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DIPARTIMENTO

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LAB
Agrifood and
Cultural Heritage

Research activity



Agri-food chemistry – analysis of the inorganic component, metabolomics and characterization of the geographical origin

Analysis of the mineral fraction (content of metals and metalloids in bulk, trace and ultra trace) of soil samples (focus on olive grove and vineyard soils) and of products of the entire olive and wine production chain (leaves, fruits, finished product) in order to study the correlation between territory and commercial product.

Analysis of secondary metabolites using HPLC DAD and MS of the products of the entire olive and wine supply chain (analysis of hydro-alcoholic extracts of leaves, fruits and finished products) in order to study the different varieties and geographical origins of products such as oil and wine

Analysis of organic compounds in plant matrices (leaves and fruits, in particular olive trees and grapevines) and in commercial products (oil and wine) by mass spectrometry based on orbitrap® technology and isotopic ratio mass spectrometry IR-MS. Combination of targeted and untargeted approaches for the determination of key compounds in order to identify the geographical origin of products in agri-food supply chains, through the application of statistical and chemometric methods.

Analysis of the chemical and molecular structure of plant matrices and final products by nuclear magnetic resonance (NMR) spectroscopy to detect the presence of marker metabolites for the study of the correlation between geographic origin, different cultivars, and environmental effects on the final properties of commercial products belonging to different agrifood supply chains.

3D fluorescence spectroscopy for the acquisition and interpretation of fluorescence maps to determine the presence of specific metabolites containing chromophore groups (chlorophylls, polyphenols) within plant matrices and commercial products, which can be useful for monitoring different parameters such as vegetative state of plants, alterations or frauds in agricultural and food products, and discrimination of geographical origin.

L'attività di ricerca



Chemistry of cultural heritage

Research activity in this area is carried out in two directions. On the one hand there is the development and characterization of innovative systems and materials for restoration and conservation, while on the other the diagnostics and study of the materials constituting the art objects, with the aim of identifying their chemical nature, state conservation and, consequently, to suggest suitable strategies for intervention by qualified operators.

The range of instruments available to the group allows for a complete and in-depth characterization of the chemical-physical properties of materials. The synergy with research activities on the environmental/agri-food front also allows us to carry out chemometric analyzes that are particularly useful in the study, for example, of archaeological objects.

Images





ICP-MS Agilent 8900 with autosampler



HPLC Dionex UltiMate 3000 coupled with Thermo Scientiific LTQ XL MS with autosampler



Microwave-assisted digestor ETHOS Easy

Images





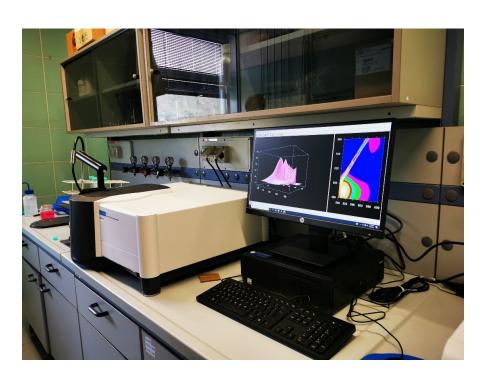
Orbitrap (Exploris 240, Thermo-Fischer)



NMR (Advance - 600 MHz, Bruker) with a 24positions autosampler



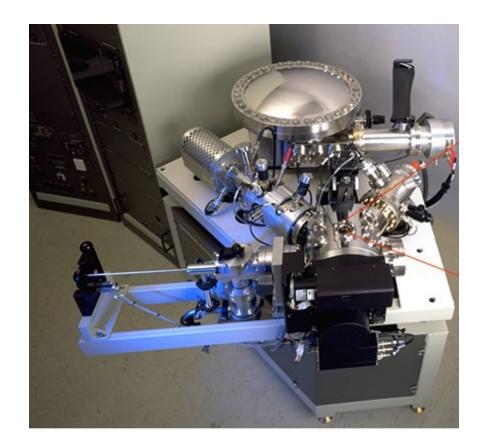
IR-MS (Delta Q, Thermo-Fischer)



Spectrofluorometer (Cary Eclipse, Agilent)

Disegni e Immagini





ToF-SIMS (Trift III, Physical Electronics)



DSC (TA Instruments)



ATR-FTIR (iS-10, Thermo-Fischer)



TGA (TA Instruments)

Disegni e Immagini

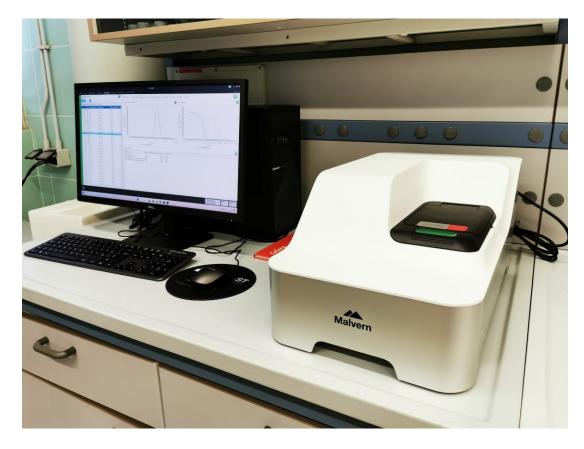




Spectrophotometer UV-Vis (Agilent)



