Emory @ Unisi

Summer School

Chemistry for Life & Environment
Education, Collaboration, Innovation

XI Edition, 28 May - 03 July 2014

Università di Siena 1240

Dipartimento
Biotecnologie
Chimica & Farmacia

CHEMISTRY @ EMORY
celebrating scientific discovery and innovation

EMORY UNIVERSITY

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Summer School Emory @ Unisi
Chemistry for Life & Environment
11th Edition, 28 May - 03 July 2014

Time Table

28 May, Wednesday	
5.00 pm	Arrival of Emory Group Check-in at Refugio residence
6.30	Introductory meeting at Refugio by summer program coordinator. Introduction to the program, teaching aids, internet connection, notes about Siena City, restaurants, pharmacies, supermarkets, laundries, etc…
7.00	Welcome Pizza in the Refugio's Garden
29 May, Thursday	
8.45 am	Emory Classes at Refugio
12.30	Lunch at Mensa Universitaria at Bandini, cards validation
2.00 pm	Free tour: Unisi scientific and didactics sites in town, libraries, selected monuments (Town Hall, Piazza del Campo, Duomo, Churches, post office, bus station, Contrade, police office, museums, sport facilities, theaters, Accademia Musicale Chigiana, Unisi Botanical Garden, Accademia dei Fisiocritici, etc…)
30 May, Friday - OPENING OF THE SUMMER SCHOOL (San Miniato, Room #14)	
10.00	Introduction and greetings Daniela Valensin - Unisi Coordinator of General Cooperation Agreement Emory/Unisi Francesco Frati - Prorector Unisi Maurizio Taddei - Director Department Biotechnology Chemistry & Pharmacy Stefano Mangani - Director of Doctorate School Michael McCormick- Emory Representative Simon Blakey - Emory Representative Gabriella Tamasi – Executive Coordinator of Summer School *Introduction of summer program and its educational purposes*
11.15	Coffee break & Poster session
11.30	Presentations by Unisi research groups Gianluca Giorgi - *Mass spectrometry in bioorganic chemistry* Fabrizia Fabrizi de Biani – *Modern applications of electron transfer processes* Daniele Spinelli - *Laccase immobilization onto nanofibers and mesoporous materials* Claudia Perini & Thomas Evans - *The mysterious fungi: the good, the bad and the ugly*
12.45 2.00 pm	Buffet & Posters session Conclusions
31 May, Saturday	
	Free Morning in Siena
2.00pm	Guided visit to the "Museo Civico, Palazzo Comunale, Piazza del Campo"
01 June, Sunday	
	Free Day in Siena

02 June, Monday - Italian Civic Holiday (Festa della Repubblica)	
8.45 am	Emory Classes at Refugio
03 June, Tuesday	
08.45 am 2.30-5.30 pm	Emory Classes at Refugio Parallel Unisi Laboratory Session at San Miniato Gianluca Giorgi – *Mass spectrometry in bioorganic chemistry: from structural to stereochemical and conformational characterization* Fabrizia Fabrizi de Biani – *Modern applications of electron transfer processes*
04 June, Wednesday	
8.45 am	Emory Classes at Refugio
05 June, Thursday	
8.45 am 11.30 2.30 -5.30 pm	Emory Classes at Refugio First Evaluation about accommodation, facilities and first week activities at Siena, form filling for Emory Students Unisi Laboratory Session at San Miniato Daniele Spinelli – *Laccase immobilization onto nanofibers and mesoporous materials*
06 June, Friday	
	Emory Students and Faculties visit Florence
07 June, Saturday	
	Free Day in Siena
08 June, Sunday	
	Free Day in Siena
09 June, Monday	
8.45 am 11.00 3.00 pm	Emory Classes at Refugio Lecture at Refugio Neri Niccolai - *The beauty of bioinformatics* Lecture by Emory Speaker at San Miniato Simon Blakey – *C–H Functionalization: An enabling technology for pharmaceutical and materials chemistry*
10 June, Tuesday	
8.45 am 2.30 5.00 pm	Emory Classes at Refugio Parallel Unisi Laboratory Session at San Miniato Gabriella Tamasi - *Chemical analysis for food quality control: AAS & HPLC* Agnese Magnani & Gemma Leone – *Rheological characterization of biomaterials and infrared characterization of biosensors*
11 June, Wednesday	
9.30 am	Half a day at Novartis Vaccines Italia, Siena
12 June, Thursday – Two Days Cultural trip to Montalcino territory (D. Picciolo)	
10.30 12.00 12.15 1.30 pm 4.00 7.30	Departure to Montalcino (by line bus) Arrival to Montalcino Welcome & Lunch Check-in to the B&Bs and free time Guided visit to the Montalcino's museum and Fortress Typical Montalcino/Tuscany Dinner

