The drugs were detected simultaneously by using a Zorbax Extend C-18 column (250 mm × 4.6 mm; 5 μm particle size) in gradient elution mode. The chromatographic analysis was performed in 15 minutes. The analytical method was calibrated and validated from 0.1 to 18 μg/mL for both drugs. Rat plasma was used as biological samples during the analysis; while the 3-methylxanthine was used as internal standard. The performance of analytical method was further tested in rat plasma samples collected after single dose administration of drug or their association. Results demonstrated that HPLC-PDA method allows to detect the drugs in the range of concentrations herein reported and the analytical method is accurate and selective. The limit of quantification of the method was 0.1 μg/mL. These values are similar or little higher to data published in literature, which are performed using sophisticated and expensive detectors such as mass spectrometer, and wich consider merely only one drug and not their association. The weighted-matrix matched standard curves showed a good linearity until 18 μg/mL. The parallelism tests were also performed to evaluate if over-range samples can be analyzed after dilution, without affecting the performance of validated method. The intra- and inter-day precision (RSD%) values were ≤7.14% and ≤11.5%, respectively, for the full range of analysis. The intra- and inter-day trueness (Bias%) values ranged from -11.5% to 1.70% for the two drugs. At the best of our knowledge, this is the first HPLC-PDA method which allows to detect simultaneously Irinotecan Hydrochloride and Gemcitabine Hydrochloride in rat plasma, both after single and drugs association administration in order to evaluate how can interact and modify the pharmacokinetic parameters.

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P091

FPSE-HPLC-PDA METHOD FOR THE DETERMINATION OF INFLAMMATORY BOWEL DISEASE TREATMENT DRUGS IN WHOLE BLOOD, PLASMA AND URINE

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This communication reports a novel fabric phase sorptive extraction-high performance liquid chromatography-photodiode array detection (FPSE-HPLC-PDA) method for the simultaneous extraction and analysis of three drug residues (ciprofloxacin, sulfasalazine, and cortisone) in human whole blood, plasma, and urine samples, generally administered in human patients to treat inflammatory bowel disease (IBD). The drugs of interest were well resolved using a Luna C18 column (250mm×4.6 mm; 5 µm particle size) in gradient elution mode within 20 min. The analytical method was optimized and validated in the range 0.05–10 µg/mL for whole blood, 0.25–10 µg/mL for human plasma, and 0.10–10 µg/mL for human urine. Blank human whole blood, plasma, and urine were used as the sample matrix for the method development and validation; while methyl-*p*-hydroxybenzoate was used as the internal standard (IS). Weighted-matrix matched standard calibration curves showed a good linearity up to a concentration of 10 µg/mL. The intra- and inter-day accuracy values (precision and trueness) were found in the range from −10.9% to 12.3%, and the performances of the validated FPSE-HPLC-PDA were further tested on real IBD patient samples.

This is the first FPSE procedure applied simultaneously to whole blood, plasma, and urine samples for the determination of residual IBD drugs, which possess a wide range of polarity (logP values ranging from 2.30 for Ciprofloxacin, to 1.66 for Cortisone, and 2.92 for Sulfasalazine). The new approach exhibits high potential for immediate adoptation as a rapid, robust and green analytical tool for future clinical and pharmaceutical applications.

P092

FAST METHOD FOR THE DETERMINATION OF MAJOR AND TRACE ELEMENTS IN BREAST MILK: OPTIMIZATION AND VALIDATION

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Breast milk, the first and irreplaceable source of nourishment for the infant, and the well-being of both the mother and baby are increasingly threatened by contamination from environmental toxic agents. In particular, elements can be used as good indicators/tracers of environmental and food contamination. In turn, as well as urine [1–3], and serum [4], breast milk can be considered as suitable biological matrix for biomonitoring studies.
Taking all the above aspects into account, the aim of this study was to optimize and validate a fast method for the determination of a total content of 34 elements (Al, As, B, Ba, Be, Bi, Ca, Cd, Co, Cr, Cs, Cu, Fe, K, Li, Mg, Mn, Mo, Na, Ni, P, Pb, Rb, Sb, Se, Si, Sn, Sr, Te, Ti, Tl, U, V, and Zn) in liquid and lyophilized breast milk. The samples (0.5 g) were subjected to HNO_3:H_2O_2 (2:1) digestion in open polypropylene tubes heated in a water bath (80 °C) and subsequently analysed by inductively coupled plasma mass spectrometry (ICP-MS). The analytical performance and quality control of the proposed method were evaluated in terms of selectivity, detection and quantification limits, linearity, accuracy, and robustness by using standard reference materials and filed samples of breast milk. The number of samples that can be handled in parallel was only limited by the number of available electric plates.
The proposed method allows a significant reduction in treatment time and sample handling compared to microwave acid digestion, thereby resulting in a precise and accurate method (trueness and recovery percentages 80–111%; coefficient of variation <10%; and relative repeatability <15%) with satisfactory detection limits. Furthermore, simple application and high sample throughput make it suitable for routine and biomonitoring studies.

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P093

POLAR LIPID PROFILE OF SPIRULINA MICROALGA BY LIQUID CHROMATOGRAPHY COUPLED TO HIGH RESOLUTION MASS SPECTROMETRY

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Microalgae are a rich source of organic macromolecules, such as lipids, proteins, carbohydrates, and pigments. Due to the high content of lipids in microalgae, they have been attracting increasing attention as a source of lipids for various commercial applications, for example in the manufacturing of food supplements or in the chemical, pharmaceutical and cosmetic industries [1]. In the literature, investigations of the lipid profile of microalgae are mainly focus on free fatty acids and triacylglycerols, whereas information on the occurrence of glyco-, sulpho- and phospholipids is rather scarce [2].
As the amount of lipids in microalgae is relatively small (15–30 % on average depending on the species), the extraction procedure must be as efficient as possible to maximize lipids recovery. For this reason, in this work a fractional extraction was employed, based on the use of CH_3OH:$CHCl_3$:H_2O, 8:4:3 (v/v/v). The upper layer, containing microalgae polar lipids, was collected, dried and analyzed by Ultra High Performance Liquid Chromatography coupled to high resolution tandem mass spectrometry (MS) followed by a bioinformatics analysis by Lipostar, a comprehensive platform-neutral cheminformatics tool for lipidomics.
Before analyzing real samples, a chromatographic evaluation, based on the type and concentration of mobile phase additives, gradients and pH of mobile phase, was carried out in order to separate the largest number of individual lipid classes with emphasis on glyco-, sulpho- and phospho- lipids under MS-compatible conditions. The best separation was obtained using a C18 Kinetex EVO column, at 0.4 mL min^{-1} flow rate, 50 °C column temperature and the following mobile phase gradient: 0 min—60% B, 5 min—70% B, 30 min 99% B, where mobile phase A was 100 mmol L^{-1} formic acid with 1 mmol L^{-1} ammonium formate and mobile phase B was methanol with 1 mmol L^{-1} ammonium formate and 100 mmol L^{-1} formic acid.
The optimized procedure was applied to the analysis of Spirulina microalgae and the entire lipidomic platform led to the identification of 117 lipids belonging to the three main investigated classes.

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P094

AUTHENTICATION OF "NOCCIOLA ROMANA" PDO HAZELNUT BY NIR COUPLED WITH CHEMOMETRICS

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Hazelnuts (fruits of the deciduous tree Hazel) are widely consumed because of their organoleptic characteristic and their positive effect on the human organism. Several studies have demonstrated that the area of harvesting influence the quality of these nuts; as a consequence, it is relevant to develop analytical methodologies which allow tracing these fruits. In addition, some particular cultivars of Italian hazelnuts have got the PDO label, clarifying the added value the area of growth confers to the nuts.

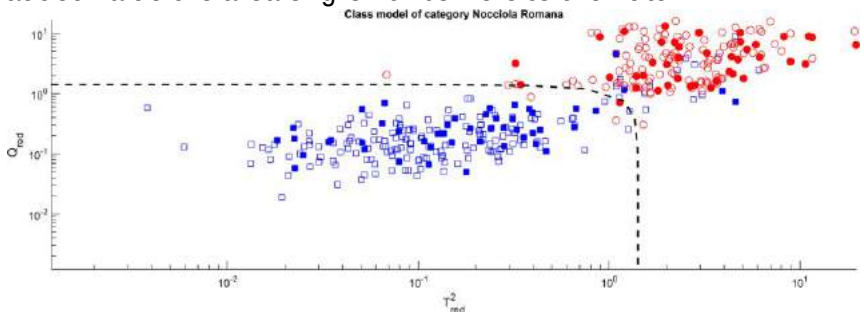

Figure1*: SIMCA analysis: projection of hazelnuts samples onto the T^2 vs Q model space of class Nocciola Romana PDO*. Legend: Class PDO-blue squares, class Others-red circles. Empty symbols: training objects; Filled symbols: test objects. The dashed line defines the acceptance threshold for the category.

Starting from this scenario, the possibility of developing a non-destructive methodology for the authentication of a particular Italian PDO hazelnut, the "Nocciola Romana PDO" has been tested. For this reason, 376 nuts (Nocciola Romana PDO or common hazelnuts) have been unshelled and analyzed by NIR spectroscopy. Then, classification models, aimed to distinguish Nocciola Romana samples (Class "PDO") from common hazelnuts (Class "Others") have been created by SIMCA [1] and PLS-DA [2-3]. The best results (in terms of predictions) were given by SIMCA. In Figure 1 samples (projected onto the T^2 vs Q model space of class PDO) are shown: 4 test objects belonging to Class PDO (blue filled squares) are rejected and 1 sample from Class "Others" (red filled circles) was accepted from the model.

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P095

DIRECT QUANTIFICATION OF CHEMICAL SPECIES BY MULTIVARIATE STANDARD ADDITION AND NET ANALYTE SIGNAL METHOD

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Analytical interferences, such as instrumental noise or matrix effect, can make a quantitative analysis very difficult, thus increasing the experimental error associated to the analysis.
Multivariate methods, such as Principal Component Analysis (PCA) and Partial Least Square (PLS), offer a valid alternative to classical univariate ones, due to their better skill in managing noise, and because they do not require a single variable directly related to the analyte. PLS, in particular, is able to quantify the analyte of interest taking into account the entire spectra obtained by samples, computing a multivariate calibration line with the standards onto which the unknown-sample(s) spectra can be interpolated.
Sometimes it is not possible to prepare standard samples for a PLS-interpolation, so it is better to use a standard addition method. However, in this case, the matrix effect strongly affects the results of PLS, and a blank sample is necessary; it is not so simple, and sometimes it is impossible, to obtain such a blank.
We propose a novel chemometric approach for quantification based on Net Analyte Signal (NAS) procedure [1,2]. This approach is based on multivariate standard addition method and PLS, but the "blank" signal is mathematically calculated, and the blank sample is not required. Moreover, the NAS procedure is able to extrapolate from multivariate spectra only the signal(s) due to the analyte of interest and the multivariate model can be reduced to an easier-to-interpret univariate one.
NAS procedure was successfully applied to quantification of salts in solution by UV-Vis spectroscopy, biosilica in marine sediments by IR-ATR spectroscopy, and polymorphs of pharmaceutical ingredients in drugs by XRPD.

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P096

DETERMINATION OF PLANT-DERIVED CONTAMINANTS IN SAFFRON BY MEANS OF SPME-HS/GC-MS AROMA PROFILING COMBINED WITH CHEMOMETRICS

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Saffron, the dried stigmas of *Crocus sativus L.*, is a spice known since ancient time and worldwide used in culinary and food industry for its colouring, flavouring properties and bioactivity. Obtaining one gram of dry saffron requires processing of 150-200 Crocus flowers by time-consuming procedures, most of them carried out still manually. For these reasons, saffron is the most expensive spice in the world and one of the foodstuffs most frequently subjected to fraudulent adulterations. Common saffron sophistications by economic frauds include addition of artificial dyes, cheaper parts of other plants or inorganic materials able to simulate the Crocus stigmas and increase the spice weight.
Analysis of the saffron volatile profile by means of solid-phase micro-extraction (SPME) coupled with gas-chromatography (GC) has been previously used to identify the chemical substances responsible for the saffron aroma or to attempt geographical discrimination of spices cultivated in different sites [1-3].
In this work, SPME-GC has been applied for the first time to detect plant-derived adulterants in saffron. In particular, we investigated the volatile profiles of *Calendula officinalis L*. (calendula) petals, *Carthamus tinctorius L.* (safflower) petals and *Curcuma longa L*. powdered rhizomes (turmeric), which are the bulking agents of plant origin most frequently used in fraudulent saffron adulteration. To maximize the GC signals of the adulterants as compared to that of the saffron volatiles, we evaluated the effect of the kind of sorbent by testing three different SPME fibers. Moreover, an experimental design combined with surface response methodology was applied to evaluate the influence of temperature and exposure time of the SPME fiber on the detectability of the target adulterants. Finally, the potentiality of SPME-GC analysis for the detection of saffron adulteration with cheaper parts of other plants was evaluated by application of unsupervised and supervised multivariate statistical methods to the volatile profiles collected from genuine and artificially sophisticated spices.

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P097

GEOGRAPHICAL CLASSIFICATION OF SAFFRON (CROCUS SATIVUS L.) BY MEANS OF MULTIVARIATE STATISTICAL ANALYSIS OF UHPLC DATA

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Saffron is a precious spice obtained by drying of the stigmas of *Crocus sativus L.* used since ancient times as colouring and flavouring additive of foods and in folk medicine. Because of high price, saffron is one of the most frequently adulterated foodstuffs. Adulteration of certified saffron produced in specific territories with low-quality spices cultivated elsewhere is one of the most common frauds that cannot be easily detected by conventional quality control methods. Therefore, geographical classification of saffron has a great commercial relevance. Reversed-phase high performance liquid chromatography (HPLC) coupled with photometric or mass-spectrometry detection has been extensively used in saffron analysis aimed at the characterization of the spice phytochemicals, for quality control and geographical classification [1-3]. The crocetin esters (commonly known as crocins), picrocrocin and its derivatives, safranal and several flavonoids can be detected by HPLC analysis of saffron aqueous extracts. Most of these chemical species, apart from being responsible for the organoleptic properties of saffron, are promising markers of the spice geographical origin. However, previous evidences revealed that resolution of the chromatogram has a great impact on the classification performance based on HPLC data [3]. In this work, we used ultra-high performance liquid chromatography (UHPLC) to enhance separation of polar saffron constituents, crocins in particular, and improve information on the qualitative chemical composition of the spice. Metabolomic profiles determined by UHPLC were handled by means of classification and class-modelling methods to attempt geographical discrimination.

