

## SEPARATION SCIENCES

Fundamental investigations in separation sciences are nowadays made in chemical and biological sciences as well as different topics of engineering. Separation sciences involve understanding of processes and materials interaction with solutes for chromatographic separation and analysis of specific molecules. Analytical determination occurs usually from complex matrices, such as environmental, food, biological, pharmaceutical or industrial.

### GOALS

The ultimate goal is to study fundamental aspects of physico-chemical phenomena, both from experimental and theoretical viewpoints, and understand how they rule separation processes (i.e., adsorption processes onto micro- and nano-porous materials, molecular and chiral recognition processes, effects due to surface heterogeneity, mass transfer phenomena in porous media, etc. This knowledge is fundamental also to improve technologically the employed adsorbent media, optimization of efficient, selective, sustainable analytical methods (i.e., determination of chiral compounds, emerging contaminants, nanoparticles, biologically active compounds, rare earth, etc.). Finally, all this can be pivotal for implementation of advanced separation systems (i.e., multidimensionally hyphenated, bioreactors on-flow, etc.).

### INSTRUMENTS AND METHODS

Laboratories of Separation Science Research Group at the University of Ferrara are well equipped with modern, advanced instrumentation, such as liquid chromatographs (standard and micro systems) for HPLC and UHPLC analysis, LC-MS (linear ion trap analyzer), LC-ICP/MS (triple quadrupole analyzer), GC-MS (both single quadrupole and ion trap analyzers), CE (both UV-Vis and fluorescence detectors), Field Flow Fractionation.

### MAIN SUBJECTS

Separation Science; Environmental Analytical Chemistry; Food Chemistry; Organic Chemistry; Pharmaceutical Chemistry.

### RESEARCH GROUP

Prof. A. Cavazzini, Prof. L. Pasti, Dr. N. Marchetti, Prof. M. C. Pietrogrande, Dr. C. Contado, Prof. M. Remelli, Dr. V. Costa.

### COLLABORATIONS

Research activities has active collaborations with other Departments of the University of Ferrara (i.e., Physics and Earth Science), numerous national (i.e., Eastern Piedmont University, University of Rome "La Sapienza") and international (A. Galarneau, Istitute Montpellier, France; A. Felsing, University of Pécs, Hungary; G. Desmet, University of Brussels, Belgium; N. Delunay Paristech, Colloïdes et Sciences Analytiques, Paris, France) scientific partnerships.

## **DIMENSIONAL AND COMPOSITIONAL ANALYSIS OF NANO- AND MICRO-PARTICLES USED IN FOOD, PERSONAL CARE PRODUCTS AND PHARMACEUTICAL FORMULATIONS**

### *GOALS*

- Development of methods for the separation and/or extraction and pre-concentration of particulate material from complex matrices.
- Development of separation methods, based on the Field-Flow Fractionation techniques to determine physico-chemical parameters (mass, sizes, density) of nano- and micro-particles in food products and personal care products.
- Physico-chemical characterization of nano- and micro-particles used as drug-delivery systems.

### *INSTRUMENTS AND METHODS*

Several analytical techniques are needed to achieve the aims of this research, such as the Field Flow Fractionation (FFF), the optical emission spectroscopy (AES) and the optical absorption spectroscopy (AAS), the liquid chromatography (HPLC) and the electron microscopy.

### *MAIN SUBJECTS*

Separation Sciences; Food Chemistry; Pharmaceutical Technologies.

### *RESEARCH GROUP*

Dr. C. Contado, Prof. A. Cavazzini, Prof. L. Pasti, Prof. M. Remelli, Prof. M. C. Pietrogrande, Dr. N. Marchetti, Dr. A. Pagnoni

### *COLLABORATIONS*

The team collaborates with colleagues within UniFe (Prof. A. Dalpiaz, Prof. R. Cortesi, Dr. E. Esposito) and with International teams (University of Namur - Belgium, University of Bordeaux – France, Postnova – Germany).

## **DEVELOPMENT, OPTIMIZATION AND VALIDATION OF ANALYTICAL METHODOLOGIES FOR THE DETERMINATION OF BIOACTIVE COMPOUNDS IN FOODS, PHARMACEUTICAL PRODUCTS AND BIOLOGICAL SAMPLES**

This research topic is aimed to characterize vegetable matrices, such as agri-food products, with short term purposes (i.e., give value to these products from a nutritional and functional point of view, determination of bioactive compounds) and long term objectives (increase biodiversity for local agri-food products, contribute to point out typical agri-food products, enhance the use of functional foods with supporting scientific data). Bioactive compounds are studied also on pharmaceutical or cosmetic matrices (i.e., stability studies), and biological samples (i.e., pharmacokinetic studies).