XRF (Tracer 5g, Bruker)



Dynamic light scattering (DLS, Malvern)



Rheometer (TA Instruments)

Technologies and services



ICP-MS: The samples (as they are or already mineralized by acid attack in an oxidizing mixture) can be analyzed in order to quantify the metal content for quality control and to identify the geographical origin of the product (EVOO or Chianti wine)

HPLC-DAD/MS: analysis of secondary metabolites (e.g. polyphenols) for quality control (e.g. identifying the percentage of certain varieties within an oil blend) and for the zoning of agricultural products

ORBITRAP®: Obitrap® allows high-resolution detection of organic compounds in plant samples (leaves, fruits), enabling the interpretation of molecular complexity and contributing to the metabolomic study of matrices. Statistical analysis of the results, using multivariate methods, provides a pivotal contribution to the determination of the geographical origin of products in agri-food chains

IR-MS: IR-MS (isotopic ratio mass spectrometry) determines the isotopic ratios of light elements such as H, C, N, O and S, providing fundamental information on the geographic origin and metabolic characteristics of the tested samples

Technologies and services



NMR: Nuclear magnetic resonance spectroscopy can be used to explore the molecular structure and the chemical composition of plant matrices (leaves, fruits) and final products (wine, oil), providing a key contribution to the metabolomic analysis of samples. Spectra can be examined and used for subsequent analyses that include chemometric methods, such as multivariate analysis, which are particularly efficient in the context of determining the geographic origin of products in agrifood supply chains

SPECTROFLUORIMETRY: This technique analyzes the fluorescence emitted by plant extracts (from leaves or fruits) upon an appropriate light excitation. The fluorescence excitation-emission maps can be examined and deconstructed through statistical models, typically the PARAFAC methodology, that provide relevant information on the metabolomic profile of the investigated matrices

XRF: This instrumentation, portable - and therefore also usable *in situ*, allows the identification and quantification - through appropriate calibration - of the elements present in the samples, allowing rapid and efficient analysis of soil, leaves and fruit. Particularly effective in the analysis of metals and metalloids, the X-ray fluorescence technique is a versatile, practical and complementary alternative to the ICP-MS technique.

It can also be used very effectively in the analysis of cultural heritage, in archaeometry and on pictorial matrices, for the study of alteration patinae, pigments, metal alloys, etc.

Strumenti, Tecnologie e Servizi



TOF-SIMS: This mass spectrometry is a powerful surface analytical technique, capable of detecting molecular elements and fragments in solid matrices of any composition, with high sensitivity. Also in this case it is possible to apply multivariate statistical methods to the analysis of mass spectra, taken both from the external surface of fruits or leaves and from sections of them.

This technique can also be used for the analysis of cultural heritage, for the identification of organic binders, for the characterization of metallic and ceramic matrices or in general for the microinvasive and non-destructive analysis of samples of various nature.

ATR-FTIR: This spectroscopic technique is one of the most versatile and powerful investigation techniques for the chemical analysis of complex, organic and inorganic matrices of unknown composition, in terms of molecular groups present. Effective in identifying salts in alteration patinae, pigments, pictorial binders, polymeric coatings, adhesives, it can also be used as a diagnostic tool for evaluating the state of conservation of a material, or for determining the outcome of a cleaning intervention.

DSC: This calorimetric technique allows you to obtain information on the thermal properties and state changes of the sample. It is an effective technique for the chemical-physical characterization of polymer systems and gels and can be used both in the development of new materials and in the study of samples taken from works of art.

Strumenti, Tecnologie e Servizi



TGA: Thermogravimetry allows to monitor the weight loss of a sample subjected to a thermal ramp. Particularly relevant for monitoring the degradation processes (thermal and not only) of organic materials (polymers) and inorganic (salts), it is an extremely sensitive technique, which - despite being destructive - requires a minimum quantity of sample, and is therefore very indicated for analysis in the context of the conservation of cultural heritage.

UV-Vis spectrophotometry: This extremely versatile technique counts several applications in almost every scientific field and even in conservation of cultural heritage it can be used both as a diagnostic tool (presence and/or quantification of salts or compounds with specific absorptions in unknown mixtures), or for characterization in the development of new materials.

Rheometry: Rheological analyses represent a fundamental step in the chemical-physical characterization of viscous or viscoelastic systems, such as polymeric solutions, polymeric films, gels and so on. In the field of cultural heritage, the main use of this technique concerns the development of new materials.

Applications and collaborations



Agri-food

Collaboration with multiple farms located in Tuscany in the context of the PNRR-funded AGRITECH project for the analysis of their products with the techniques aforementioned

Possibility of extending the use of the experimental techniques to other products from different agricultural and food supply chains (i.e. not limited to grapes, olives, wine and oil), expanding the focus of inorganic analysis and metabolomic study.

Involvement of producer associations belonging to different supply chains to study the quality of raw materials and final commercial products.

Cultural heritage

Collaboration within the restoration project of the copy of the Fonte Gaia by Tito Sarrocchi (Piazza del Campo, Siena), through an analysis campaign which showed the chemical composition of the alteration patinas, removed through mechanical/laser action.

In the future, similar collaborations and/or research projects may be activated, aiming at the study and characterization of samples from works of art under restoration or at the development of new conservation strategies.



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