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P098

DISCRIMINATION OF ARABICA AND ROBUSTA COFFEE SPECIES BY HS-SPME-GC-MS ANALYSIS OF VOLATILE ORGANIC COMPOUNDS OF GREEN BEANS AND A CHEMOMETRIC APPROACH

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Observing unroasted seeds, Arabica can be distinguished from Robusta by inspecting the morphological characteristics such as size and shape. However, nowadays a number of different cultivars are farmed with prevalent characteristics of one species and some characteristics of the other, thus making not so straightforward the species identification by visual inspection. Several literature studies report chemical approaches to identify markers for the discrimination of the species by HPLC-MS and using e.g. NMR and Raman spectroscopy. A recent study using PTR-ToF-MS technique and a chemometric approach on 13 stock samples produced a model which distinguished Arabica and Robusta at different stages of roasting with the exception of green coffee. Few studies have been conducted on green coffee, mainly aimed at the identification, by HS-SPME-GC-MS, of defective coffee beans' markers [2]. In the present study we propose a survey on 35 coffee samples obtained by different producers located in Trieste (Italy), the identification of nearly fifty VOCs in the green coffee volatilome by HS-SPME-GC-MS and the selection of twenty possible markers of difference in species by use of Principal Component Analysis and Discriminant Analysis [3].

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P099

IMAGE TEXTURE ANALYSIS ON HYPERSPECTRAL DATACUBES: A COMPARATIVE STUDY

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Surface texture is an important feature for evaluating physical nature of analytical samples, allowing to highlight differences between matrices with a very similar chemical composition. To measure such a property, several algorithms of image texture are available in literature and are typically applied on mono-layer images, usually the grey scale ones. The aim of the work is to compare and evaluate the ability of three different approaches of image analysis on hyperspectral data; the fact that these data are organised in three-dimensional data cubes may constitute a limiting factor in applying image texture algorithms directly on the hypercube. In more detail, two algorithms typically applied on mono-layer images are taken into consideration: GLCM (Grey Level Co-occurrence Matrix) and AMT (Angle Measure Technique), while for multivariate approaches an algorithm proposed by Bharati e MacGregor and based on PCA was considered [1]. Different types of data compression, such as integral images and PCA, were applied to extract the information related to physical properties of the samples, before performing the procedures under study. In the flour case study, images of 5 types of flour (durum wheat flour, strong flour – Manitoba, wholemeal, plain flour and soft flour) were recorded by a hyperspectral camera SWIR3 (SPECIM Ltd, Finland), working in the spectral range 1000-2500 nm. These images were submitted to combinations of data compression and image texture algorithms to distinguish between the five commercial types of flour.
This work allows to deeply evaluate the reliability of well-known image texture approaches on HSI-NIR images; pros and cons of each procedure were highlighted.

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Acknowledgement
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P100

FROM CHEMOMETRIC MODELS TO CHEMICAL INTERPRETATION: TOOLS AND CAVEAT

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Chemometrics can be defined as the "art of extracting relevant information from chemical data", and it performs this task by encoding such information in the form of models [1]. Depending on the hierarchy of the problems to be solved, such models could be "only" exploratory, focusing on describing the main trends and characteristics within the data set, or predictive, if the final aim is to be able to reliably relate the chemical measurements to one or more responses (be them of quantitative or qualitative nature). Whatever the nature of the problem to be solved, and the corresponding level of complexity of the chemometric model to deal with it, one of the fundamental aspects to be considered is how to interpret the final outcomes in chemical terms. In this respect, since the chemical information is encoded in the chemometric models, interpretation has to rely on the inspection of the model parameters, be them scores, loadings, weights or, in a predictive fashion, e.g., the regression coefficients. However, especially if careful validation, not only of the predictions, where available, but also of the whole data processing pipeline, including the final interpretation, is not undertaken, the risk of being misled or, even, overinterpreting the results is always present [2].
Accordingly, in the present communication, the different tools available to support the chemical interpretation of the outcomes of chemometric modeling will be critically revised and discussed, especially focusing on strategies and good practices which are often neglected by most of the practitioners. On the other hand, some critical issues and the risks connected to the misuse of some interpretation tools will also be addressed.

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P101

A SURVEY OF DATA FUSION APPROACHES IN CHEMOMETRICS CONTEXT

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The adoption of data driven discovery paradigm in science has led to the need of handling large amount of diverse data. Drivers of this change are on one hand the increased availability and accessibility of hyphenated analytical platform, imaging techniques, the explosion of omics data, and on the other hand the development of information technology.
Data driven research in general deals with an inductive attitude that aims at extracting information and building models capable of inferring the underlying phenomena from the data itself. In other words, data-generated hypotheses are by large replacing the deductive attitude of generating data according to prior hypotheses.
Hence, the main challenge is how to face these multiple data sources and how to retrieve all possible available information. One of the salient aspects is the methodology to integrate data from multiple sources, analytical platforms, different modalities, varying timescale, including also unstructured data. This is generally referred to as Data Fusion [1-2].
Aim of this presentation is to provide an overview of the different available methodologies, mainly proposed/used in Chemometrics, framing as well the nature of coupled data and how data fusion can enhance knowledge discovery.
Applications will be presented concerning food authenticity [3], process monitoring and a recently developed approach for exploratory analysis of weak structured data [4].

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P102

EXPLOITING THE PERFORMANCE OF NEAR-INFRARED HYPERSPECTRAL IMAGING: TRANSFLECTANCE AND TRANSMISSION ANALYSES

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Hyperspectral imaging is usually considered as a surface analysis method. Nevertheless, electromagnetic rays may penetrate in depth, inside the upper layers of the sample, including information from the inner parts in the recorded spectra. Moreover, such an effect depends on the matrices analysed and on the specific wavelengths at which spectra are recorded.
In the present study, penetration depth was evaluated for a near infrared hyperspectral imaging system working in the 1000–2500 nm spectral range, at 8 nm spectral resolution (HSI-NIR SWIR3 camera equipped with a LabScanner 40x20).
To the aim, a chessboard background was assembled using two polymeric materials characterised by different total reflectance values (about 0% and 90%, respectively) and with different and characteristic spectral profiles. The use of a geometrical pattern, in comparison with uniform backgrounds, adds spatial information to the penetration depth evaluation. Images were recorded placing samples (sliced cheese), both sliced at different thickness and wedge-shaped, between the source and the chessboard background.
Univariate and multivariate image analysis was carried out in order to highlight both spatial and spectral features, allowing to evaluate the penetration depth. First of all, a region of interest (ROI) within the hyperspectral image, including a representative portion of the sample was selected. Then, principal component analysis (PCA) was carried out, reducing data dimensionality and removing non-useful information to confirm the level of penetration on the basis of score images.
On the basis of these outcomes, in many practical applications, hyperspectral imaging should be regarded as a transflectance approach, depending, of course, on the physico-chemical characteristics of the matrix, such as the chemical composition and the physical microstructure, and on characteristics of the electromagnetic radiation involved (wavelengths and intensity).
A further interesting topic concerns the possibility of acquiring hyperspectral images in the transmission mode. To this aim, an in-house instrumental setup was adopted, allowing to transmit electromagnetic radiation across samples. Particular strategies for focusing and normalising image intensities were developed. Transmittance images obtained on samples of biological interest allowed capturing important chemical information on the internal structures of biological tissues, complementary to information acquired in the reflection mode.

Acknowledgement: Financial support by the Italian Ministry of Education, Universities and Research (MIUR) is acknowledged – Research Project SIR 2014 “Advanced strategies in near infrared spectroscopy and multivariate data analysis for food safety and authentication”, RBSI14CJHJ (CUP: D32I15000150008).

P103

ELECTROCHEMILUMINESCENT DNA SENSOR FOR THE DETECTION OF SPECIFIC DNA SEQUENCES

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Electrochemiluminescence (ECL) is a powerful transduction technique that has rapidly gained importance as a sensitive and selective transduction technique in analytical science gathering the advantages of the electrochemical sensitivity and the spatial resolution.[1]
Methods for the detection of specific DNA sequences have attracted significant attention due to possible applications in different fields such clinic diagnostics, food safety, environmental pollution analysis, and forensic identification. DNA sensors, the electrochemical equivalent of molecular beacons, appear to be a promising tool to detect oligonucleotides. [2,3]
In this work, an electrochemiluminescent DNA (ECL-DNA) sensor was investigated. The system is comprised of a luminophore attached to a DNA "stemloop" probe by crosslink chemistry, which is immobilized on a gold electrode via self-assembled monolayer chemistry. ECL is generated according to the "oxidative-reduction" strategy using Tripropylamine (TPA) as co-reactant and Ru(bpy)32+ as luminophore. When the DNA target sequence we observed a variation DNA signaling arises due binding-induced changes in the conformation of the stem-loop probe.
Here, effect of probe density on the electrode surface, hybridization signal suppression were investigated.

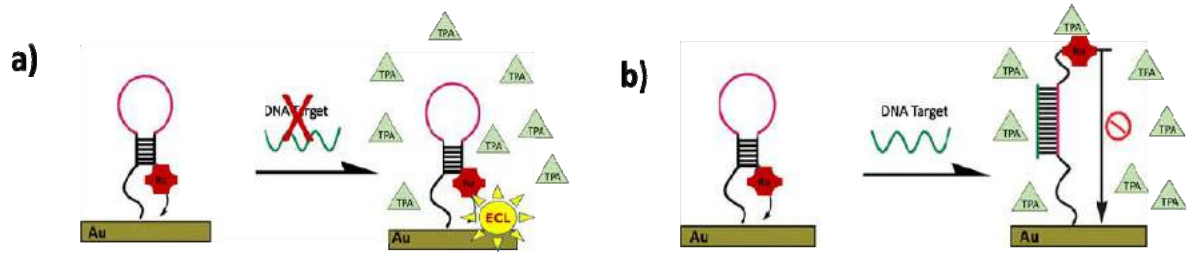

Figure 1. Scheme of the DNA sensor in a) before and b) after hybridization with the target DNA sequence.

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P104

THALLIUM VOLTAMMETRIC DETERMINATION IN PRESENCE OF METAL INTERFERENCE IN FOOD AND BIO-MONITOR SPECIES: APPLICATION TO MUSSELS, CLAMS AND OYSTERS

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Heavy metals are very dangerous pollutants owing to their bioaccumulation and toxicity, and in particular thallium is a new emerging pollutant. To establish reasonable water quality criteria it is therefore necessary to determine this metal at trace and ultra-trace level, especially in aquatic ecosystems. Moreover, toxic metals accumulate in certain marine species and thus enter the aquatic food chain. In particular, mussels, clams and oysters sequestrate and concentrate several metals from their aqueous environment, possibly becoming dangerous to human health in consequence of their consumption. These filtering organisms require particular attention and inspections before being sold on the market: an adult organism is able to filter even up to 5 L h-1, depending on its weight.
In addition to this important and fundamental aspect of public health, the determination of toxic metals in mussels and clams, that are not only filtering organisms but also sessile species, can be usefully employed for bio-monitoring campaigns, evaluating the long-term trend of the pollution load of an aquatic ecosystem: this information evidently cannot be provided by punctual determinations. For completely mapping environmental pollution, the sampling duration and cadence are very important. In our opinion, the use of bio-monitors, just proposed by several authors, but certainly not scientifically supported, is possible only in the case of a long sampling plan. In any case, the metal determination in oysters, mussels and clams must be evidently accurate and especially characterized by very low limits of detection.
The present work reports and discusses the analytical procedure for the voltammetric determination [1,2] of thallium in oysters, mussels, clams and oysters sampled in a bay in proximity of the northern Adriatic coast (Goro Bay). Interferences from Pb(II), Sn(II) and Sb(III) are considered, while a critical comparison with spectroscopic measurements is also discussed, comparing the results obtained from voltammetric determinations with those of spectroscopic measurements.

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P105

ELECTROCHEMICAL AND SPECTROSCOPIC INVESTIGATION ON THE STABILITY OF POLY ORTHO- AMINOPHENOL (PoAP), GROWN AS A VERY THIN MEMBRANE ON PLATINUM, UNDER PROLONGED IMMERSION IN WATER

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We have recently reported on the use of the modified electrode Pt/PoAP [1] as biosensor for amyloidogenic peptides, particularly performing when 'recognizer' peptides are firmly entrapped within PoAP chains during electrosynthesis.
The synthesis steps of this 2D MIP-inspired biosensor, using an elastin-like peptide, ELP, as a self-similar receptor of amiloidogenic peptides, having the same repeat sequence, VGGVG, are schematized in the graphical abstract of reference 1.
The stability of PoAP membrane is thus crucial for the biosensor efficiency, considering the prolonged immersion of the Pt/PoAP/ELP system into the aqueous suspension of amyloids.
At first, in this contribution we have investigated on the stability of 'as prepared' Pt/PoAP systems that are produced, in neutral media, either by CV and potentiostatic growth of an insulating PoAP membrane, ultrathin and strongly adherent to the underneath platinum.
The inertness of the membrane, acting as impermeable protecting barrier to electrodes poisoning, was monitored after increasing time of residence in water, using ferrocyanide as electrochemical probe having a well-known redox activity on platinum at the given potential range.
Results from *in situ* electroanalyses and *ex situ* investigation by XPS and AFM techniques will be provided which unequivocally show the importance of the post characterization of these layered electro synthesized systems, after periodic 'resting and working' hours, in order to better control the process optimization, particularly, in view of bio-application with the more complex Pt/PoAP/ELP system.

R.I.P. 4 February 2018

† In memory of Innocenzo G. Casella, Full Professor CHIM01- University of Basilicata (Italy)

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P107

3D FLOWER-LIKE Pt NANOSTRUCTURES ON POLYPYRROLE NANOWIRE MATRIX FOR ENHANCED METHANOL OXIDATION

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Platinum electrocatalytic properties are well-known since long and have stimulated extensive research leading to several applications, mainly related to its use in chemical sensors and as catalysis [1,2]. It is generally accepted that both catalytic efficiency and selectivity are highly dependent on the size and shape of platinum material, thus explaining the growing research efforts in the synthesis of Pt nanoarchitectures [1,2]. Among these, very recently nanoflowers have emerged as compelling materials due to their three-dimension structure, which provides favorable surface areas and active centers for electrocatalysis supplying enough adsorption sites for all involved molecules in a narrow space [3].