### *GOALS*

Set-up of selective, reliable, sensitive analytical methods for determination of bioactive compounds in complex matrices, such as food, pharmaceutical products and biological ones. From one hand, separation techniques allow identification and quantification of bioactive molecules (i.e., pharmacokinetics) and their stability and distribution in living organisms (tissues, plasma, cerebrospinal fluid) are determined. On the other hand, separation techniques have to give enough power to identify and fully characterize food matrices (mainly vegetables) and/or identify metabolites that might have a certain bioactivity.

### *INSTRUMENTS AND METHODS*

Different analytical techniques for sample treatment (extraction of bioactive compounds) molecular identification and quantitative determination are used. Most important methodologies involve: liquid-liquid extraction with enzymatic hydrolysis, solid-phase extraction, gas chromatography-mass spectrometry (GC-MS), liquid chromatography-mass spectrometry (LC-MS). Regarding LC-MS ion interfaces, Electrospray (ESI) and Chemical ionization (APCI) are available in our laboratories.

### *MAIN SUBJECTS*

Separation Science; Analytical Chemistry; Food Chemistry; Organic Chemistry; Pharmaceutical Chemistry.

### *RESEARCH GROUP*

Dr. N. Marchetti, Prof. A. Cavazzini, Prof. L. Pasti, Prof. V. Brandolini, Dr. A. Maietti, Prof. M. Remelli, Prof. M. C. Pietrogrande, Dr. C. Contado, Dr. V. Costa, Dr. P. Tedeschi.

### *COLLABORATIONS*

The research group has active collaborations with other groups of the same Department (Prof. A. Dalpiaz, Prof. S. Scalia), European Universities (Spain, Hungary, France) and many Italian local enterprises.

## **DEVELOPMENT, CHARACTERIZATION AND APPLICATION OF ADSORBENT MATERIALS FOR WATER DECONTAMINATION AND RECOVERY OF SECONDARY RAW MATERIALS**

This research topic has the ultimate aim of studying nano- and meso-porous materials with respect to their characteristics as adsorbents towards different organic pollutants in waters (emerging and persistent organic contaminants). Additionally, this project can give impulse to develop new materials for liquid chromatographic applications and/or solid-phase extraction (on-line, too) and pre-concentration steps in environmental, pharmaceutical and food chemistry.

### *GOALS*

Interaction mechanisms between organic molecules and chiral or achiral stationary phase are studied and investigated. Specific separation issues are solved through the development and characterization of new adsorbent materials. These will be employed in analytical applications for separation, extraction and/or pre-concentration. These studies can have remarkable fallouts in different research area, such as environmental chemistry or agri-food. Innovative decontamination techniques will be developed in order to treat waters and recover secondary raw materials from waste waters.

### *INSTRUMENTS AND METHODS*

Research goals are reached by using instrumental techniques such as liquid chromatography (HPLC), gas chromatography (GC), capillary electrophoresis (CE), atomic emission and absorption spectroscopy (AES and AAS), field flow fractionation (FFF). Advanced equipment are already present within the research group laboratories and they couple separation techniques and mass spectrometric detection (HPLC-MS, GC-MS, ICP-MS). Moreover, sample treatment approaches are used, such as solid-phase extraction (SPE) and solid-phase micro extraction (SPME).

### *MAIN SUBJECTS*

Separation Science; Environmental Analytical Chemistry; Food Chemistry; Organic Chemistry.

### *RESEARCH GROUP*

Prof. L. Pasti, Prof. A. Cavazzini, Dr. N. Marchetti, Prof. M. C. Pietrogrande, Dr. C. Contado, Dr. V. Costa, Dr. A. Pagnoni

### *COLLABORATIONS*

The research group has many active collaborations inside the Department and the entire University of Ferrara (Physic and Earth Sciences Department). Also, national (Eastern Piedmont University) and international (A. Galarneau, Istitute Montpellier, France) collaborations can be counted.

## **AIR QUALITY MONITORING: CHEMICAL CHARACTERIZATION OF ATMOSPHERIC AEROSOL**

There are evidences that chemical composition of atmosphere can be associated to risks for human health, particularly in towards quantity and quality of disperse atmospheric particulate matter (PM). Investigation of air quality is dedicated to both well-known toxic compounds (for environment and habitants), and specific molecules that have been recognized as markers able to give information about sources and processes taking place in the atmosphere. These studies have interesting fallout facts for Environmental Chemistry and Toxicology because they are primarily important for determining atmospheric pollution sources and for identifying strategies to reduce the impact on human health.