13 June, Friday - Two Days Cultural trip to Montalcino territory	
7.30 am	Breakfast
8.00	Trekking from Montalcino Fortress to Abbazia di Sant'Antimo (ca 10 km)
11.30	Guided visit to Azienda Agraria "La Mágia". Class on Sangiovese Grosso variety and Brunello winemaking and aging processes
12.30	Lunch and wine tasting at Agriturismo
1.30 pm	Leaving from Agriturismo towards Abbazia di Sant'Antimo
2.45	Attendance to *Ora Nona* and Canto Gregoriano by Monaci Premonstratensi
3.00	Visit to Abbazia di Sant'Antimo, its history, architecture, …
4.00	Return to Siena
14 June, Saturday	
	Free day in Siena
15 June, Sunday	
	Free day in Siena
16 June, Monday	
8.45 am	Emory Classes at Refugio
11.00	Lecture at Refugio Riccardo Basosi - *Energy from the principles of thermodynamics to the sustainable development*
2.30 pm	Emory students meet Unisi Students at Refugio Welcome and Introduction by Emory and Unisi Teachers Teachers excluded! Students present their own experiences at Universities
5.00 – 7.00pm	Sport activity at CUS, University of Siena Sport Center
17 June, Tuesday	
8.45 am	Emory Classes at Refugio
11.00	Lecture at Refugio Enrico Tavarnelli - *The depositional and tectonic history of ridges and basins of Southern Tuscany: geological controls on the quality of wines and food produced in Val d'Orcia and in the Chianti mts*
2.30-5.30 pm	Unisi Laboratory Session at San Miniato Maria Camilla Baratto - *EPR spectroscopy for the study of antioxidant activity*
18 June, Wednesday	
8.45 am	Emory Classes at Refugio
11.00	Lecture at Refugio Michele Gregorkiewitz – *Full structural characterization through global diffraction pattern fitting. A contribute to the International Year of Crystallography IYCr2014*
2.30-5.30 pm	Unisi Laboratory Session at Laterino Michele Gregorkiewitz, Enrico Mugnaioli, Sonia Mugnaini *Full structural characterization through global diffraction pattern fitting*
19 June, Thursday	
8.45 am	Emory Classes at Refugio
11.00	Lecture at Refugio Stefano Mangani - *100 years of Crystallography from quasicrystals to proteins*
3.00 pm	Lecture by Emory Speakers at San Miniato James Kindt – *Computer simulations of lipid bilayers*

20 June, Friday **FIELD-TRIP TO BARONE RICASOLI SPA AGRICOLA** **(BROLIO, GAIOLE IN CHIANTI, SIENA)**	
9.30	Departure from Porta Romana
10.00	Arrival at Brolio Guided visit and class in two vineyards by the Agronomist about Sangiovese and other vines growing, treatments, …
11.00	Guided visit and class in the cellars by the Enologist about wine production and aging
12.00	Wine tasting
12.30	Lunch at Restaurant Cantine Barone Ricasoli, typical Chianti foods
2.00 pm	Guided visit to the Ricasoli Castle, old enological laboratory of Baron Bettino Ricasoli, History of Chianti and Italy
4.30	Return to Siena
21 June, Saturday	
	Free day in Siena
22 June, Sunday	
	Free day in Siena
23 June, Monday	
8.45 am	Emory Classes at Refugio
3.00 pm	Guided visit to a Contrada Museum, Church, …
24 June, Tuesday	
8.45 am	Emory Classes at Refugio
2.30-5.30 pm	Unisi Laboratory Session at San Miniato Manuela Benvenuti - *Lysozyme crystallization*
25 June, Wednesday **FIELD-TRIP TO VILCA (COLLE DI VAL D'ELSA, SIENA)** **AND TO SAN GIMIGNANO**	
9.00 am	Departure from Porta Romana Introductory class on bus by Unisi teachers about the day activities
9.40	Arrival at ColleVilca
10.00	Guided visit and class about chemistry of glass and glass-blowing methods
11.30	Departure to San Gimignano
12.00	Arrival at Fattoria Sovestro in Poggio, and visit to the Vineyards and Cellars
13.00	Lunch at Fattoria Sovestro in Poggio
2.30 pm	Visit to San Gimignano, the town and main historical places
5.00 pm	Departure to Siena
26 June, Thursday	
8.45 am	Emory Classes at Refugio
2.30-5.30 pm	Unisi Laboratory Session at Toscana Life Science Foundation (TLS): Laura Salvini - *Confocal microscopy and mass spectrometry: two important methodologies in biotechnology*
27 June, Friday	
8.45 am	Emory Classes at Refugio
2.30-5.30 pm	Unisi Laboratory Session at Orto Botanico & Accademia dei Fisiocritici Claudia Perini & Thomas Evans - *The mysterious fungi: the good, the bad and the ugly*

28 June, Saturday	
	Free day
29 June, Sunday	
	Free day
30 June, Monday	
	Free day
4.00-6.00 pm	Sport activity at CUS, University of Siena Sport Center (optional activity)
01 July, Tuesday	
8.45	Emory Classes at Refugio
11.30	Second and final Evaluation, forms filling for Emory Students
12.00	Meeting of Evaluation Committee of Unisi and Emory Teachers Conclusions and remarks Planning for 12th Edition Emory@Unisi 2015 and 4th Edition Unisi@Emory 2015
7.00 pm	Horse trials in Piazza del Campo
8.30	Eve Dinner in a Contrada
02 July, Wednesday - Palio Day	
07.00 am	Blessing Mass celebrated by Archibishop in Piazza del Campo for Fantino, the Jockey
02.00 pm	Attending to the horse blessing in a Contrada
03.00	Attending to Contradas blessing from the Archbishop at Duomo
04.30	Piazza del Campo …waiting for Palio race
07.00	Palio Race
03 July, Thursday	
10.00 am	Check-out