In the present work, for the first time, the synthesis of Pt flower-like nanostructures (PtNFs) is performed on a conducting polymeric support consisting of a three-dimension polypyrrole nanowires (PPyNWs) matrix, obtaining a composite material with excellent catalytic performances in methanol oxidation. Both PtNFs and PPyNWs are prepared by an electrochemical approach without using any seed, template or surfactant. The morphology and chemical composition of the resulting PtNF/PPyNWs hybrids are characterized by scanning electron microscopy and by X-ray photoelectron spectroscopy, respectively. The electrocatalytic performance of the as-prepared PtNF/PPyNWs system has been evaluated by cyclic voltammetry and chronoamperometry, evidencing that these 3D materials exhibit excellent electrocatalytic activity and high level of poisoning tolerance to the carbonaceous oxidative intermediates [4]. Such performances can be ascribed to the combined effect of the flowerlike structure promoting the exposure of more sites and the polymer nanowires matrix endorsing high dispersion of PtNF on a high electrochemically active surface area, besides the removal of sub-products from electrocatalytic sites.

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P108

Electrodeposition of thin films for the galvanic industry

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The interest in scientific research within the metal finishing sector is growing. The demand for durable metals and adaptable manufacturing processes are increasing across a wide range of applications, from aerospace and automotive to machinery and jewelry. An essential step in the production line is the surface engineering of metals, as this determines the final appearance and functionality of a product. Therein electroplating is recognized as a mature technology allowing the low cost fabrication of defined surfaces with extensive property profile. Galvanic electrodeposition accounts today for almost 40% of the global market value share with North America and Western Europe leading the scenery. Although technological and processing advancements occurred in the past forty years, industrial firms are still struggling to provide solutions to corrosion protection as well as reduction of toxic wastes. Specifically, large-scale industrialization of electroplating techniques will continue to be limited by strict environmental regulations. Due to adverse ecological impacts, the adoption of plating processes involving toxic metals such as lead or cadmium is prohibited. Moreover, price volatility of the highly demanding electroplated materials gold, copper and nickel is expected to impact the market share for more than 60% by 2026.
In that respect, alloy plating offers better answers in terms of economic growth and environmental sustainability due to fine tuning composition, morphology and crystallinity [1]. Here, current trends on alloy electrodeposition research are reviewed highlighting open challenges and process innovations from an industrial perspective. The main categories of alloy compounds are presented and the most important properties for the manufacturing process discussed. Particular attention is devoted to advances in industrial quality control and viable solutions for the reduction of precious metal content in electroplated accessories as well as replacement of cyanide and nickel baths with non-toxic compounds.

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Acknowledgments. Financial support from Oroplac srl, Freschi & Vangelisti srl, LEM srl and Tecnomet srl is acknowledged.

P109

VOLTAMMETRY IN HYDROGEL FOR THE ANALYTICAL CHARACTERIZATION OF WATER SENSITIVE SURFACES

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Biopolymer hydrogels, prepared with starch, pectin or agar, have been extensively applied in different fields varying from biology to electrochemistry [1]. The coupling of microelectrode voltammetry with the closely related electroanalytical techniques Micropipette (MP) and Scanning Electrochemical Microscopy (SECM) allows extending analytical measurements to a variety of interfaces and surfaces, thus achieving high spatial resolution.
In this paper, it is shown that the use of gelled media along with the above mentioned techniques opens new roads for the characterization, from an electrochemical point of view, of micro areas on surfaces which suffer the direct contact with liquid electrolytes. In particular, the uncharged polysaccharide agarose is used as medium to avoid large impregnation with electrolyte and/or redox mediator solutions of water-sensitive substrates, though allowing free diffusion of the electroactive species within the gel, as happens in conventional solutions. A series of voltammograms have been performed either in bulk (Fig. 1a) or gel/solid interfaces (Fig. 1b,c). Different charged and uncharged redox systems, of known electrochemistry and different formal potentials, have been considered to characterize either conducting or non-conducting substrates. The usefulness of the proposed voltammetric, SECM and MP strategies has been proved by performing measurements above paper-based substrates of cultural heritage and food industry interest.

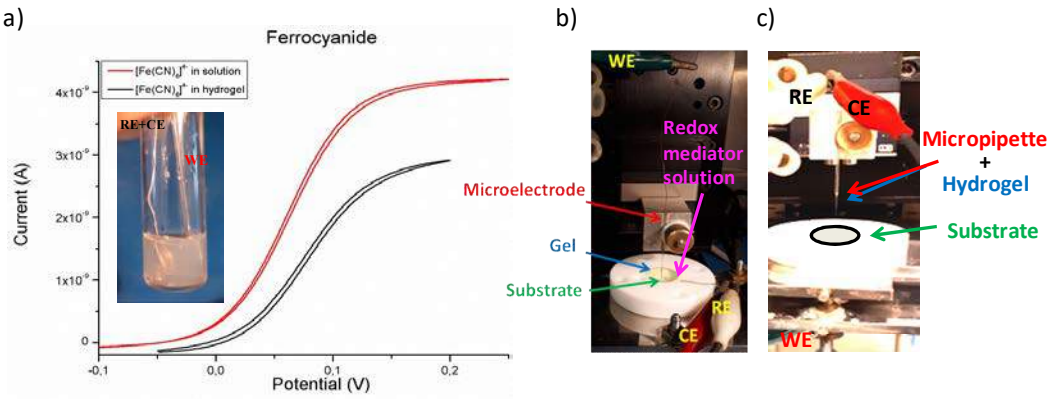

Figure 1. Voltammetric measurements performed with a Pt microdisk electrode in: (a) bulk Agarose hydrogel; (b) at the solid/gel substrate with a SECM and (c) MP apparatus.

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P111

Determination of pharmaceuticals in surface waters by an electro-activated glassy-carbon electrode

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Pharmaceuticals have been recently detected in natural water bodies and could have an impact on the biological activity of natural waters [1]. The increasing use of pharmaceuticals [2] and the unsuitability of the current Waste Water Treatment Plants (WWTPs) to decrease the concentration of these molecules [3,4] are the major reasons for their occurrence in surface waters.
In this work an electro-activated glassy carbon electrode (aGCE) was tested as sensor for the detection of acetaminophen (APAP) in surface water samples. The best measurement conditions for the determination of APAP by Differential Pulse Voltammetry (DPV), assisted by the aGCE, were optimized by means of a Design of Experiment approach. The analytical performance of the electrochemical procedure was than assessed in synthetic solutions and in real samples. The system can detect APAP concentrations higher than 4.4 $\mu g\ L^{-1}$ in untreated river-water samples, and higher than 0.2 $\mu g\ L^{-1}$ in river-water samples that were pre-treated by solid phase extraction. The analytical response had a linear trend with concentration between 5.5 and 33 $\mu g\ L^{-1}$. The electrochemical technique based on DPV with aGCE was then used for the quantification of APAP in river water samples collected in the Turin area (Piedmont region, NW Italy) with the collaboration of ARPA-Piedmont (Agenzia Regionale per la Protezione Ambientale). The results were successfully compared with those obtained by liquid chromatography-mass spectrometry (HPLC-HRMS) to assess the reliability of the electrochemical measures.
The same electrode was then tested as sensor for the detection of the diclofenac. The drug can be easily absorbed on the surface of the activated GCE allowing the revealing of the analyte at very low concentration levels.

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P112

DOPAMINE QUANTIFICATION IN RAT STRIATUM TISSUES TREATED WITH PERMETHRIN BY HLPC-ECD

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Pyrethroids are the most commonly pesticides used for residential pest control and public health purposes. Although pyrethroid pesticides are often considered a safer choice because they are generally not as acutely toxic as organophosphates, previous studies indicated that exposure to pyrethroid compounds such as permethrin (PERM), in neonatal age, may not be innocuous [1]. In particular, pesticides are known as environmental factors involved in the etiopathogenesis of Parkinson's disease. The correlation between the PERM exposure and a significant decrease in striatal dopamine (DA) levels has been demonstrated in rats [2].
The aim of the present work was to develop an analytical HPLC method coupled with electrochemical detection to quantify DA in the striatum of rats treated with PERM from 6 to 21 postnatal days. Rat striatum tissues were homogenized with a solution of perchloric acid, sodium metabisulphite and Na_2EDTA. Samples were homogenised and centrifuged, and after filtration, aliquots of 10 µL were analysed by HPLC [3]. The column employed for the analysis was a Phenomenex Luna C_{18} (250 × 4.6 mm, 5 µm), the mobile phase was a mixture of methanol, sodium acetate, n-octyl-sodium sulfate and Na_2EDTA in water (pH adjusted to 4.1). The liquid chromatography apparatus was coupled with an Antec Leyden Decade II detector. The dihydroxybenzoic acid (DHBA) was employed as internal standard. Results revealed that DA levels were significantly different in the control and PERM-treated groups. These data provide some evidence the *in vivo* damage induced by PERM on dopaminergic neurons, highlighted by the lowest levels of DA measured in the striatum of rats groups treated with PERM in comparison with the control groups. The possibility to perform highly sensitive analyses with a reduction of the well-known issues connected with the dopamine low concentrations present in biological tissues was one of the main benefits of this investigation.

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P113

CHARACTERIZATION OF DUSTY AND DUST FREE PM SAMPLES COLLECTED IN A SUBURBAN SITE IN SOUTHERN ITALY

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PM10 and PM2.5 samples simultaneously collected at a suburban site of south eastern Italy have been analysed with the main aim of determining the atmospheric dust contribution and investigating the dust source impact. Low volume samplers were used to collect 24-h PM10 and PM2.5. Organic and elemental carbon, inorganic ions, and selected metals were measured in the collected samples. EC and OC were determined by thermal optical transmittance technique (Sunset Carbon Analyzer), soluble ions (SO_4^{2-}, NO_3^-, NH_4^+, Cl^-, Na^+, K^+, Mg^{2+} and Ca^{2+}) were analysed via High Performance Ion Chromatography (HPIC, Dionex DX-500 System); eight trace elements (Ni, Cu, V, Mn, As, Pb, Cr, Sb) were analyzed via Graphite Furnace Atomic Absorption Spectroscopy (GF-AAS, Perkin Elmer Analyst 600 System); four trace elements (Fe, Al, Zn and Ti) were analysed by Inductively Coupled Plasma Atomic Emission Spectroscopy (ICP-AES, Varian Liberty 110 spectrometer). Moreover, ATR-FTIR analysis were performed on samples of Saharan Dust event and samples characterized by mass air transported from NE Europe. ATR-FTIR analysis let identify organic functional groups including non-acid organic hydroxyl C-OH group (eg sugars, anhydrosugars, and polyols) and carbonyl C=O group, carboxylic acid COOH group, aromatic and aliphatic unsaturated C=C-H group, aliphatic saturated C-C-H group, and amine NH2 group. Some inorganic ions have also been identified: carbonates, sulfate, silicate and ammonium. In this work, the X-ray photoelectron spectroscopy (XPS) has been used to investigate surface chemical composition of particulate matter.
The mass closure analysis have been applied to the chemically speciated PM10 and PM2.5 samples to identify main natural and anthropogenic sources and determine the atmospheric dust contribution. Analytical back trajectories combined with statistical analyses and satellite true colour images were used to know about the location of potential source regions and to determine the contribution of long range transported air masses. In particular the effect of Sahara dust outbreak on PM composition was evaluated.

P114

DETERMINATION OF POLYSTYRENE ACCUMULATION IN MUSSELS (*Mytilus galloprovincialis*) BY PYROLYSIS AND GC-MS

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In recent years microplastics (<5 mm) and nanoplastics (<100 nm) are becoming recognised with increasing concern as main contaminants of aquatic environments due to their ubiquity, interactions with living organisms and carriers of priority pollutants (e.g. PCBs). Polystyrene (PS) is among the most largely used plastics worldwide and one of the most frequently detected types of microplastics in surface oceans. However, the knowledge on the occurrence of PS particles in aquatic environments and biota is limited. Quantification of microplastic particles often relies on visual sorting from a processed sample and recording the number of particles observed. Pyrolysis (Py) with GC-MS, Fourier transform infrared spectroscopy (FTIR), focal-plane array FTIR, Raman spectroscopy, and scanning electron microscopy are techniques used for identifying and characterizing microplastic polymers. These techniques are typically used after isolating microplastic particles via a separation procedure and principally adopted for qualitative analysis. Previous studies showed that Py-GC-MS can be a valid method for quali-quantitative analysis of synthetic polymers and has been applied to analyse PS in environmental matrices. The method is based on the analysis of pyrolysis products specific of the polymer released by thermal degradation. The present study aimed at developing a protocol based on thermal degradation and GC-MS analysis for the determination of PS microparticles in biological tissues. Protocols of alkaline digestion followed by solvent extraction or filtration with quartz filter have been tested on tissues fortified with PS with different particle size. Extracted/filtered samples were thermally degraded by two different techiques: thermogravimetric analysers (TGA) and Py with a CDS pyroprobe heated platinum filament. Evolved pyrolysis products (styrene, styrene dimer and trimer) were captured by an ORBO activated carbon sorbent tubes and determined by GC-MS for the identification and quantification of PS by internal standard calibration. The principal figures of merit were determined using calibration standards and internal reference materials. The optimised protocol was applied to the analysis of haemocytes and gills from marine bivalve *Mytilus* spp exposed in seawater tanks at different concentration of 45-µm PS particles. Results indicated the accumulation of 45-µm PS consistent with microplastic translocation to the different mussel organs through haemolymph.

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P115

ASSESSMENT OF PARTICULATE MATTER DIMENSIONAL PROFILES AT AN INDUSTRIAL SITE BY MEANS OF SELF ORGANIZING MAP ALGORITHM APPLIED TO OPTICAL PARTICLE COUNTER DATA

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Civil dwellings close to productive activities can be subject to perceptible pollutants as malodors, particulate matter (PM) of different size and noise. Some of these environmental health determinants as PM of size smaller than 2.5 micrometers are not regulated adequately in Italy, but they deserve attention, especially in the case of population living very close to intense pollution sources. Nowadays instruments as optical particle counters (OPCs) are available for continuous monitoring of ambient air at the receptors which are able to produce highly dimensional data (e.g multivariate data per minute or second). Therefore, there is the need of a tool to manage millions of single data and extract information for assessing the impact on population.