### *GOALS*

Ultimate goals of this research topic is: i) to investigate chemical composition (both metals and organic fractions) of atmospheric particulate matter; ii) to develop and to optimize analytical methods for trace analysis of atmospheric samples; iii) to set-up methodologies for better environmental monitoring; iv) real case studies aimed at monitoring the air quality; v) data mining and processing for results interpretation.

### *INSTRUMENTS AND METHODS*

Several instrumental techniques are used in order to reach purposes of this research activities: gas chromatography (GC), liquid chromatography (HPLC), atomic emission (AES) and absorption (AAS) spectroscopy. Research group laboratories are equipped with modern, advanced instruments that hyphenate separation techniques as mentioned above with sensitive and selective detection methods (i.e., Mass Spectrometry): HPLC-MS, GC-MS and ICP-MS are fully available in our group. Additionally, modern approaches for sample treatment are used (i.e., solid-phase extraction, SPE, and solid-phase micro extraction, SPME).

### *MAIN SUBJECTS*

Analytical Chemistry; Environmental Chemistry; Separation Science.

### *RESEARCH GROUP*

Prof. M. C. Pietrogrande, Prof. A. Cavazzini, Prof. L. Pasti, Prof. M. Remelli, Dr. N. Marchetti, Dr. C. Contado, Dr. A. Pagnoni.

### *COLLABORATIONS*

The research group is involved in active national (Istituto ISAC-CNR Bologna, ARPAE Emilia Romagna, ARPA Lombardia) and international (Department of Analytical Chemistry, University of Helsinki, Finland; Department of Analytical Chemistry, University of Santiago de Compostela, Spain) collaborations.

## **COMPLEX-FORMATION SOLUTION-EQUILIBRIA BETWEEN METALS AND LIGANDS OF BIOLOGICAL AND/OR PHARMACOLOGICAL SIGNIFICANCE**

Many metals are involved in the biological processes that support plant and animal life. Some of them are called "minor" metals, since they are present only in trace amounts although they are part of fundamental molecules of life, such as metal-proteins and metal-enzymes. The formation of these complexes is regulated by a large number of environmental factors including the competition of other ligands and metal ions. Therefore, it is important to understand the behavior of these systems under dynamic conditions, such as those occurring in solution, in biological fluids.

### *GOALS*

The main goals of this research are as follows: a) measurement of acid/base properties of the considered ligands; b) definition of the speciation model relative to complex species formed between the ligands and metals investigated; c) calculation of distribution and competition diagrams; d) study of the structure in solution of the main complexes. This scheme of investigation has recently been applied in different fields: metal-peptide equilibria (used as models for metal-protein complexes, e.g. SPARC or Prion proteins); potential drugs for chelation therapy (used in the treatment of heavy-metal poisoning); macro-chelate complexes (e.g. metallacrowns), possible candidates as contrast agents in diagnostic imaging.

### *INSTRUMENTS AND METHODS*

The most widely used method for studying solution equilibria involving molecules with acid-base properties is potentiometry with the glass electrode. In special cases other electrodes can be used, e.g. electrodes sensitive to the metal ion. The laboratory has two automatic titrators, each consisting of a motor-driven microburette and a precision pH-meter, both operated by a computer. In order to complete the thermodynamic characterization of solution equilibria, the laboratory has an isoperibol titration microcalorimeter (Tronac, mod. 450). To obtain information about the structure of the species formed in solution several spectroscopic techniques are used, including UV-Vis spectrophotometry (available in the lab), circular dichroism spectroscopy, EPR and NMR spectroscopies. In addition, among the techniques available in our Department, the following are also widely employed: ESI-MS spectrometry, useful to confirm the stoichiometry of the species in solution, and the X-rays diffraction, giving the solid state structure of complex species. In collaboration with the Department of Life Sciences and Biotechnology tests of biological activity in vitro of both the ligands and complexes are performed.

### *MAIN SUBJECTS*

Analytical Chemistry, Physical Chemistry, Bioinorganic Chemistry, Organic Chemistry, Biochemistry.

### *RESEARCH GROUP*

Prof. M. Remelli, Prof. A. Cavazzini, Dr. C. Contado, Dr. N. Marchetti, Dr. A. Pagnoni, Prof. L. Pasti, Prof. M. C. Pietrogrande.

### *COLLABORATIONS*

Intra moenia: Prof. Valerio Bertolasi, Prof. Remo Guerrini, Prof. Riccardo Gavioli. Extra moenia: Prof. H. Kozlowski (University of Wroclaw, PL), Prof. D. Valensin (University of Siena), Prof. M.A. Zoroddu (University of Sassari), Prof. G. Crisponi (University of Cagliari), Dr. M. Tegoni (University of Parma).