CLASSES AND LAB EXPERIMENTS
ORAL PRESENTATIONS & POSTERS
THE LISTING IS BASED ON THE ALPHABETICAL ORDER OF THE FIRST AUTHOR SURNAME

Maria Camilla Baratto
EPR spectroscopy for the study of antioxidant activity

Riccardo Basosi
Energy from the principles of thermodynamics to the sustainable development

Manuela Benvenuti
Lysozyme crystallization

Caterina Bernini, Lorenzo Zani, Massimo Calamante, Gianna Reginato, Alessandro Mordini, Maurizio Taddei, Riccardo Basosi, Adalgisa Sinicropi
Excited state properties of organic sensitizers for DSSC evaluated at the PCM/TD-DFT level

Fabrizia Fabrizi de Biani
Modern applications of electron transfer processes

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Spectroscopic studies of interactions between β-amyloid peptide fragments and metals

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Mass spectrometry in bioorganic chemistry: from structural to stereochemical and conformational characterization

Michele Gregorkiewitz, Enrico Mugnaioli, Sonia Mugnaini
Full structural characterization through global diffraction pattern fitting.
A contribute to the International Year of Crystallography IYCr2014

Gemma Leone
Rheological characterization of polymeric hydrogels

Agnese Magnani, Nicola Nelli, Claudio Rossi
Biosensors: useful tools for diagnostic purposes

Stefano Mangani
100 years of Crystallography from quasicrystals to proteins

Chiara Nesti, Riccardo De Ricco, Marek Luczkowski, Henryk Kozlowski, Daniela Valensin
Spectroscopic investigation on -KLVFF- amyloid β sequence

Neri Niccolai
The beauty of bioinformatics

Rebecca Pogni, Francisco Javier Ruiz-Dueñas, Maria Camilla Baratto, Adalgisa Sinicropi, Verónica Sáez-Jiménez, Dolores Linde, Angel T. Martínez, Riccardo Basosi
From P. eryngii Versatile Peroxidase to A. AURicula-Judae Dye-decolorizing Peroxidase: an epr work in progress

Rebecca Pogni, Daniele Spinelli, Riccardo Basosi, Maria Laura Parisi, Enrico Fatarella, Luciano Tacconi, Luigi Ricceri, Mehmet Sener, Rezzan Karaaslan, Christian Marie Bols
Laccase-mediated Synthesis of new dyes for applications in textile industry

Laura Salvini, Laura Tinti
Confocal microscopy and mass spectrometry: two important methodologies in biotechnology

Daniele Spinelli, Enrico Fatarella, Riccardo Basosi, Rebecca Pogni
Laccase immobilization onto nanofibers and mesoporous materials

Gabriella Tamasi, Daniele Pagni, Zeno Tabani, Renzo Cini
Analysis of top quality Chianti wines from the years 2010-2013 grape harvests. The content of polyphenols and selected metal ions

Enrico Tavarnelli
The depositional and tectonic history of ridges and basins of Southern Tuscany: geological controls on the quality of wines and food produced in Val d'Orcia and in the Chianti mts

EPR spectroscopy for the study of antioxidant activity

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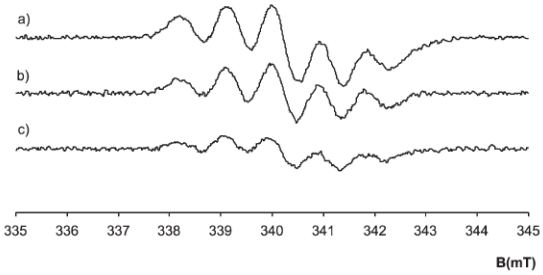
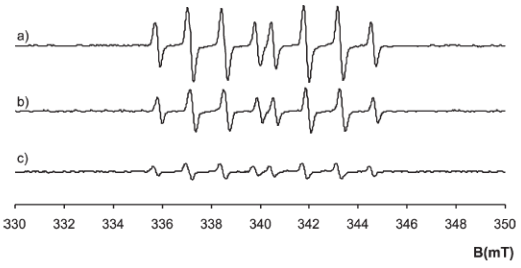
Electron Paramagnetic Resonance (EPR) spectroscopy is able to directly measure species with unpaired electrons and it has been used in several research field such as physics, chemistry, biology, life science, material science, medicine, nutrition, nutraceutical and food science. The spectroscopic technique can be applied for free radical scavenging capacity estimation, antioxidant activity investigation and food oxidative stability evaluation.
For food and nutraceutical research, EPR can be used with two methodologies: direct measurements and spin-trapping technique. EPR direct measurements allow to detect stable radical species, to define the radical stability and to quantify its formation. The most common assay is applied towards DPPH (2,2-diphenyl-1-picryhydrazyl radical). The stable EPR signal of the radical is acquired before and after the addition of the antioxidant species and the estimation of the scavenging capacity of selected antioxidant samples in function of EPR signal reduction gives a measurement of the antioxidant activity. The spin-trapping technique is applied to short-lived radicals, not directly detectable by EPR. The addition of a diamagnetic molecule (spin trap) will allow to intercept short-lived radicals and form relatively stable paramagnetic adducts which can be easily detected by EPR. This method is of great significance to investigate Reactive Oxygen Species (ROS) which have relatively short half-life time. Examples of commonly used spin trapping agents are: 5,5-dimethyl-1-pyrroline N-oxide (DMPO), N-tert-butyl-α-phenylnitrone (PBN), 5-diethoxyphosphoryl-5-methyl-1-pyrroline-N-oxide (DEPMPO).
In the following figures, EPR spectra of DPPH and ROS radical in the presence of antioxidant molecules are reported.