In the present study we propose a data elaboration by Self Organizing Map algorithm [1] of a three months' survey near civil dwellings at an industrial site by an 8-channels OPC (from 0.3 μm to 10 μm particle diameter) which records data per minute, proposing a description of variability of size distribution of PM in a concise form. The model output can undergo to a second level abstraction by means of k-means clustering algorithm [2] to obtain a reduced number of clusters (usually 2 up to 10) which represent the different "air types" perceived at the receptor. The clusters can be characterized in terms of PM classes profiles, frequency and persistence. Recently we applied this method to data about gaseous composition related to odour impacts, collected by an electronic nose near dwellings in proximity of an industrial plant [3]. The model can be used for effectively visualizing the dynamical evolution of PM size distribution at the receptor site.

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P116

IDENTIFICATION OF POLICYCLIC AROMATIC HYDROCARBONS IN POLYHYDROXYALKANOATE BIOPOLYMERS OBTAINED FROM URBAN SOLID WASTE BY GAS CHROMATOGRAPHY/MASS SPECTROMETRY ANALYSIS

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Polyhydroxyalkanoates (PHAs) are completely biodegradable polymers that can be produced from renewable resources. In recent years, the attention to organic wastes as a new feedstock for PHA production is increased to reduce their high cost and increase their sustainability. However, because PHAs can be obtained from heterogeneous bio-waste (organic fraction of urban waste, food processing waste etc.), before they can be introduced into the market, it is necessary to assure the absence of chemical contaminants that could be incorporated from the feedstock to the final product. Among the several organic contaminants which could be pass from waste to PHAs, there are the polycyclic aromatic hydrocarbons (PAHs), known for their dangerous effects on human health and environment compartments. For this reason, we have developed a rapid analytical method for the determination of the main sixteen PAHs in PHAs. Since the PHA is a solid but biodegradable sample, the main challenge was to find out the most suitable solvent for analyte extraction. After that, the extract was purified by solid phase extraction using florisil as adsorbent. High recoveries were obtained for all the analytes, except for the three with the lowest molecular weight, likely due to their volatility and/or limited retention on florisil cartridge. Gas chromatography/mass spectrometry was used for analyte determination. Method limit of quantification were suitable to assure that the presence PAHs in PHA biolpolymers is much below the limits set by European law for plastic materials. Indeed, analysis of two different PHA samples showed that contamination is limited to few compounds and at not concerning levels.

Funding This work was funded by the REsources from URban BIo-waSte" - RES URBIS (GA 7303499) project in the Horizon2020 (Call CIRC-05) program.

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GAS AND AEROSOL COMPOSITION DURING THE AEROCLO-SA CAMPAIGN IN HENTIES BAY (NAMIBIA)

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The South East (SE) Atlantic represent a natural laboratory for studying the effects of aerosol-radiation and aerosol-cloud interactions on climate. A mixture of emissions from biomass burning during the dry season, transport of dusts from the Namibian desert, marine emissions, particularly rich in nutrients from the Benguela upwelling system, together with local emissions makes this site particularly interesting to study different aerosol typologies and their interactions with coexisting fogs and stratocumulus clouds. The AErosol RadiatiOn and CLOuds in southern Africa (AEROCLO-sA) project aims at studying the interactions between aerosols, clouds, and radiation, along the Atlantic coast of austral Africa through airborne, ground-based and satellite measurements of clouds, aerosols, and their radiative impacts. The one-month long AEROCLO-sA field campaign took place in August-September 2017 in Henties Bay (Namibia). In this context, ground-based measurements of volatile organic compounds (VOCs) and trace gasses were continuously done together with measurements of aerosol concentration, composition, optical and hygroscopic properties. The relation between VOC peak emissions and new particle formation events will be discussed with the aim of understanding the underlying mechanisms and their impacts on the Earth's energy budget.

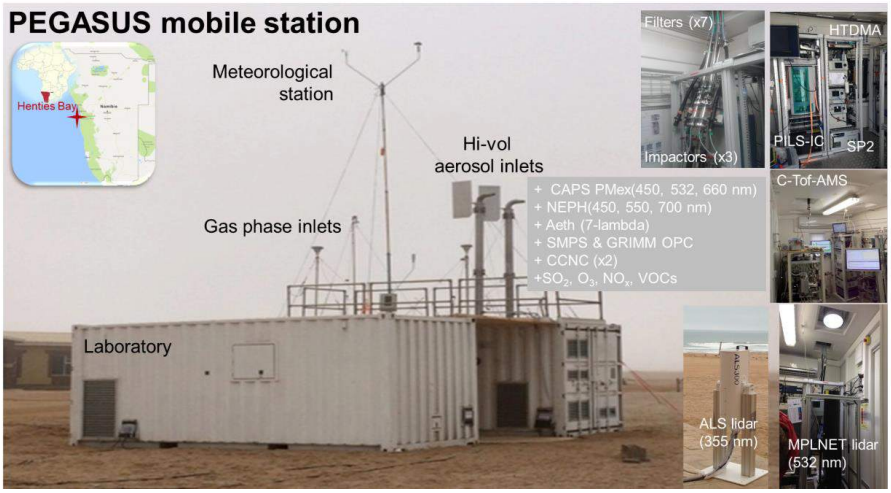

Figure 1. The PEGASUS (Portable Gas and Aerosol Sampling UnitS) mobile station with instruments deployed during the ground-based measurement campaign in Henties Bay (Namibia).

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DETERMINATION OF CONTAMINANT SORPTION CAPABILITY OF BIOCHAR IN CULTIVATED SOILS: MODEL VS REAL SYSTEM APPROACH

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Biochar is the solid carbonaceous residue generally derived by biomass pyrolysis or gasification. Biochar satisfying regulated quality parameters can be used as a soil amendment. Furthermore, due to the very good sorption properties, addition of biochar to soils can reduce the mobility of contaminants and improve their removal efficiency from runoff water and thus preserve riverine and ground water quality.

Within two Emilia-Romagna Region projects PSR misura 16 Focus Area 4B and 5E, biochar synthesized with an innovative up-draft gasifier prototype operating under direct combustion of syngas/tar, has been utilized as amendment in several agricultural soils. The main objective of this study was the assessment of pollutant immobilization capability of biochar itself and of biochar in field-like conditions. To this purpose, conventional adsorption isotherms and a new approach aimed at recreating real system conditions were compared.

Sorption capacity through adsorption isotherms was evaluated for representative inorganic (cadmium) and organic (Broamacil, an herbicide) species at high and low concentration of pollutant. Results revealed that different methods and conditions provided different values of sorption capacity that can be considered only for relative comparative purposes. Therefore, more specific evaluations were performed for real soil/biochar systems, by determining the amount of pollutant released in water by soil and by soil/biochar systems. Soil were enriched in pollutant artificially, by a technique developed *ad hoc* in order to simulate gradual pollution conditions. Soils added with biochar exhibited significantly higher sorption capacity for cadmium and especially for Bromacil. Biochar sorption enhancment was observed in soils with low and high content of inorganic carbon. In conclusion, biochar can be effective in absorbing pollutants in real soil systems.

Acknowledgments

This study was conducted within the projects PSR misura 16 Focus Area 4B and 5E Emilia-Romagna Region. Sauber srl and Super Taurus srl are sincerely acknowledged for their help with the study.

P119

THE HIDDEN MICROPLASTICS: SEPARATION AND CHARACTERIZATION OF MICROPLASTICS AND OF THEIR DEGRADATION BYPRODUCTS IN COASTAL SEDIMENTS

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The environmental pollution by plastic debris directly dispersed in or eventually reaching marine habitats is raising increasing concern not only for the vulnerability of marine species to ingestion and entanglement by macroscopic debris, but also for the potential hazards from smaller fragments down to a few micrometer size, often referred to as "microplastics". A novel procedure for the selective quantitative and qualitative determination of organic solvent soluble microplastics and microplastics degradation products (<2 mm) in shoreline sediments was adopted to evaluate their concentration and distribution over the different sectors of a Tuscany (Italy) beach. Solvent extraction followed by gravimetric determination and chemical characterization by FT-IR, Pyrolysis-GC-MS, GPC and ^{1}H NMR analyses showed the presence of up to 30 mg microplastics in 1 kg sand, a figure corresponding to about 5.5 g of generally undetected and largely underestimated microplastics in the upper 10 cm layer of a square meter of sandy beac. The extracted microplastic material was essentially polystyrene and polyolefin byproducts from oxidative degradation and erosion of larger fragments, with accumulation mainly above the storm berm. Chain scission and oxidation processes cause significant variations in the physical and chemical features of microplastics, promoting their adsorption onto sand particles and thus their persistence in the sediments.

A. Ceccarini, A. Corti, F. Erba, F. Modugno, J. La Nasa, S. Bianchi, V. Castelvetro, The Hidden microplastics: new insights and figures from the thorough separation and characterization of microplastics and of their degradation byproducts in coastal sediments, *Environmental Science & Technology*, in press, available on line, DOI: 10.1021/acs.est.8b01487

P120

ADSORPTION OF FLUORIDE ONTO TUFF VARIETIES OF THE NEAPOLITAN AREA

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Fluoride is a natural and anthropic pollutant of ground waters that can have harmful effects on human health. Concentrations in drinking water exceeding 1.5 mg/L have been shown to cause dental fluorosis, whereas concentrations exceeding 4.0 mg/L cause fluorosis of the bone .[1]. According to the World Health Organization (WHO) recommendation and Italian drinking water standards, the maximum permissible limit of fluoride in drinking water is 1.5 mg/L F-. A recent hydrogeochemical and hydrogeological study, carried out on the groundwater of volcaniclastic aquifers of the Neapolitan area (Fig. 1), showed concentrations of F- greater than 3.0 mg/L.

In this work, we intend to study the acid-base behavior of the tuff varieties Neapolitan area, (Campanian Ignimbrite and Neapolitan Yellow Tuff) and the adsorption equilibria of the fluoride at 25° C, in 0.1 M NaClO4. Furthermore the adsorbent properties of pyroclastic soils, sampled at different depths in a borehole, towards fluoride ions have been studied. Finally, a comparison was made between the adsorbent properties of stale samples with solid phases such as $AlPO_{4(S)}$ and $Al_2O_{3(S)}$, used for the removal of fluoride Ion from the water (Fig.2).

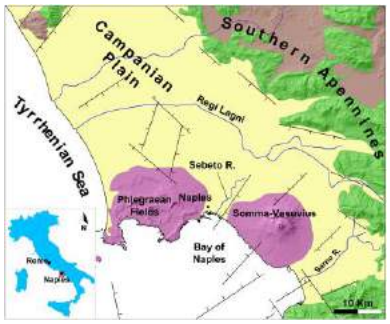

Fig.1. Location of study area

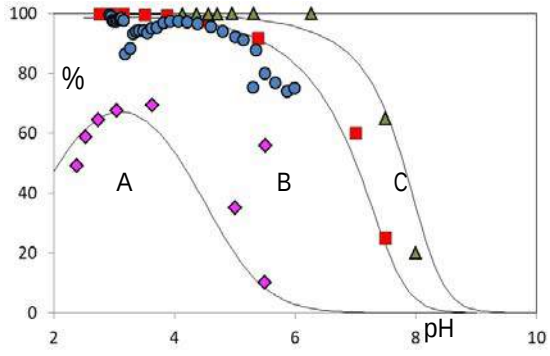

Fig.2. % adsorbed fluoride as a function of pH for solids yellow tuff (A), $AlPO_{4(S)}$ (B) and $Al_2O_{3(s)}$ (C), in suspensions 2.0 g/L at 25° C in 0.1 M $NaClO_4$.

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P121

USE OF ZEOLITES FOR THE ABATEMENT OF AMMONIUM INTO NATURAL WATER AND SAWAGE BREEDING

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Nitrogen, as well known, is a valuable nutrient for plants. The extreme use of nitrogenous fertilizers and zootechnical waste into soil could release high quantities of nitrogenous compounds (such as ammonium) in the groundwaters.
This study has been focused on use of zeolites for the ammonium abatement in polluted waters by ammonia and in a sewage digestate with a high ammonium content.
Zeolites are hydrated aluminosilicate characterized by reversible dehydration, high selectivity and molecular absorbent capacity, a catalytic behavior and high cationic exchange capacity. Key property of those materials is the high number of interconnect porosity and cavity, that is an advantage for ions and water molecules housing.
Making the most of this last property, in this work the zeolites efficiency for the effective ammonium abatement and their utilization in a sewage treatment plant was tested. Several tests in batch were conducted, with and without stirring, using standard solutions and real samples (sewage digested). Different experimental conditions were applied. Laboratory tests have shown positive results for standard solution with an ammonium abatement between 60% to 73%. Higher abatement values were achieved for the real samples, reaching an ammonium abatement of 90%. In particular, these tests showed that ammonium abatement was facilitated by a concentration increase. For this reason the same aliquote of zeolite has been used several times in new different solutions with higher concentration, in order to fill all the active sites until saturation.
The zeolites saturated could be used as slow release fertilizer into the soil. This characteristic was studied with a desorption kinetic in a water solution.
So the use of zeolites in agriculture field could have several advantages:

- An environmental advantage (reducing ammonium and nitrates pollution in waters)
- An economical advantage, because of their cheap costs
- Saturated zeolites could be re-use as fertilizer in the soil.

P122

RELEASE AND SORPTION OF HEAVY METALS FROM BIOCHAR PRODUCED AT DIFFERENT TEMPERATURES

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Biochar, a solid by-product generated during biomass pyrolysis or gasification in the absence (or near-absence) of oxygen, has recently garnered interest for both agricultural and environmental management purposes owing to its physicochemical properties. Biochar is applied to soil systems for soil improvement, mitigation of climate change, and waste management [1]. Although a series of positive effects are associated with biochar application, it's necessary pay attention to the levels of potentially toxic elements including polycyclic aromatic hydrocarbon (PAHs) and metal elements within biochars.
In this study, the release and the sorption of heavy metals from biochars produced at different temperatures were evaluated. In addition, how the metal contents of biochar change according to different conversion temperatures and elements properties was discussed. To this end, in laboratory, spruce chips were pyrolysed at 350, 400, 550, 700 and 1100 °C for 15 or 60 minutes in inert atmosphere. The initial biomass and obtained biochars were characterised. Parameters characterised include: IR analysis, surface area, CHN elemental composition, and element composition. The release tests of metals from produced biochar were performed in water and acetate buffer solution (pH 4) while the sorption tests in acetate buffer solution (pH 4) added with metals (2 mg/l of Al, Fe, Cr, Co, Mn, Ni, Pb, Zn, and Cd).
The biochar yield depends on the temperature and changed approx. from 38% to 23% at 350 and 1100 °C, respectively. The different time of pyrolysis (15 or 60 minutes) has little influence on biochar yield. The concentration of the elements increased with pyrolysis temperature due to the decrease of the carbonaceous matrix. However, some deviations were present depending on the properties of the elements (e.g. Cd, Pb, Zn).
The element release tests showed that K is the more extracted element while Pb, Ni, Cr and Co were negligibly extracted or not at all. The release trends as a function as pyrolysis temperature varied according to considered element. The element sorption tests showed that all considered elements were sorbed, and the sorption increases as function as pyrolysis temperature.
Therefore, the results showed that the release and sorb of elements is affected by element properties and pyrolysis temperature. The ability of biochars, in particular of those produced at high temperatures, to sorb a variety of compounds including heavy metals, is favourable for agricultural field or treatment of contaminated soil.

