CHEMISTRY OF ENVIRONMENTAL PROCESSES

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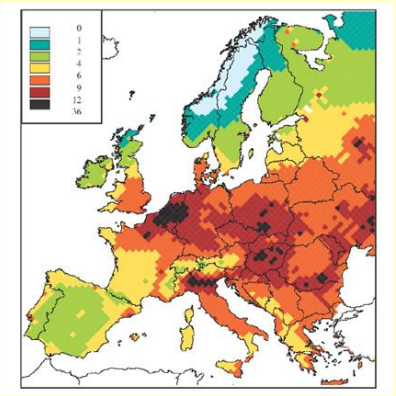
Our search is devoted to the study environmental pollutants and their bio-remediation through microbiological attack, with the aim to obtain good degradation yields at low cost. Our search is devoted also to the spectroscopic characterization of organic compounds of environmental and historical artistic value, to obtain information about their structure and their degradation products

Keywords: micropollutants, particulate matter, FTIR spectroscopy, soil remediation, molecular modeling.

1. Characterization of organic micropollutants



The aim of our research was to obtain a better knowledge of the relation between chemical composition of the particulate matter and the dimensional distribution. Moreover we study the effects of the seasonality and the geographic location on the composition of the particulate matter.
The toxicity and mutagenicity of particulate matter was studied on size-segregated samples obtained using an high volume multistage impactor. The collection of fine and ultrafine fractions allowed to measure the concentrations of toxic compounds in the respirable particles in different environmental conditions. Some samples showed a genotoxic activity, as detected. by the high level of cytogenetic damages on exposed in vitro cell culture systems.
The image shows the decrease in life expectancy (months) due to anthropogenic PM2.5.

2. Advanced characterization methods of organic materials of environmental and historical-artistic relevance by Micro-FTIR Mapping and Raman Microscopy

Infrared and Raman spectroscopy are the most powerful tools for the identification and characterization of chemical structures (Figure 1). They represent two complementary and versatile techniques to obtain chemicals information in many scientific fields.
These techniques were used for the characterization of paper from ancient books and for identification of their degradation products. It is important to figure out the current physico-chemical state of the artefact, in order to identify appropriate methods of preservation and restoration of such property.
The spectroscopic techniques were also applied for the characterization of particulate matter (PM) collected in Catania using an high-volume cascade impactor. Assignment of PM vibrational bands has

been studied too.
FTIR and Raman spectra data obtained with different sampling techniques will be compared in order to figure out the influence of these different spectroscopic methods in the measurements.

Figure1: FTIR and Raman spectrometer Thermo Scientific

3. Advanced biodegradation processes for the soil remediation of polluted sites in Sicily

The Project has developed some key points regarding the issue of soil remediation in sites contaminated by polycyclic aromatic hydrocarbons (PAHs) such as:

- Developing modified enzymes through molecular modelling techniques for the degradation of PAHs.
- Testing in vitro and in situ PAHs enzymatic biodegradation using bacterial (*Stenotrophomonas maltophilia*) and fungal (*Rigidoporus lignosus*) strains.

The first step has allowed to assess (by computational simulations), the interactions between an enzymatic macromolecule (naphthalene dioxygenase-NDO) (Figure 2) and its ligand. "In-silico" NDO enzyme chain breaking was produced by number of proteolytic enzymes.

Figure 2: NDO ($\alpha 3\beta 3$)

Finally it was also tested the ability of the enzyme laccase, extracted and purified from a fungal strain *Rigidoporus lignosus* (Figure 3), to degradate PAHs both in an in-vitro solution and into a soil dispersion, getting significant degradative yield in some samples.

Figure 3: *Rigidoporus lignosus*

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Selected Publications

- Librando V., Minniti Z., Perrini G., Pappalardo M., Federico C., Motta S., Saccone S. (2010). Distribution of Nitro-Pahs in Size-Segregated Particulate Matter Fractions from an Elevated Car Transit Area. *Fresenius Environmental Bulletin, 19*, 2282-2286.
- *Librando V., Pappalardo M., Minniti Z. (2010). Progress in Bioremediation Processes. a Computational Study of the Interaction of a Novel Enzyme with Selected Polycyclic Aromatic Hydrocarbons. Journal of Biotechnology, 150; 567.*
- *Librando V., Alparone A. (2008). Prediction of Mutagenic Activity of Nitronaphthalene Isomers by Infrared and Raman Spectroscopy. Journal of Hazardous Materials, 154 (1-3), 1158-1165.*
- *Librando V., Cambria M.T., Minniti Z., Cambria A. (2008). Degradation of Polycyclic Aromatic Hydrocarbons by Rigidoporus Lignosus and its Laccase in the Presence of Redox Mediators. Applied Biochemistry And Biotechnology, 149 (1), 1-8.*
- *De Guidi G., Catalfo A., Perrini G. (2008). Spectroscopic Properties of Some Derivatives of PAHs. Applied Spectroscopy, 61,1233-1237.*
- *Lorusso S., Librando V., Minniti Z. (in press). Ancient and modern paper characterization by FTIR and Micro-Raman spectroscopy. Conservation Science in Cultural Heritage, In press.*