Room temperature EPR spectrum of DPPH radical a) in the absence of antioxidant, b) in the presence of 5-O-galloyl quinic derivative and c) 3,4,5-O-trigalloyl quinic derivative



Room temperature EPR spectrum of DEPMPO-OH adduct a) in the absence of antioxidant, b) in the presence of gallic acid and c) in the presence of 3,5-O-digalloyl quinic derivative

In this laboratory the scavenger activity of antioxidants, such as polyphenols, against radical species will be determined using EPR.
Lecture (1h): Theoretical introduction to the EPR spectroscopy and its applications.
Laboratory Session (2h): EPR detection and analysis of radical intermediates.

References

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9. Electron Paramagnetic Resonance: Elementary Theory and Applications, J.R. Bolton, J. Weil.
10. New Applications of Electron Spin Resonance: Dating, Dosimetry and Microscopy, M.Ikeya.

ENERGY from the principles of thermodynamics to the sustainable development

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Clean energy does not exist. The only clean energy is the one saved, i.e. the one which is not necessary to use. The choices on the energy resources should be done in terms of environmental impact minimization and in terms of cost/benefit analysis. This derives from the basic concepts of Thermodynamics. In fact the unidirectional time flowing, implicit in thermodynamics laws, allows to connect apparently distant worlds like the one of order, the one of probability and the one of information. The information content of energy resources is specific and not unlimited in nature, with the only exception of renewables. This suggests the rationale and efficient use of energy (commonly said energy saving) as the first pillar of environmental sustainability. The second pillar, which is equally necessary, is the use, compatible with their characteristics, of the renewable resources. All of them are directly or indirectly bound with solar activity. In the presentation, examples of thermodynamic saving taken by everyday experience will be shown. and a general view on the recent developments of renewables will be given.

The presentation will end with a summary of a good practices, in agreement with thermodynamic principles, for building and environmentally sustainable society.

Lysozyme crystallization

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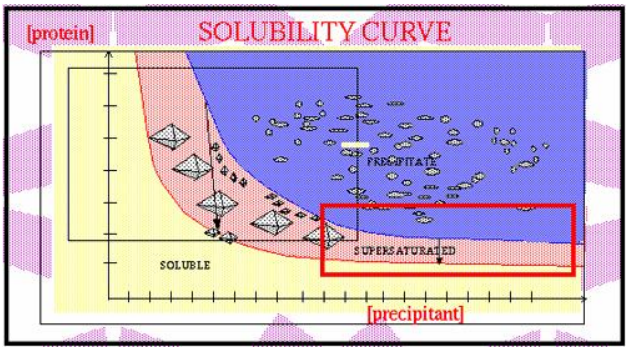
Crystallization is the process, governed by both thermodynamic and kinetic factors, by which molecules arrange themselves in a natural manner to form a repetitive three-dimensional reticulum we call crystal. Thermodynamically, protein crystallization is not very different from the crystallization of NaCl. In both cases, we need to bring the solution into a supersaturated state after which the salt or the protein will hopefully start to crystallize. However, protein crystallization methods are very different. In the case of NaCl supersaturation may be achieved by first preparing a saturated solution of the salt at some high temperature (for example, 40°C) and then leaving it at room temperature for some time. At room temperature the solution will be in a thermodynamically metastable state. The result is that after a short while salt crystals will be found at the bottom of the glass. In the case of proteins, heating is not a method to use, proteins may quickly denature at high temperatures (unless it is a protein from a thermophilic organism). We are helped by the fact that protein solubility depends on many factors and not only on temperature. Among these factors is the concentration and type of salt present in the buffer, the pH of the buffer, the presence of possible co-factors, etc. Depending on the protein, different crystallization methods may be used to bring the solution into supersaturation, normally through a gradual decrease of the solubility of the protein. The most common way to reduce protein solubility for crystallization is by the addition of so-called precipitants (see Diagram). A precipitant binds water molecules, essentially competing with the protein for water, thus reducing water availability, which mimics higher protein concentration. Popular precipitants include polyethylene glycol and ammonium sulfate, probably the most widely used, but there are many other precipitants. When precipitant concentration is gradually increased, for example by using the method of vapor diffusion, the amount of solvent available for the protein is decreased, which in turn may lead to protein precipitation, or if the conditions are correct, to crystallization of the protein.
The objective of the Laboratory session is to provide "hands on" experience on the crystallization of Enzyme Lysozyme, which has been well characterized with respect to crystallization properties.
We will use the sitting drop methods that rely on vapor diffusion, in which a drop containing lysozyme/precipitant solution is allowed to equilibrate in a closed system containing a reservoir of precipitant.
With vapor diffusion, the sample is at 50% of the concentration of the precipitant compared to the reservoir solution and is less than that required for protein crystallization. Thus because the precipitant is the major solute present, vapor diffusion in the closed system results in the net transfer of water from the protein solution to the reservoir, until the precipitant concentration is the same in both solutions. Upon equilibration this transfer of water ceases and the resultant protein solution stays at the optimal precipitant concentration for crystallization.