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P123

STRATIGRAPHIC DATING OF A 80 M DEEP FIRN CORE DRILLED IN COASTAL EAST ANTARCTIC ICE SHEET (EASTERN WILKES LAND)

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The Antarctic ice sheet and the surrounding ocean play a key role in climate dynamics [1]. Causes and control factors of the current climate change are not yet fully understood; for these reasons, increasing attention has been recently paid to natural climate variability over the last millennium, as compared to anthropogenic climate forcing occurred during the last century [2].
In this work we present the stratigraphic dating of the most superficial 80 m of the 250 m firn core, drilled in coastal East Antarctica at GV7 site (70° 41' 17.1" S; 158° 51' 48.9" E; 1950 m a.s.l.). The GV7 drilling was accomplished through a bilateral Italy - South Korea collaboration, during the 2013/2014 Antarctic summer field. Snow pit samples, shallow firn cores and a 250 m deep ice core were collected [3].
Firn core dating is the first step for a correct interpretation of climatic and environmental changes.
The firn core sections were firstly decontaminated, subsampled at 5 cm resolution and analysed using an ion chromatography system that allowed the simultaneous detection of main and trace ions.
Among the analysed ions, nssSO_4^{2-} (sulphates not coming from sea spray) was chosen as chemical marker for dating as it is characterized by a seasonal pattern with summer maxima. Stratigraphic dating was validate by using the volcanic eruptions, well visible in the nssSO_4^{2-} profile as concentration peak lasting more than one year, as historically known as tie point.
The GV7 (B) firn core dating showed clear snow layers from 2008 (first summer peak) to 1775 and six clear volcanic events: Pinatubo (Philippines 1991), Agung (Indonesia, 1963), Krakatoa (Indonesia, 1883), Cosiguina (Nicaragua 1835), Tambora (Indonesia, 1815) and Unknown (1809).
The accumulation rate for the 2008-1775 time period was 191 mm we/yr, slightly lower than 242 mm we/yr found for recent period (2013-2008) from snow pit analysis.

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P124

PAHs AND PCPs IN THE LOWER ADIGE RIVER: AN UNDEREVALUATED MATTER

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Freshwater is an essential resource, vulnerable to several human pressures: the water quality is globally stressed by different anthropogenic pollutants, typically originating from industry, domestic practices and agriculture. Adige is the second longest river in Italy, nevertheless few studies investigated the distribution of anthropogenic organic pollutants in its waters [1]. Even less information is available about the plain part of the basin, where the river is exploited as a water resource for irrigation. Consequently, the river represents a sink for pollution in the upper catchment, turning to a potential source in the lower agricultural plain areas. This study is aimed to evaluate the contamination of the Adige river waters due to Polycyclic Aromatic Hydrocarbons (PAHs) and Personal Care Products (PCPs), including UV-filters (EHS, BP-3, 4-MBC, IMC, EHMC) and Musk fragrances (ADBI, HHCB, AHTN, MM, MX, MK, MT). A single analytical method was developed: water samples were extracted with SPE (HLB Oasis 200 mg) and analyzed by GC coupled to a triple-quadrupole (QqQ) mass spectrometer (Agilent). The coupling of PAHs with PCPs may help the identification of the major environmental drivers [2]: the different classes of the analytes are representative of urban and industrial contamination, potentially reflecting the inputs deriving from the cities (e.g. Bolzano, Trento, Verona) set in the upper river catchment.

Figure 1. Map of the Adige river basin [1]

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P125

CHARACTERIZATION OF THE OXIDATIVE POTENTIAL OF WATER SOLUBLE FRACTION OF ATMOSPHERIC AEROSOL IN AN URBAN BACKGROUND SITE IN SOUTHERN ITALY

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Several studies point out oxidative potential (OP) as a quantitative indicator of multiple particulate matter (PM) health effects, since OP of ambient particles causes high concentrations of reactive oxygen species (ROS).

ROS concentrations, in excess of the antioxidant capacity to neutralize them, lead to oxidation of other cellular components, which eventually translates into numerous health consequences. Indeed, although the human body is capable of settle with ROS, diseases can overcome or weaken the defense mechanisms. In that case, ROS can generate a series of damaging events. Oxidative potential (OP) is defined as a measure of the capacity of PM to oxidize target molecules. It has been proposed as an indicator related to biological reactions to PM exposures and thus could be more revealing than mass concentration alone. Over the years, several methods for testing OP have been developed. In this work, we evaluated the OP of the water-soluble fraction of $PM_{2.5}$ and PM_{10} using the a-cellular DTT (dithiothreitol) test. The consumption of dithiothreitol (DTT) is based on the ability of redox active compounds to transfer electrons from DTT to oxygen.

Briefly, aliquots of $PM_{2.5}$ and PM_{10} water extracts were incubated with DTT. The reaction was stopped at designated time points, adding 5,5′-Dithiobis(2-nitrobenzoic acid) (DTNB). The absorbance at 412 nm was recorded and the rate of DTT consumption (δDTT, pmol/min) was determined from the slope and intercept of linear regression of measured absorbance versus time. Three replicates were done, for each sample, and the standard deviation among the replicates was taken as uncertainty of the measured DTT activity.

Daily (from 15/11/2016 to 15/11/2017) $PM_{2.5}$ and PM_{10} samples were simultaneously collected, on quartz substrates, using a dual channel low-volume (2.3 m^3/h) sampler (SWAM, Fai Instruments). The samples were collected at the Environmental-Climate Observatory of Lecce, regional station of the Global Atmosphere Watch (GAW-WMO) network, that could be considered an urban background station located at 4 km from the town of Lecce and between 30 km and 80 km from large industrial sites of Brindisi and Taranto. Finally, seasonal variability of measured DTT activity was investigated and correlated with aerosol concentrations observed on collected samples.

P126

VARIATION OF LEVELS OF FATTY ACIDS COMPOSITION IN THE LIVER OF ANTARCTIC FISH *TREMATOMUS BERNACCHII* IN FUNCTION OF TIME AND TEMPERATURE: A MODELLING APPROACH

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Global climate change is causing an increase in mean world temperature and an increase in seawater temperature. A variation of temperature corresponds at local changes in species composition and acclimation to higher heat tolerance [1].
The present research aimed at modelling the effect of the variables time and temperature as a function of the levels of fatty acids in liver of Antarctic fish *Trematomus bernacchii*. This fish is an ubiquitous specie of stenothermal Antarctic teleost (family Nototheniidae), well adapted to the extremely low temperatures of the Antarctic region (-1.86°C) and considered a key indicator for monitoring anthropogenic impact [2].
During the 28th Italian Antarctic Expedition (austral summer 2014–2015), sexually mature specimens of *T. bernacchii* were caught by a fishing rod in Tethys Bay (74°42'052'' S, 164°02'267'' E) at the depth of ~30 m, Ross Sea, Northern Victoria Land. After a period of acclimation at -1.8 °C, fishes were kept in tanks at 0, +1 or +2 °C, and sacrificed after 1, 5 and 10 days. The choice of these temperatures as thermal stress was based on shelf water warming until +0.8-+1.4 °C predicted around 2200 for the Ross Sea region. The fatty acid composition of the liver was determined by gas chromatography coupled with a flame ionization detector. Changes in fatty acid composition of liver from *T. bernacchii* were studied as a function of the time and temperature of exposure by using polynomial models.
Major changes in fatty acid composition were observed at 1 day of exposition to a higher temperatures. At 5 days, the fish start adapting to the new temperature condition. The concentrations of saturated fatty acids were almost constant throughout the various conditions. The monounsaturated fatty acids (in particular 18:1n-9) decreased after 1 day of exposure to higher temperatures. In contrast, the polyunsaturated fatty acids (in particular 20:5n3 and 22:6n-3) increased throughout the various conditions.
The proposed models were in agreement with reported studies on polar and temperate fish, indicating possibly similar adaptation mechanisms for teleost to cope with global warming.

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P127

DETERMINATION OF KEY COMPOUNDS IN ANAEROBIC DIGESTION AND BIOMETHANE PRODUCTION: VOLATILE FATTY ACIDS AND METHYL SILOXANES

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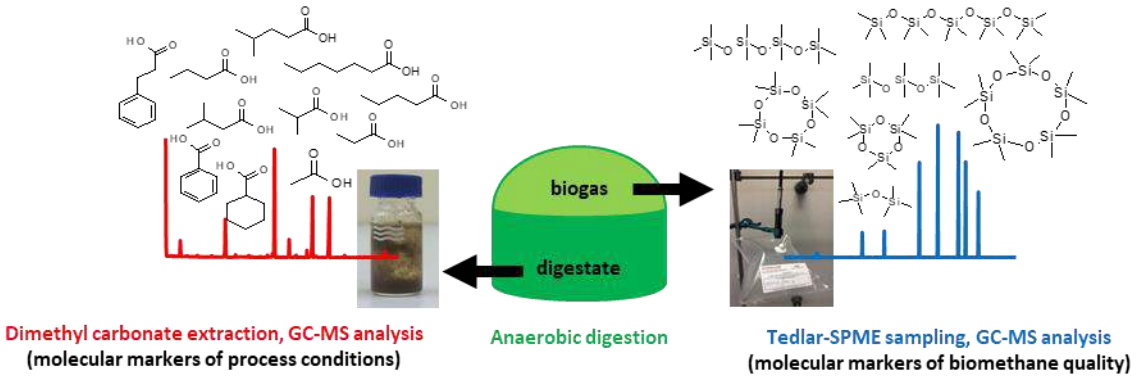
Anaerobic digestion of waste biomass produces biogas that can be upgraded to biomethane and subsequently injected in the natural gas grid or used as a transportation biofuel. Within the biomass to biomethane route, monitoring anaerobic digestion process is fundamental to maximize biogas production. Volatile fatty acids (VFA) are key intermediate products of biopolymers degradation that can suitably indicate the occurrence of system stress [1]. Moreover, the quality of biomethane is determined by the concentration of impurities. Siloxanes are widely used in consumer and industrial products, and their degradation products (volatile methyl siloxanes, VMS) are considered emerging contaminants in the environment. VMS can hamper biomethane combustion performance due to the formation of microcrystalline silicon dioxide [2]. Currently there are no standardized methods for the quantification of VFA in digestate of anaerobic digestion and VMS in biogas/biomethane. VFA are commonly analyzed by direct injection into GC-MS after aqueous extraction, but this procedure can cause rapid deterioration of GC apparatus. VMS are sampled from biogas streams through adsorption onto cartridges and thermally desorbed or solvent-extracted. The present study reports the development of a new method of extraction of VFA from digestate samples with dimethyl carbonate (DMC), followed by GC-MS analysis. The method was applied to a wide set of samples from anaerobic digesters operating with several biomass feedstocks and allowed the detection of new molecular markers (aromatic and alicyclic carboxylic acids). The use of solid-phase microextraction (SPME) was investigated for the first time as fast method for the analysis of VMS in raw biogas and upgraded biomethane.
Acknowledgements: "GoBioM" POR-FESR 2014-2020 Regione Emilia-Romagna.



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P128

SYNCHRONIZATION OF FIVE ANTARCTIC ICE CORES ACROSS THE LAST ICE AGE.

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A bunch of information about the atmospheric composition in the past can be extracted from polar ice cores, and the accomplishment of this knowledge represents a key step toward a better understanding of past climate changes in order to predict future global changes. The huge potential of the ice archives can be exploited only when a fully reliable age scale is available; this holds true especially when comparing different ice cores drilled at the same site or, to a major degree, drilled at sites far away from each other.
Volcanic reference horizons provide the most precise way to synchronize ice-core age scales. Within the last decade, progress has been made in volcanically linking the EPICA (European Project for Ice Coring in Antarctica) Dome C (EDC) ice core to the EPICA Dronning Maud Land (EDML) core, the Talos Dome (TAL) core, and the Dome Fuji (DF) core. Here we provide new volcanic stratigraphic links between the WAIS (West Antarctic Ice Sheet) Divide ice core (WDC) and the EDML, EDC and TAL cores, based on pattern matching of volcanic peaks in high-resolution records of either sulfur (WDC) or sulfate (EDML, EDC, TAL).
The period covered by our volcanic synchronization among these ice cores reach 60.000 years BP (i.e before 1950 CE). The high resolution sulfur/sulfate data for each core were achieved using different analytical techniques. For the EDC and Talos Dome cores we used two different Fast Ion Chromatographic (FIC) methods able to analyze chloride, nitrate and sulfate with a resolution ranging from 2 to 4 cm. The EDML core was analyzed using an Ultra-FIC method able to measure only sulfate with a depth resolution of about 0.8 cm. The WAIS core was analyzed at the Desert Research Institute (DRI) using two Thermo Element-2 HR-ICP-MS measuring the total sulfur amount in the ice.
The synchronization among these five ice cores will represent a key tool in highlighting the relationships between several climate-related markers such as stable isotopes, sea-spray components, etc.