Generic diagram showing the different areas of a protein-precipitant equilibrium in terms of the concentrations of both components.

Excited state properties of organic sensitizers for DSSC evaluated at the PCM/TD-DFT level

Caterina Bernini[a], Lorenzo Zani[b], Massimo Calamante[b], Gianna Reginato[b], Alessandro Mordini[b], *Maurizio Taddei*[a], *Riccardo Basosi*[a], *Adalgisa Sinicropi*[a]

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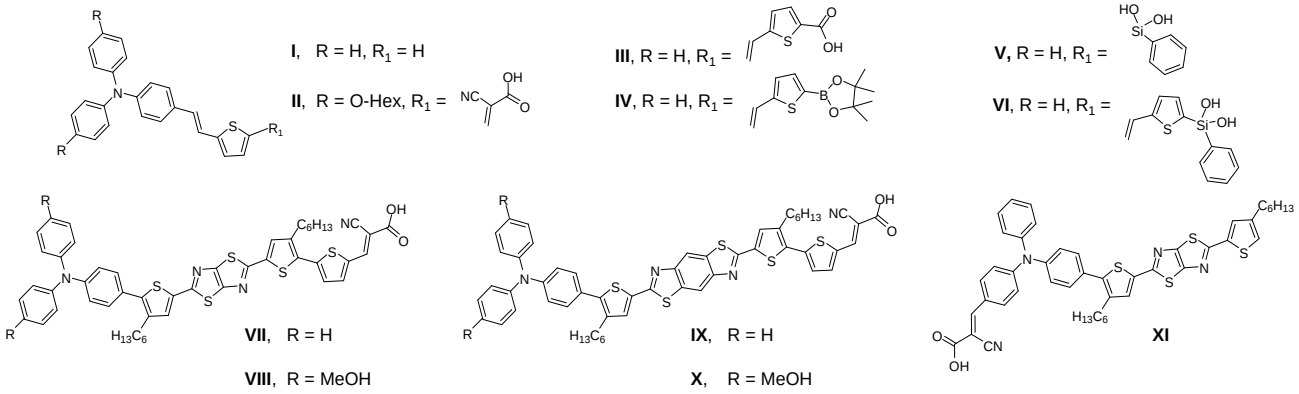
Excited state geometries and emission maxima of 11 organic dyes used as sensitizers in Dye-Sensitized Solar Cells (DSSC) have been computed using a PCM/TD-DFT strategy. The investigated dyes can be divided into few groups: triarylamine-thiophene derivatives with different conjugation lengths and bearing various anchoring groups (**I**-**VI**), thiazolothiazole- (**VII**-**VIII**, **XI**) and benzobisthiazole-containing (**IX**-**X**) sensitizers.



The results showed that the computed emission energies are in good agreement with the experimental values [1-3] (mean absolute error ~ 0.10 eV). The obtained accuracy opens the way to the design of improved compounds, in terms of excited state stability, to be used as photo-sensitizers in DSSC.

References

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Modern applications of electron transfer processes

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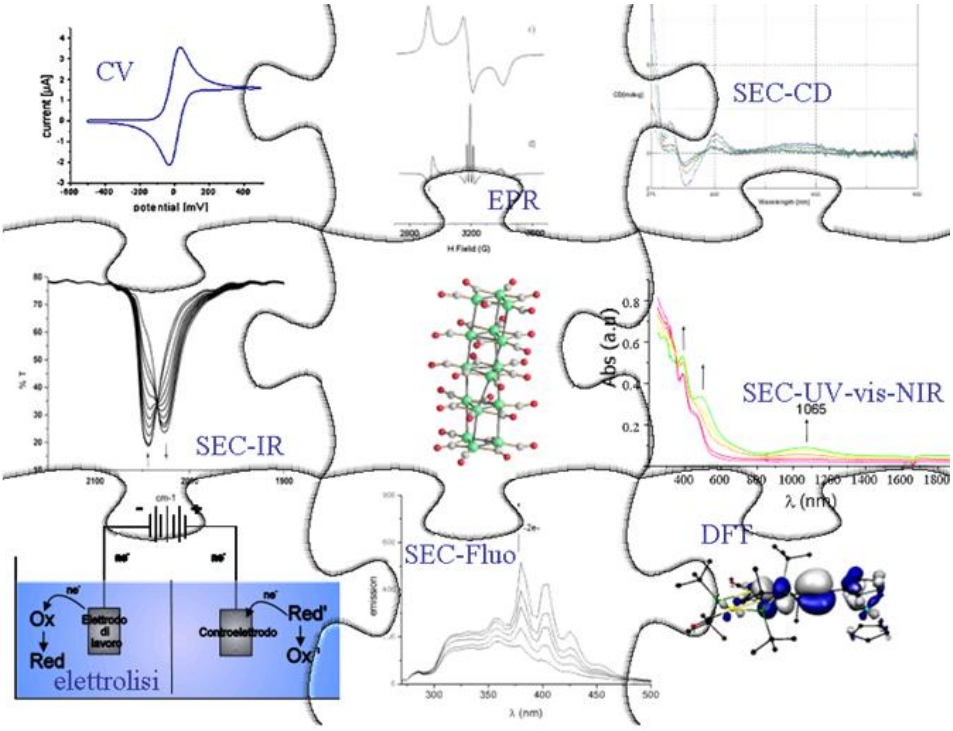
Electron transfer [1] is the key-step in many chemical processes brought into play in many applications: as an example it plays a role in nanotechnologies, in biochemistry and in the solar energy exploitation. Electrochemistry collects a branch of techniques dedicated to the study of the many aspects concerning the electron transfer phenomena, their energetic and kinetic aspects and their consequences from a chemical and physical point of view. As a further bonus, electrochemistry can be used in tandem with many spectroscopies extending the potentiality of this approach. In this short presentation we will give a short survey of the activity of the inorganic electrochemistry group of the Department.