P129

DETERMINATION BY GC-MS/MS AND GCXGC-TOFMS TECHNIQUES OF PERSISTENT ORGANIC POLLUTANTS IN BIOTA: DEVELOPMENT AND VALIDATION OF A MODIFIED QUECHERS EXTRACTION

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Environmental monitoring plays an important role in pollution prevention and human health protection. As reported in the Directive 2000/60/EC, establishing a framework for Community action in the field of water policy, "community water policy should be based on a combined approach using control of pollution at source through the setting of emission limit values and of environmental quality standards (EQS)". EQS means the concentration of a particular pollutant or group of pollutants in water, sediment or biota which should not be exceeded in order to protect human health and the environment. Environmental pollution prevention is one of the main goals of world environmental legislation; recently, the new law n. 68/2015 introduces a specific chapter on environmental crimes such as environmental pollution.
Our topics focus on the development and validation of analytical methods in order to evaluate persistent organic pollutants in biota matrix. In particular, a fast and easy modified QuEChERS (quick, easy, cheap, effective, rugged, safe) [1,2] extraction and gas chromatography mass spectrometry (GC-MS/MS and GCxGC-TOFMS) methodologies were developed and implemented for the quantification of 23 polycyclic aromatic hydrocarbons (PAHs), 29 polychlorinated biphenyls (PCBs) and 23 pesticides in fish matrix (*Mullus Surmuletus*). Different extraction and clean-up methods were investigated to clearly enhance the recoveries of analytes. The QuEChERS method was based on extraction with acetonitrile and, prior to dispersive solid-phase extraction (SPE) clean-up, the extract was freezed to remove fatty acids. Internal standard calibration was employed to quantified IPA, PCB and pesticides. The developed method was validated: recoveries at 10 and 25 µg/kg were within 70-120% for many analytes with coefficient of variation, CV<15%; the quantification limit (LOQ) were 5-10 µg/kg for PAHs, 1-5 µg/kg for PCBs, 10-20 µg/kg for pesticides. This method was successfully applied for preliminary analysis of *Mullus Surmuletus* samples from the local fish market.

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Acknowledgements: Piano per la ricerca linea di intervento 2

P130

INSIGHT ON THE OCEAN-ATMOSPHERE INTERACTION IN POLAR SOUTHERN EMISPHERE BY LONG TERM AEROSOL MEASUREMENTS IN CENTRAL ANTARCTICA.

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The complex interconnection between ocean and atmosphere is a critical issue in understanding feedback processes related to climate change. Within this issue the polar region are critical environment due to the presence of sea ice. Ice-covered seas are particularly important for biological activity producing large amount of marine biogenic aerosol. The understanding of factor affecting biogenic activity also in relation of sea ice dynamic is a hot topic in a climate changing word due to the effect on CO_2 uptake from the atmosphere by photosynthesis and the production of biogenic aerosol having direct and indirect effect on solar radiation. Biogenic sulphur aerosol is produced by the oxidation of the dimethylsulphyde produced by phytoplankton. Atmospheric records of sulphur aerosols in polar region are one of the most important tools to achieve such a knowledge. In particular, central Antarctic Plateau offer the unique possibility to obtain information of large aerosol source areas of Southern Ocean.
Ten years data of atmospheric oxidised sulphur compounds (methanesulphonic acid-MSA) and non-sea salt sulphate, $nssSO_4^{2-}$) from the east Antarctic Plateau at Dome C (75° 06' S, 123° 20' E, 3220 m a.s.l. and 1100 km away from the nearest coast) are here presented. The two sulphur-derived species exhibit a seasonal cycle characterised by maxima in the summer from October to March. In particular MSA presents two summer maxima the first one in November and the second in February, the latter with MSA concentrations higher than the first-one. The two maxima are characterized by different size distribution and are related to different source area of DMS characterized by different timing of primary production.

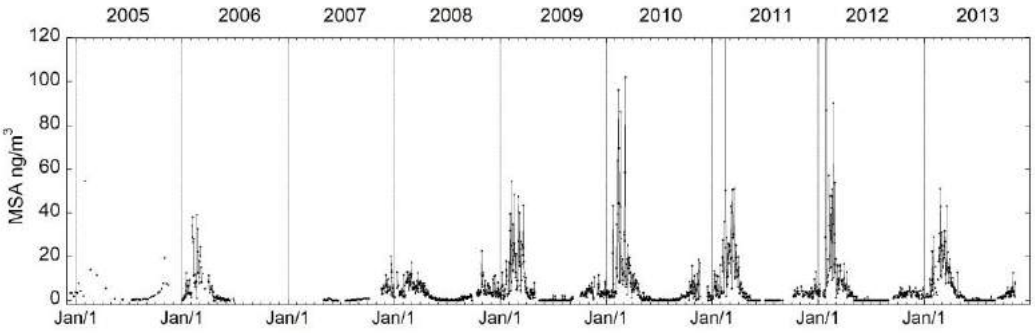

Figure 1. Time evolution of MSA in PM10 sampled at Concordia Station (East Antarctic Plateau).

P131

Thermodynamic properties of Levulinic acid, a sustainable platform molecule

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Levulinic acid (LA) was considered by the US Department of Energy [1] one of the chemicals on the list of green chemical building blocks that can help to reduce dependence on fossil fuels. The knowledge of its thermodynamic behavior is required for optimization of reaction conditions for production of useful platform chemicals from the renewable sources. LA acid–base properties were studied by potentiometry and calorimetry. We determined the protonation constant ($logK^H$) in $NaCl_{(aq)}$ (at 298.15 and 310.15 K) and in $Et_4NI_{(aq)}$ (at 298.15 K) at different ionic strengths (*I*), and also the formation constants of Ca^{2+} and Mg^{2+} complexes at different *I* of $NaCl_{(aq)}$ at 298.15 and 310.15 K. In addition, we performed distribution measurements between 2-methyl-1- propanol/pure water (or NaCl aqueous solutions up to *I* = 1.00 mol kg^{-1}) to determine the salting parameter and consequently the activity coefficient of the neutral species by means of the Setschenow equation. The dependence of the $logK^H$ on *I* was modeled using the DH type, SIT and Pitzer approaches. For the $logK^H$, the thermodynamic value $logK^{H0}$ = 4.62 ± 0.01 was obtained at infinite dilution at T = 298.15 K, in the molal concentration scale, while the Setschenow coefficient k_m= 0.08±0.01. At infinite dilution and at T = 298.15 K the protonation enthalpy change is ΔH^0 = -2.5±0.5 determined by calorimetric titrations.

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P132

As(III) INTERACTION WITH NITRILOTRIACETIC ACID DERIVATIVE COMPOUNDS IN AQUEOUS SOLUTION

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Arsenic is a metalloid easily found in the environment, both for natural and anthropogenic processes. Its toxicity is related to the speciation and, in fact, arsenate and arsenite are considered more dangerous in comparison with the organic forms. They also are the most common species in natural waters and its distribution mainly depends on the pH and redox potential [1-2]. In literature some studies related to As(III) interaction with biological molecules are reported, since it shows a very good affinity for the thiol groups of proteins. The aim of this contribution is to investigate the interaction of As(III) with ligands of environmental interest, such as phosphonate compounds, since their chelating properties are well known and they could represent an alternative method to remove this pollutant from natural waters. In the last years, a study based on the complexation of some particularly toxic cations with molecules derived from the nitrilotriacetic acid by systematically substitution of the three acetate groups with one (NTAP), two (NTA2P) or three (NTA3P) phosphonates was carried out [3]. In this work, we extend this study to As(III), developing a thermodynamic investigation performed at different ionic strengths in order to evaluate the dependence on the ionic strength of the complexes stability constants by means of a Debye-Hückel type equation. For all the systems, the speciation model is featured by the ML, MLH and MLH_2 species. Moreover, for As(III)-NTA2P and As(III)-NTAP a mixed hydrolytic species (MLOH) was determined and MLH_3 and MLH_4 complexes were observed for As(III)-NTAP and As(III)-NTA3P respectively. As regards the ML species, the stability constant value follows this trend: NTA3P > NTA2P > NTAP. For all the ligands, the sequestering ability was investigated using an empiric parameter, $pL_{0.5}$, which represents the total concentration of ligand required to sequester the 50% of the metal in trace amount [4]. It was determined at pH and ionic strength typical of a fresh water and seawater.

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The authors thank FSE regional fund for PhD support to D.C.

P133

METAL-BINDING ABILITY OF CALCITERMIN, AN ANTIMICROBIAL PEPTIDE OF HUMAN AIRWAYS

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Calcitermin is a 15-mer peptide recently isolated in the human airways [1]. Its sequence (VAIALKAAHYHTHKE) exactly corresponds to the C-terminal domain of Calgranulin C, a calcium-binding protein of the S100 family which have been shown to have antimicrobial properties. While Calcitermin did not show any antimicrobial activity in phosphate buffer at pH 7.4, when pH was lowered to 5.4, it was active against *E. coli*, *P. aeruginosa* and *C. albicans*. In addition, it was demonstrated that zinc improves the antimicrobial activity of Calcitermin against both *E. coli* and *L. monocytogenes* [1].

Calcitermin possesses a putative metal-binding domain, containing three histidines separated by one different amino acid. The above results prompted us to deeply investigate complex-formation equilibria of Calcitermin with Zn(II) and Cu(II), two endogenic and competing metal ions. Three peptide analogues, where one His residue has been substituted by an alanine (VAIALKAAAYHTHKE, VAIALKAAHYATHKE, VAIALKAAHYHTAKE) have been also studied, for the sake of comparison, in order to shed light on the role played by each histidine in the sequence. The experiments have been performed in aqueous solution, at 25 °C and I = 0.1 M (KCl), by potentiometry, mass spectrometry and several spectroscopic techniques.

The preliminary results show that all the investigated peptides are good ligands for the considered metal ions (see Fig. 1), although copper complexes are far more stable than zinc ones. The presence of three His residues makes wild-type Calcitermin the best ligand among the four peptides.

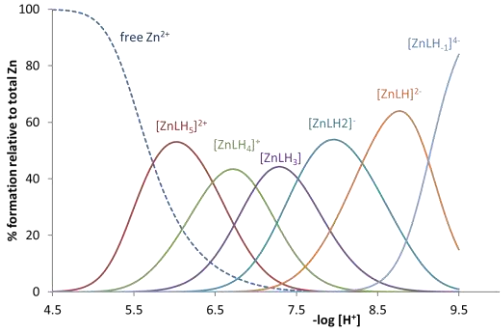

Figure 1.

Representative distribution diagram for the formation of Zn^{2+} complexes with Calcitermin (L^{3-}) at 25°C and I = 0.1 M (KCl). $[Zn^{2+}]_{total}$ = 0.36 mM; Zn/L molar ratio = 0.9:1.

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P134

STUDY ON THE INTERACTION OF Ca^{2+} WITH AMPICILLIN AND AMOXICILLIN IN AQUEOUS SOLUTION

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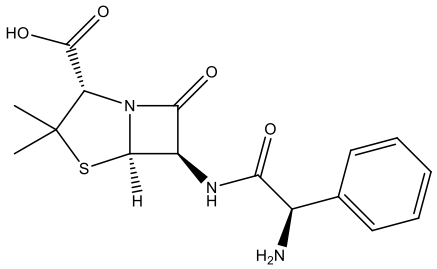
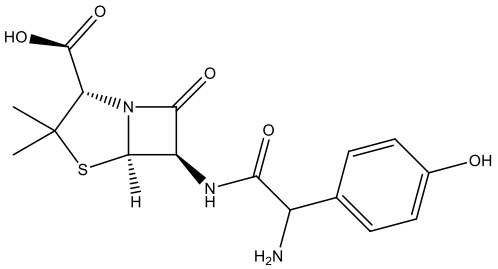
Ampicillin (*Amp*) and amoxicillin (*Amox*) (Figure 1) are the most important amino-penicillins for their wide spectra/mechanisms of action. Owing to the biological relevance of calcium, a study on its ability to interact with *Amp* and *Amox* was undertaken. More in detail, a potentiometric and UV spectrophotometric investigation on the interaction of Ca^{2+} with *Amp* and *Amox* was conducted in NaCl aqueous solution at I = 0.15 mol L^{-1} and at different temperatures (15, 37, 45°C). At t = 25°C the dependence of formation constants on ionic strength was also investigated in the range $0.15 \leq I$ / mol $L^{-1} \leq 1$.

The speciation models proposed on the basis of potentiometric results include MLH, ML and MLOH species for Ca^{2+}-*Amp* system and MLH_2 and MLH species for Ca^{2+}-*Amox* one. For the common species MLH, log$K$ = 2.05, 2.69 for *Amp* and *Amox*, respectively, under physiological conditions (t = 37°C and I = 0.15 mol L^{-1}). The agreement between the formation constants of the species of both systems, obtained by potentiometry and UV spectrophotometry, at t = 25°C and I = 0.15 mol L^{-1}, is very good, fully confirming the potentiometric findings. The results at different temperatures have shown the decrease of formation constants with the increasing of the temperature. By Van't Hoff equation the enthalpy change values were obtained for all the species. For example, for Ca^{2+}-*Amox* system, ΔH = -61, -43 kJ mol^{-1}, for MLH_2 and MLH species, respectively (t = 25°C and I = 0.15 mol L^{-1}), fairly close to -54 and -38 kJ mol^{-1}, for Mg^{2+}-*Amox* species with the same stoichiometry (t = 25°C and I = 0 mol L^{-1}) [1].



Amp



Amox

Figure 1. Structures of ligands understudy.

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P135

ON METAL-LIGAND SYSTEMS AS CONTRAST AGENTS IN DIAGNOSTICS (MRI)

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Magnetic Resonance Imaging is a non-invasive medical imaging technique based on the magnetic fields of protons within the body, producing two-dimensional views of internal organs or tissues. The technique is based upon the principles of nuclear magnetic resonance, and MRI contrast agents are chemical compounds that are able to markedly alter the relaxation times (T1 and T2) of water protons in tissues where they are distributed. Paramagnetic and ferromagnetic materials can act as contrast agents. On the basis of different mechanisms of action, they affect the relaxation time of water[1]. Positive contrast agents are commonly made up of paramagnetic materials, mainly those based on metal ions with large numbers of unpaired electrons, such as Mn^{2+}, Fe^{3+}, and Lanthanides (typically Eu^{3+}, Gd^{3+}, Tb^{3+}).
Lanthanide complexes with ligands such as 1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid (DOTA, Figure 1) and its derivatives are used as contrast agents for Magnetic Resonance Imaging (MRI). The use of complex ions originates in the toxicity of most of the paramagnetic metals. To prevent their bond with molecules inside the body, and therefore to reduce their toxicity, these metal ions are masked with ligands able to chelate. The DOTA ligand has four pendant carboxylated arms linked to the amines of the cycle. This molecule turns out to be an excellent complexing agent of metals, in particular of lanthanides. The M-DOTA complexes are characterized by a structure that incorporates a water molecule (the chelator shows an octaedric geometry) in the coordination, which makes them monitorable[2]. In this work we present a thermodynamic study on metal ions-DOTA aqueous systems. Complex formation between Zn(II), Eu(III) and DOTA was investigated in 0.5mol/dm^3 NaCl as ionic medium. The study has been conducted at 25.00±0.02°C by using electrochemical techniques, such as potentiometry and polarography, and spectroscopic, such as infrared spectrophotometry (FTIR) and mass spectrometry (MALDI, ESI).