Reference

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Spectroscopic studies of interactions between β-amyloid peptide fragments and metals

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Alzheimer' s disease (AD) is the most common neurodegenerative disease. It affects roughly thirty million people in the world and this number will increase drastically in the next forty years[1]. A common hallmark of AD is the presence of extracellular amyloid plaques, which are constituted of fibrils and aggregates of β-amyloid peptide (Aβ)[2]. It is well accepted that high concentration of transition metal ions, such as copper, zinc and iron are present in Amyloid plaques of AD brains, and these metals are involved in AD pathogenesis[3]. The complexes of Cu(II)-Aβ and Zn(II)-Aβ have been well-characterized at different experimental conditions. The stoichiometry ratio metal/Aβ is always 1:1, while the coordination environments are dependent on pH conditions[4]. The coordinations of Fe(II)/(III) and Cu(I) to Aβ species is less known. A Faller' s study have assumed a hexa-coordination of Aβ to the Fe(II) ion[5], while a two-coordinate linear model with two imidazole ligand is established for the complex Cu(I)-Aβ[6]. Many studies have demonstrated that the binding site of metals to Aβ is located in the first sixteen amino-acid residues. The aim of this work is to investigate different complexes of transition metal and peptide fragments of Aβ, at physiological pH, through Nuclear Magnetic Resonance spectroscopy (NMR), in order to understand the differences of every single amino—acid in the chelation of metal. The interaction of Ag(I) to Aβ peptide is also taken into account to assess the possibility to use Ag(I) ion as a probe for Cu(I)-Aβ complexes. Finally the structural transitions occurred in Aβ in presence of different surfactants has been monitored by means of Circular Dichroism (CD).

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Mass spectrometry in bioorganic chemistry: from structural to stereochemical and conformational characterization

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Mass spectrometry (MS) is a powerful methodology for identifying, structurally characterizing, investigating the reactivity and quantitating wide classes of naturally occurring organic molecules or obtained by different synthetic approaches.
A number ionization techniques, depending on the chemico-physical properties of the molecules, and a wide range of analyzers are available.
Given an organic molecule, a lot of information can be obtained by mass spectrometry: molecular weight, elemental formula, structural characterization (tandem mass spectrometry), quantitation, but also it is possible to determine stereochemical properties, to study conformations (ion mobility mass spectrometry), to make a mapping of the analytes on a surface, such as a tissue or a leaf (mass spectrometry imaging), to make ion spectroscopy in the gas phase [1-2]. The use of soft ionization techniques, such as electrospray and MALDI, allows to characterize non covalent complexes and to study supramolecular aggregates.
The mass spectrometer can be used as a complete chemical laboratory for gas phase studies of the reactivity of radical ions, cations and anions, collision-induced dissociation reactions, ion activation by photons, ion-molecule and ion-ion reactions.
The coupling of mass spectrometry with different separative techniques, such as gas chromatography and HPLC allows the study of complex mixtures.
Applications of mass spectrometry in organic chemistry developed by this research group [3-4]will be presented.

Laboratory session

Mass Spectrometry in Practice: What is Your Weight and What is Your Structure?

ESI MS and MS/MS experiments on different matrices (food, biological samples, plants) will be carried out.

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Full structural characterization through global diffraction pattern fitting. A contribute to the International Year of Crystallography IYCr2014

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Powder diffraction is a widely used technique to characterize solid materials. A tiny quantity (from 10^{-1} down to 10^{-6} g) of a polycrystalline sample, either prepared in the lab or in situ, is irradiated with X-rays or neutrons which are diffracted (reflected, but only at certain angles) giving a series of of tens to hundreds of peaks, depending on the complexity of the material under study. Each of these peaks is characterized by a position, an intensity, and a width. Positions are related to the unit cell dimensions which may range from a few Å in simple structures like NaCl up to ~1000 Å and more for an enzyme or virus. Intensities are related to the coordinates of all the atoms (1 to several 1000) inside the unit cell, and the widths reflect several phenomena from grain size to internal strain and pseudosymmetry.
The correct ("global") simulation of all these aspects of a powder pattern through curve fitting is therefore able to give a very detailed description of a solid including crystal structure, phase quantification (in mixtures), grain size and anisotropy, specific surface area (e.g. for catalysts), texture and preferred orientation of grains which is important to explain the history of rocks or the mechanical strength of an alloy, and more.
The simulation of the latter, or "microstructural", parameters has not been possible until a few years ago when sophisticated maths became available to describe the peak shape. Here, we give an introduction to the philosophy and working principle of the fitting procedure in order to enable the student to realize the role of the different parameters and eventually make use of the power of powder diffraction in his own research.

Lecture program (90 min, at Rifugio)

Diffraction, structure, and the International Year of Crystallography
Unit cell and crystal structures
About Gaussians, Lorentzians and real peak shapes
Powder diffraction techniques: tools and tricks
Principles of Rietveld powder pattern fitting

Exercises (3h, groups of max 4 students, at Dip SFTA, via Laterina 8)

Setup of data and instruction parameters for Rietveld refinement
Use of databases to find crystal structure parameters
Instrument parameters and calibration
Stratiegy and criteria for a successful refinement
Interpretation of results and errors

Rheological characterization of polymeric hydrogels

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Rheology is defined as the flow of fluids and deformation of solids under stress and strain. Some materials are intermediate between solids and fluids and the viscosity is not enough to characterize them. A solid material can be described by its elasticity or resilience: when it is deformed it will store the energy and fight back, as a spring that regains its original shape after being deformed. The other extreme is a fluid which stores no energy while deformed and just flows. A viscoelastic material is intermediate and stores some energy and flows a little when deformed. It moves partly out of phase. This can also be expressed mathematically. The solid-like component at any particular frequency is characterised by the storage modulus G', and the liquid-like response is described by the complementary loss modulus, G". The unit of both these moduli are pascals and their values vary with applied frequency, ω, which is given by 2πf, where f is the frequency in hertz (Hz) [1].

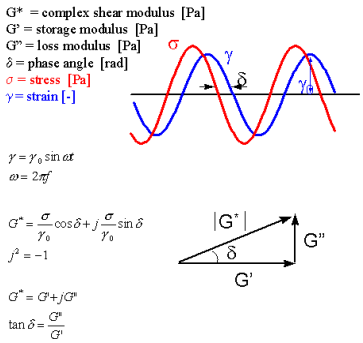

Figure 1: Mathematical relations between the basic parameters G' and G" and other derived parameters δ (loss tangent) and G*(complex modulus).

A classical example of viscoelastic material is hydrogel, or crosslinked network of hydrophilic polymers and possess the ability to absorb large amounts of water and swell, while maintaining their three-dimensional (3D) structure.

Laboratory Activity

Hydrogels, in the swollen state, will be tested in a strain-controlled AR2000 Rheometer (TA-Instruments, Leatherhead, United Kingdom) in the parallel plate configuration. Smooth and rigid plates will be used for testing. Strain sweep tests at a fixed oscillation frequency (consisting in monitoring the viscoelastic properties while logarithmically varying the strain amplitude γ0) will be performed on the materials to determine the strain amplitude at which linear viscoelasticity is valid. A dynamic frequency sweep test will be performed in a frequency range basing on strain sweep results. The following parameters will be determined: the shear storage modulus G' (provides information about the elasticity or the energy stored in the material during deformation), the shear loss modulus G" (describes the viscous character or the energy dissipated as heat) and the loss tangent (tanδ = G"/G'; a measure of the ratio of the energy lost against the energy stored in a cyclic deformation) A series of stress-relaxation experiments will be also performed to evaluate the shear stiffness at the equilibrium increasing the strain from 5% up to 20%.

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Biosensors: useful tools for diagnostic purposes

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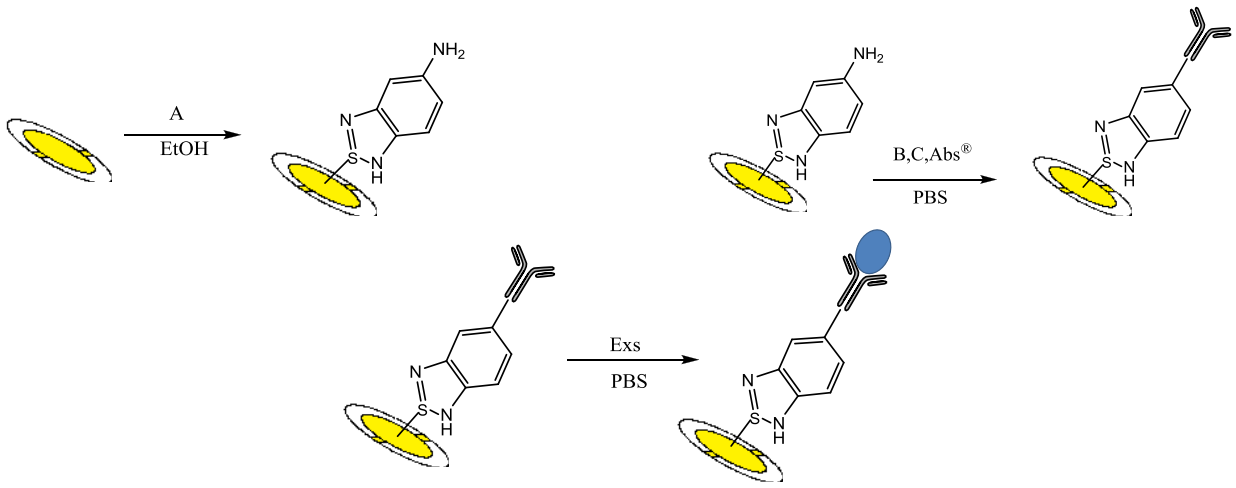
The *in situ* detection of biological species is a topic of great interest in several fields including environmental, food, safety, diagnostic and biomedical areas. Consequently, it is of huge importance to develop simple systems with high specificity towards the species of interest, able to reveal them through a simple interaction mechanism with high sensitivity and accuracy. In this contest, biosensors represent useful tools, because of their quick response with high sensitivity.
A strategy to develop a biosensor model system is presented. Specific antibodies for specific cancer biomarkers, are immobilised without modification on a QCM (quartz microbalance) substrate by combining the SAM (self-assembled monolayers) methodology with a simple chemical route. In particular, the gold substrate of the QCM sensor was functionalised with benzymidazol which was further led to react with the antibody, the carboxylic moiety of which was activated through N-Hydroxysuccinimide (NHS) and 1-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (EDC). The substrates were characterised at each step of modification by reflection absorption infrared spectroscopy (RAIRS) and the ability to specifically recognise biomarkers was demonstrated by QCM measurements.