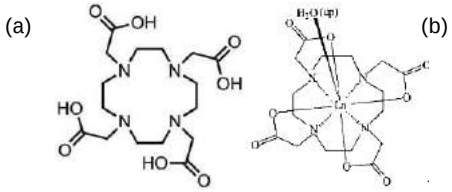

Figure 1. (a)1,4,7,10-Tetraazacyclododecane-1,4,7,10-tetraacetic acid and (b) Ln-DOTA.

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P136

AUXINE: THERMODYNAMIC PROPERTIES, COMPLEXING ABILITY AND DOSAGE IN HUMAN SERIUM

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The Auxins are phytohormones that govern and regulate the growth and development of plant organisms, as well as being the most abundant hormones present in plants. All natural and synthetic auxins are structurally similar to 2-(1H-indol-3-yl)acetic acid, the mother molecule of this class of photons. The 2-(1*H*-indol-3-yl)acetic acid, IAA, is a carboxylic acid (acid function) containing an indolic group, a heterocyclic system consisting of a benzene ring and a pyrrole ring, see figure 1.
The IAA, defined as "growth hormone", acts as a modulator for the growth and development of plants, intervening in cell elongation, vascular differentiation, fructification, lateral formation and root and regulates apical domination. Recent studies have shown that IAA has also been found in the blood of mammals including humans, but the effects are clearly different, in fact in this case is considered a uremic toxin, the increase in its concentration is directly proportional to the decline in renal function. For this reason, the 2-(1*H*-indol-3-yl)acetic acid is considered a biomarker of renal function.
As consequence of the importance of this ligand, the dosage in different human serum by HPLC was performed and a detailed speciation study has been carried out. In particular, the solubility and the acid-base properties of the ligand were studied in NaCl and $(C_2H_5)_4NI$ aqueous solutions at different ionic strengths ($0.15 \leq I/mol\ dm^{-3} \leq 1.0$) and at T= 298.15 K.
The complexing ability of 2-(1*H*-indol-3-yl)acetic acid was studied towards three metal cations, Zn^{2+}, Cu^{2+} and Ca^{2+} by potentiometry.

Figure 1. 2-(1H-indol-3-yl)acetic acid.

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LIPID PROFILING OF *LUPINUS LUTEUS* BY HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY COUPLED TO ELECTROSPRAY IONIZATION AND MULTISTAGE MASS SPECTROMETRY (HILIC-ESI-MS^n)

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The lupins are fruits of an annual herbaceous plant belonging to the family of the Febaceae, genus Lupinus, specie albus. There are 12 lupin species native to Europe and Mediterranean regions, two of them are fully domesticated for agriculture: the European white lupin or *Lupinus albus* and the yellow lupin or *Lupinus luteus* [1]. Edible lupins are usually cooked and stored in salts to remove some undesirable substances such as alkaloids loosing other useful substances such as vitamins. Lupins are more and more used to replace cereals or soy in baked goods or pasta, as they do not contain gluten, so they are suitable for celiac people. Lupins can be considered as a nutraceutical food since they are known to lower the glycemic index and to play a key role in opposing obesity and diseases such as diabetes and heart disease [2]. In addition, the feeding of lupins leads to a cholesterol decrease thanks to the high fiber content improving the intestinal function and to a blood pressure regulation being rich in arginine. Although lupins are currently under widespread cultivation around the world as a green manure, livestock fodder and grazing plant, and high-protein additive for animal and human foods, few studies have been focused on the characterization of fatty acids [3]. As far the total lipid characterization only the identification of major phospholipid classes is reported by recurring to thin layer chromatography with reference standards [4].
In this work, hydrophilic interaction liquid chromatography (HILIC) coupled to high resolution/accuracy Fourier-transform mass spectrometry with electrospray ionization (HILIC-ESI-FTMS) or to linear ion-trap multiple-stage mass spectrometry (HILIC-ESI-LIT-MS) was used to characterize major and minor lipids occurring in *Lupinus luteus*. The combination of accurate MS and tandem MS measurements allowed to identify more than 200 neutral and polar lipids including acylglycerols, glycolipids, glycerophospholipids and glycosphingolipids.

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P138

CHARACTERIZATION OF A SINGLE CYSTEIN-ENRICHED PHASEOLIN EXPRESSED IN TRANSPLASTOMIC TOBACCO PLANTS

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Recently, transformation of chloroplast genome has been used for the production of heterologous proteins. We transformed tobacco chloroplasts with two different versions of the storage protein of *Phaseolus vulgaris,* phaseolin (with or without signal peptide), in which a cysteine residue has been added to its C-terminal region. This modification allows for the formation of inter-chain disulfide bonds. The aim is to demonstrate the different ability of chloroplast compartments (stroma and thylakoids) in the formation of phaseolin polypeptides held together by disulfide bonds. The presence of the signal peptide should direct phaseolin into the thylakoid compartment, where the protein is able to form disulfide bridges and high molecular weight polymers[1]. It is then necessary to assess whether the extracted proteic matter consists of polymer, protein oligomers, or both. To verify the effect of the peptide modification and to quantify the polymer formation, we employed hollow-fiber flow field-flow fractionation coupled to UV and multi-angle laser scattering detection (HF5-UV-MALS). HF5 allows for the selective size-based separation of nano- and micro-sized particulate, while smaller species are filtered away in the pre-separation step[2]. Hence, HF5-UV-MALS showed its effectiveness both in sample purification and characterization of fractionated species in terms of spectroscopic behavior and molar mass.
We observed that both stroma and thylakoid-derived extracts contained phaseolin polymer (with a molar mass above 1 MDa), whereas PBS proved to be a more efficient extraction solvent than alcoholic mixtures. The formation of phaseolin polymers in these plant compartments, not detected in *P. vulgaris*, could be very interesting for industrial purposes. Chloroplasts could be employed as a reactor to produce a biopolymer derived from an edible protein. A possible application is the production of biodegradable films.

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P139

DESI-HRMS DETERMINATION OF NEW PSYCHOACTIVE SUBSTANCES IN ORAL FLUIDS BY USING NOVEL SAMPLING SUBSTRATES

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New psychoactive substances (NPS) are a large group of drugs of abuse including synthetic cannabinoids, synthetic cathinones, ketamine and ketamine derivatives. In addition to their adverse effects, one of the most alarming data relies on the age of the consumers, being mostly school-age teenagers. The development of rapid and non-invasive methods for NPS determination is a key parameter for assessing their consumption. Desorption electrospray ionization-mass spectrometry (DESI-MS) is an emerging analytical technique that enables in situ MS analysis of specimens under ambient conditions without sample preparation/pre-treatment [1]. In this context, the role of new materials as sampling substrates is of paramount importance to increase the instrumental response of the analytes. In a research program dealing with the development of new analytical strategies in forensic science using DESI-MS [2], our attention was focused on the development and validation of a screening method for the quantitation of NPS in saliva by microextraction by packed sorbent (MEPS)–desorption electrospray ionization-high resolution mass spectrometry (DESI-HRMS). Different materials were synthesized and tested as DESI-MS supports, i.e. commercial PTFE slides, homemade poly(lactic acid) (PLA)-based films and a silica-based coating. Both unfunctionalized PLA and the silica-based coating proved to be the best choice for the detection of the investigated compounds. A full factorial design followed by the multicriteria method of desirability functions was used for the optimization of the MEPS conditions. Finally, method validation proved reliability of the developed method for the analysis of NPS in oral fluid samples at trace levels.

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P140

DETERMINATION OF POLYCHLORINATED DIBENZO-P-DIOXINS (PCDDs), POLYCHLORINATED DIBENZOFURANS (PCDFs) AND POLYCHLORINATED BIPHENYLS (PCBs) IN HENS EGGS

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Dioxins (PCDDs and PCDFs) and PCBs are persistent environmental pollutants, associated with several human health effects mainly linked to endocrine interference.
The aim of this work was to validate a method for the quantitative analysis of 7 PCDDs, 10 PCDFs and 12 dioxin-like PCBs (DL-PCBs) in hens eggs which are considered one of the most common and cheap food for human consumption giving in the early years several exceedings of maximum permitted limits set by Commission Regulation EU 1259/2011 [1].
Eggs samples from different conventional production systems were used for the validation study. The method was developed in accordance with US EPA method 1613 revision B and 1668 revision C and employed the isotope dilution technique. Pre-treatment of samples consisted of freeze-drying and extraction using an Accelerated Solvent Extraction (ASE, Thermo Fisher Scientific) system, clean up using first a multilayer acid column and then a Power Prep system (FMS). The instrumental analysis was conducted using a high-resolution gas chromatograph coupled to a high-resolution mass spectrometer (DFS, Thermo Fisher Scientific) operating at a resolution of 10000.
The validation study resulted in accordance with the performance requirements fixed by ex Commission Regulation EU 589/2014 (current Comm. Reg. EU 644/2017). Accuracy and precision were evaluated in the range of the maximum levels and for the sum of PCDDs, PCDFs and DL-PCBs ranged between 91 - 110 % and 4 - 8 %, respectively. In addition, the method was accredited by the Italian accreditation body Accredia and was used for the determination of dioxins and PCBs in official samples from different types of egg farming. All analyzed samples were compliant with the maximum limits and eggs from free-range hens showed higher levels of PCDDs, PCDFs and DL-PCBs than those found in conventionally produced eggs according to the data reported by EFSA [2].

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FIRST DETERMINATION OF CYLINDROSPERMOPSIN IN DRINKING WATER CHAIN OF VICO LAKE WITH SPE-LC-MS/MS

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The incidence of cyanobacterial harmful algal blooms (CHABs) is increasing in Italy and worldwide. Cyanotoxins cause a substantial amount of human and animal poisoning from exposures in drinking-source and potable waters.
Cylindrospermopsin (CYN) is a hepatotoxin and nephrotoxic cyanobacterial produced by *Cylindrospermopsis raciborskii* and other cyanobacteria such as *Umezakia natans*, *Aphanizomenon ovalisporum* and *Raphidiopsis curvata*; it is also considered a potential carcinogen.
Cylindrospermopsin in an alkaloid compound characterized by with a guanidico tricyclic group combined with hydroxymethyl-uracil.
This study describes the first occurrence of cylindrospermopsin during a serious bloom of cyanobacterium *Aphanizomenon ovalisporum* with maximum algal density exceeding 3.5 million cells/L observed since the beginning of 2010 in Vico Lake (Lazio, Italy).
The water of this lake was even used for human consumption, so it was necessary started a monitoring activity for the identification and the quantification of the cyanobacteria presents in the water and the cianotoxins eventually produced.
The samples of raw, treated and drinking water from Vico Lake were monthly collected over a seven years-period with simultaneous determination of cyanotoxins concentration and algal population.
An analytical protocol based on solid phase extraction followed by detection with liquid chromatography–tandem mass spectrometry (SPE-LC-MS/MS) has been employed and optimized for the determination of the cylindrospermopsin in the water samples.
For determination of cylindrospermopsin, chromatographic gradient was employed, using acetonitrile (component A) and water (component B) as mobile phases, both containing 10 mM formic acid, by using a Dionex Ultimate 3000 HPLC system (Dionex Corporation, Sunnyvale, CA, USA) equipped with a Zorbax SB-Aq (4,6 mm ID x 150 mm, 5 µm, Agilent).
MS analyses were carried out using an API 3000 triple-quadrupole mass spectrometer (Applied Biosystem) operating in positive ionization mode and Multiple Reaction Monitoring acquisition.
That method was proved to be robust and very sensitive, with LOD of 0,001 µg/L. Cylindrospermopsin was sporadically observed through the entire drinking water chain, in raw, treated and distributed water from Vico basin, with maximum concentration of 0.552, 0.187 and 0.167 µg/L respectively.

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SURFACE MODIFICATION OF CHITOSAN FILMS WITH FIBRONECTIN-DNA APTAMER COMPLEX TO ENHANCE OSTEOBLASTIC CELL ACTIVITY: A MASS SPECTROMETRY APPROACH TO PROVIDE EVIDENCE ON PROTEIN BEHAVIOR

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Biomaterials are widely used to develop active medical devices capable of triggering a process of tissue regeneration and functional restoring [1]. During these processes, the extra cellular matrix with its complex and dynamic microenvironment plays a pivotal role in regulating the mechanism of cell adhesion, growth and proliferation. Thus, the direct combination of scaffold functionalized with simplified ECM proteins are widely studied as promising support for a broad range of biomedical application [2]. Direct functionalization of a surface with an active molecule could result in random non specific adsorption, loss of functionality or triggering of unwanted reactions. For these reasons, advances in understanding dynamic interaction mechanisms represent an important step for the design of supports with improved efficacy in tissue regeneration. Here mass spectrometry (MS) is successfully applied as current analytical method to study the interactions between a fibronectin fragment (FN) and a specific aptamer. First, the dynamics of FN in aqueous solution, in presence or absence of anti-FN specific DNA aptamer, are described. Thus, the same study is carried out on chitosan-based films, functionalized with the FN only or through the aptamer as selective spacer. The results obtained are compared and discussed. HDX-MS analysis showed that Fb exchanged fewer H+ atoms when bound to aptamers, indicating that some of the H+ initially available for exchange are engaged in protein-aptamer interactions. Moreover HPLC-MS analysis identified the YVVGETWEKPYQGWMM, QAQQMVQPQSPVAVSQ, YRVGDTYERPKDSMI and WERTYLGNAL fragments involved in the interaction with aptamers. Compared to Fb on chitosan, more fragments were generated by trypsin digestion of Fb bound to the chitosan-aptamer complex. These findings indicated an improved functionalization of chitosan in terms of Fb biological activity when the aptamer was used as selective spacer. The positive effect of the functionalization of chitosan films with anti-fibronectin aptamers on the colonization by murine osteoblastic cells is provided.

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P143

IMPLEMENTATION OF THE MODIFIED STANDARD ADDITIONS CALIBRATION METHOD FOR THE GC/MS QUANTIFICATION OF AMINO ACIDS

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Amino acids are non-volatile compounds with polar functionalized groups and, in general, not suitable for GC/MS analysis because very prone to decomposition during high temperature flash vaporization in the GC injector. In order to reduce the risk of decomposition, before GC/MS measurements, amino acids should be converted in other substances which are more easily detected (derivatization).
Silylation (i.e., the substitution of hydrogen atoms of carboxylic, alcoholic, amino, etc. groups with tri-alkylsilyl groups) is a very powerful and convenient single step derivatization strategy which converts a variety of polar compounds to trialkylsilyl derivatives which are suitable for GC/MS.
For qualitative applications, silylation is generally recognized as the most convenient and universal way in which a variety of functionalized substances can be made amenable to gas chromatography. On the contrary, for accurate and reproducible quantitative results, it is mandatory that the ratio between the amount of the original substance and the amount of its silylated surrogate be maintained constant throughout the whole analytical process of calibration and samples measurements.
Because of their variety and variability of behavior with respect to silylation reactions, biological amino acids hardly can all be determined on the basis of a single analytical protocol based on a fixed silylation agent, solvent and heat processing. Here we describe the analytical procedure of Modified Standard Additions Method (MSAM) which introduces flexibility and integrate in a single procedure the calibration and analysis of silylated compounds. Hence, we apply the MSAM basic experiment on a standard solution of the biological amino acids.

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CONDENSED PHASE MEMBRANE INTRODUCTION MASS SPECTROMETRY COUPLED WITH LIQUID ELECTRON IONIZATION INTERFACE (CP-MIMS-LEI): A POWERFUL TOOL TO MONITOR ON-LINE CHEMICAL REACTIONS IN NON-ACQUEOUS SOLUTIONS

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CP-MIMS uses semipermeable membrane (*e.g.*polydimethylsiloxane, PDMS) interfaces to make direct, online measurements in complex samples. Permeating analytes are transferred by a condensed (liquid) acceptor phase to a MS for detection and quantitation. The real time monitoring capabilities of CP-MIMS are ideal for investigating dynamic processes in reacting systems. Neutral species diffuse through the membrane for detection and analysis, while charged and heterogeneous components (*e.g.,* catalysts and reagents) are rejected. In LEI, a narrow capillary introduces a liquid nanoflow that is nebulized, vaporized, and introduced to an EI source. Ionization suppression from co-permeating compounds is effectively mitigated and the MS selectively monitors individual reaction components. We present the first demonstration using CP-MIMS-LEI for online reaction monitoring in organic solvents.

An HPLC pump was used to deliver a degassed methanol acceptor phase (100µL/min) through the lumen of a hollow fiber membrane (HFM) probe and to the MS. The PDMS membrane (0.30mm ID, 0.64mm OD, 170µm thick) was cut to be 5-20mm long (length of membrane exposed to sample). Passive flow splitting post membrane probe reduced the flow to the liquid electron ionization (LEI) interface to ~50nL/min, allowing direct analysis of high concentration (mM) solutions. A triple quadrupole MS/MS (Agilent 7010 QqQ) operated in MRM mode was used for online measurements. Reactions were conducted in 40 mL closed vials. Acceptor solvent and analytes were vaporized in the MS transfer line (350°C), and the mass spectrometer source was maintained at 280°C.

Initial development of the system was aimed at reducing the analytical sensitivity without compromising the operation of the LEI source. Shortened HFM interfaces were explored to reduce the mass transport of analyte permeating into the acceptor phase, and reduced flows to the LEI vaporization capillary (~50nL/min) eliminated blockages in the capillary that can interrupt continuous

measurements at higher flowrates (~500nL/min, is a more typical LEI flowrate). The current system has excellent temporal response, comparable to other CP-MIMS experiments using other ion sources such as ESI. The choice of reaction solvent was crucial, given that it should not compromise the membrane integrity, and to date, methanol, isopropanol and acetonitrile have proven successful.

To assess online measurement stability for direct reaction monitoring, stirred 25 mM solution of chlorobenzene in methanol was monitored demonstrating a steady state signal without any performance degradation. As an initial demonstration of the technique, the hydration of phenylacetylene (90 mM) in methanol in the presence of a gold chloride catalyst to yield acetophenone was studied. The loss of reactant and the formation of product were simultaneously monitored in real time at *m/z* 102 and 120, respectively.

The online, direct monitoring of chemical reactions by CP-MIMS-LEI in non-aqueous, organic solvents.

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SPRINKLER IRRIGATION: A GOLDEN BULLET TO MINIMIZE THE BIOACCUMULATION IN RICE GRAIN OF THE MOST HEALTH-THREATENING ELEMENTS?

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Among the factors affecting the bioaccumulation of toxic elements (like As and Cd) in rice, a key role is played by the nature of irrigation methods. The sprinkler irrigation method, optimized for rice in Sardinia [1], Italy, applied to several rice genotypes over a number of crop years has produced no significant differences in yields, exhibiting also many environment-friendly features. In addition, our previous studies show that the adoption of sprinkler irrigation causes, in comparison to data obtained using continuous flooding irrigation, an extraordinary As reduction (ca. -98%) [2], a meaningful Cd reduction (-20%) [3] on rice grain. In this contribution we show the outcomes of our recent studies on the effects of the different methods of irrigation (i.e. continuous flooding irrigation, sprinkler irrigation and saturation irrigation) on the bioaccumulation of a wide number of elements of health concern (i.e. Al, As, Cd, Cr, Cu, Fe, Hg, Mn, Mo, Ni, Pb, Sb, Se, Tl and Zn) in rice (grain, roots, stems, leaves and panicles) at varying of the soil composition and its pollution level, of the rice genotype and of the most representative phenological phases of the rice plant. ICPMS, GFAAS and FAAS methods of analysis have been specifically developed and validated for the measurements in all biotic matrices. Evidences for the different dynamics of the translocation of each element from soil to rice plant have been obtained and discussed. Furthermore, the effect of different soils on the bioaccumulation of the considered elements on the rice plant has been evidenced. As a general rule, the adoption of the sprinkler irrigation in place of the conventional irrigation technique (i.e. the continuous flooding irrigation) allows to minimize the total amount of the measured elements in rice grain. In addition, sprinkler irrigation allows to obtain – also on soils heavily polluted by As and/or Cd (ca. 50 mg kg^{-1} each) rice grain whose concentration of these elements is largely below the very strict limits posed by EFSA and EC (0.2 mg kg^{-1} for both elements).

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REAL-TIME MEASUREMENTS AND CHARACTERISATION OF ULTRAFINE AND SUBMICRON AIRBORNE PARTICLES NEAR AN INTEGRATED STEEL PLANT (TRIESTE-ITALY)

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Industrial activities are an important source of metal-containing ultrafine particles (UFPs), smaller than 100 nm, that are released in ambient air. Iron and steel industries can generate large amounts of coarse to ultrafine range particles associated with high concentration of metals such as Cr, Fe, Mn, Ni and Zn [1].

Metal nanoparticles can stimulate the production of ROS (reactive oxygen species) that are a major contributing factor in inflammation and toxicity [2]. Particles released by this kind of industrial activities can impact the surrounding areas. If the area is inhabited the residents can be exposed to elevated levels of atmospheric particles of a wide dimensional range and metal composition.

In Trieste (Servola district) an integral cycle steel plant, commonly called "Ferriera", is present. The dwellings of the district are positioned in very close proximity of this plant considered an "hot spot".

Given these considerations, our study is focused on the evaluation of the presence of airborne ultrafine and submicron particles in this sampling site. Real-time measurements of "number concentration" and mean diameter of particles in the range from 10 to 300 nm were performed. Moreover size-resolved sampling of particles was used to allow qualitative (by means of ED-μXRF), quantitative (ICP-AES) and morpho-chemical (TEM-EDS) analysis. Data from a "background" where UFPs emission from anthropogenic sources was expected to be minimum were used for a comparison. An optical particle counter (OPC) with eight channels has been used for real-time counting of the micro-particles in eight size ranges (0.3, 0.5, 0.7, 1.0, 2.0, 3.0, 5.0, 10.0 μm) at the hot spot site during the same sampling periods of NPs to obtain micro-particle profiles as well.

ED-μXRF analysis on the particulate matter sampled in "Servola" site showed the presence of Fe, Zn and Mn. The same elements constituted agglomerates of nanoparticles observed by means of TEM-EDS and were those with the highest concentration. The contribution of Fe concentration in the PM1 and, in particular, in the particle fraction lower than 0.25 μm seems to be not negligible in accordance with previous studies performed in similar environments [1]. This result is highly significant from a toxicological point of view.

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A RARE CASE OF DRINKING WATER CONTAMINATION BY THALLIUM: PIPE MONITORING ALONG DISTRIBUTION NETWORKS IN PIETRASANTA (LU)

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Thallium is a metal widely distributed in nature even though its abundance is very low. Although its presence in water distribution systems (WDSs) as a result of raw water contamination is an extremely rare condition, its toxicity has aroused concern in consumers.
In September 2014, a severe contamination was detected in two WDSs of *Pietrasanta*, an Italian town (about 24,900 inhabitants including hamlets) of the province of Lucca in Tuscany region. The two WDSs, fed by one drainage gallery, three springs and five wells, were connected each other by a pipe and a reservoir. Concentrations up to 14 µg/L were reached in distributed drinking water, well above the US-EPA maximum contaminant level of 2.0 µg/L. The contamination was delivered inside the waterworks by groundwater collected from one of the three springs, located close to an abandoned mining site in a mountainous area. The contaminated spring was immediately disconnected from the first WDS but a rapid increase in the concentration of thallium (up to 60 µg/l) was detected in the distributed water due to its migration from the internal surface of pipes where thallium had accumulated as sediments, sludge and adsorption products. Although system flushing for several weeks and complete replacement of steel pipes along the first WDS were performed, contamination of drinking water distributed by the second WDS remained.
150 pipe core samples (steel, cast iron, lined cement-mortar and high-density polyethylene) were collected from the second WDS to determine the extent of the remaining contamination. Samples were processed with a multiple sequential extraction, previously optimized [1]. In details, every pipe core sample was subjected to three consecutive ultrasonic-assisted extractions with reagents of increasing reactivity and eventually mineralized with concentrated nitric acid. Following the application of this extraction procedure, the concentration of Tl released in weakly acid condition (that is, the first extractant) was determined by inductively coupled plasma – mass spectrometry. The maximum detected value was 180 µg/cm^2, which represented about 5-9% of the total content present on the pipe surface. The contamination of the second WDS decreased rapidly as the distance from the two interconnection points with the first WDS increased. A negligible background concentration was found at a distance greater than 1 Km.

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Pseudomonas reduction in drinking-water and wastewater distribution systems by chlorine disinfection

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Pseudomonas aeruginosa is an opportunistic pathogen, member of the family Pseudomonadaceae, characterized by a polarly flagellated, aerobic, Gram-negative rod. It is a common environmental microorganism frequently found in faeces, soil, water and sewage. It may multiply in water and on the surface of organic materials in contact with water. It has been isolated from a range of moist environments, such as sinks, water baths, hot water systems, showers and spa pools.

Although it does not appear to represent a health concern through water consumption by the general population without some predisposing factors, it may cause a range of infections in vulnerable subpopulations, such as severely immunosuppressed people, patients with burns or extensive wounds, people with underlying disease at the respiratory tract and individuals with physically damaged eyes. From these sites, it may invade the body, causing destructive lesions or septicaemia, meningitis and serious progressive pulmonary infections. In addition, many strains are resistant to a range of antimicrobial agents, which may increase the significance of the microorganism in healthcare facilities.

Accordingly to WHO's guidelines for drinking-water quality [1], *Pseudomonas aeruginosa* has a moderate resistance to chlorine, thus colonization of water distribution systems may be minimized by adequate disinfection. A number of different authors has determined the inactivation kinetics at constant concentrations of chlorine using spot values or the conventional Chick-Watson model. These kinds of approaches do not take into account the decomposition kinetics of the disinfectant, which affects its real biocide action on the microorganism.

In the present work, we have explored the reliability of three different disinfection inactivation models (that is, Chick-Watson, Collin-Selleck and Hom) on the analysis of residual colonies measured at given time intervals (10 - 75 min) in drinking water and wastewater samples, which had been inoculated with *Pseudomonas aeruginosa* (10^2 - 10^7 CFU/100 mL) and disinfected with chlorine at different initial concentrations (0.1 - 4.0 mg/L). Residual chlorine was also determined during the contact time to assess its decomposition kinetics and correct the three-inactivation models.

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STUDY ON DISCOLORATION OF POLYVINYLCHLORIDE SHEET BY EVOLVED GAS ANALYSIS AND HEART CUTTING EGA-GC/MS ANALYSIS

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Discoloration of a polyvinylchloride (PVC) sheet material was studied by evolved gas analysis (EGA) and pyrolysis (Py)-GC/MS. One side of the material shows the original white colour (good) and the other side shows a yellow colour (bad) due to degradation. The sample surfaces of both sides were scraped to obtained fine powders used for measurements. First, FTIR and Py-GC/MS measurements were carried out, but no significant differences were observed in either sample surface. Next, EGA and heart-cutting GC/MS analysis were applied, and the results are respectively shown in Figures 1 and 2. As shown in Figure 1, a reduced level of hydrogen chloride (HCl) desorbs from the bad sample, suggesting decreased heat resistance. This can be confirmed by the reduced amount of thermal stabilizer, 2-ethylhexyl mercaptoacetate, in the bad sample, in addition to the reduction of alkyl alcohols in zone 1 as shown in Figure 2. The peak intensity of metallic soap stabilizers also decreased in the bad sample (not shown). In the chromatogram of zone 1 of EGA curve (Figure 2), desorption of higher levels of HCl is observed from the bad sample. Accordingly, the yellowing of PVC can be ascribed to the formation of conjugated polyene bonds for the discoloured sample surface.

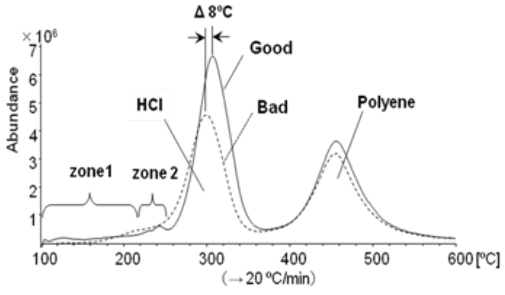

Figure 1. EGA thermograms for good and bad PVC samples

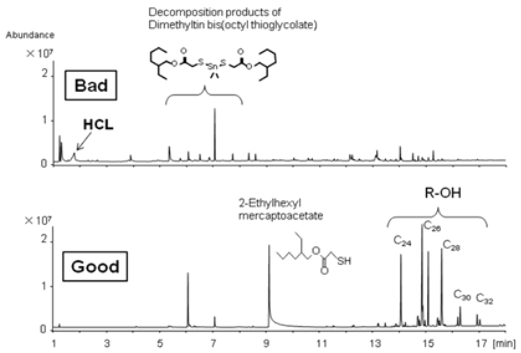

Figure2. Heart cutting GC/MS chromatograms of zone 1 for good and bad PVC samples

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