Laboratory activity

Characterisation of the single steps involved in the development of the biosensor system model by reflection absorption infrared spectroscopy (RAIRS) and evaluation of the biosensor ability to specifically recognise the biomarker *in situ* (analysis of the immobilised antibody-biomarker molecular recognition).

100 years of Crystallography: from quasicrystals to proteins

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2014 has been declared by the United Nations International Year of Crystallography to celebrate the centennial of the Nobel Prize award to Max von Laue for the discovery of X-ray diffraction by crystals (1914). Everyone uses the word "crystal" in common language, but few are aware of the true physical meaning of this word that is used both for "true" crystals, like sodium chloride, and for non-crystals such as expensive glasses (eg. Swarovski). A relevant property of crystals, from the point of view of the advancement of science, is that they are "devices" that allow us to literally see the atoms and molecules of which they are made. This relates to their interaction with X-rays.

Modern Chemistry, Solid State Physics, Biology and Medicine are based on atomic and molecular knowledge that has been acquired mostly by using X-ray crystallographic techniques. For example, we can understand how superconducting materials, or semiconductors (silicon chips) are made, but also how proteins are produced in the cell and how virus particles look, allowing us to design new materials and new drugs.

In the lecture, I will briefly introduce X-ray crystallography and review some of the most important discoveries made using crystallographic techniques. Three-dimensional molecular structures will also be displayed and discussed.

Spectroscopic investigation on -KLVFF- amyloid β sequence

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Neurodegenerative diseases, which include Alzheimer Disease (AD), are highly prevalent. These diseases are characterized by disorders in protein folding and by the progressive loss of neuron structure and function (1, 2). Moreover AD is characterized by progressive dementia and cortical atrophy. Protein folding disorders cause a specific protein rearrangement leading to the self-aggregation that finally promote the deposition of insoluble protein aggregates known as amyloid plaques (3, 4). Many amyloidogenic proteins contain simple repetitions of 6-8 amino acids involved in protein misfolding and aggregation (5). The seven residues sequence KLVFFAE is particularly interesting since it represents the amyloidogenic fragment of the Aβ peptide (6). OR2 is a short synthetic peptide based on the sequence of the amyloidogenic fragment (-KLVFF-) with added RG-/-GR residues at the N- and C-terminal ends to aid solubility. During this study the RGKLVFFGR-NH_2 peptide sequence (known as OR2 peptide) has been studied, at physiological pH, in order to understand if the presence of the -KLVFF- β sequence causes a behavior similar to the Aβ peptide. Several studies on different amyloidogenic fragments have demonstrated how the presence of phospholipid bilayer affects the aggregation phenomena of such peptides (7, 8). Spectroscopic measurements (CD, NMR and Fluorescence) were performed on OR2 in presence of different concentration of Sodium Dodecyl Sulfate (SDS). Using different techniques we demonstrate that the residues -KLVFF- strongly influence OR2 behavior. Moreover we demonstrate that the peptide in presence of SDS concentration, under and above critical micellar concentration, adopts different conformations. A similar behavior was observed for many amyloidogenic peptides, especially for $A\beta_{1-40}$ (9, 10). For these reasons Fluorescence measurements were performed (at the same OR2 experimental conditions) also to $A\beta_{1-42}$ to verify if our conclusions could be extended to the most amyloidogenic β peptide, from which OR2 derives.

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The beauty of bioinformatics

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Biomedical research in the post genomic era is characterized by huge amounts of collected data, thanks to a synergistic effect of several advances in basic knowledge and technology. For the first time in human history, high throughput procedures, such the ones routinely used in genome investigations, yield more results than the ones researchers can handle. Thus, a large number of databanks have been established to accommodate and to give some order to the obtained biological results. Once databanks are operative, algorithms must be implemented to extract information which can be relevant for the advancement of science and technology. This is what Bioinformatics do and the reason why, nowadays, it is obtaining an increasing consideration among scientists is apparent.

Structural Bioinformatics deals with the available wealth of biological information at an atomic resolution with the main goal of understanding basic mechanisms of life or, just as an example, for establishing new procedures for drug design. Protein Data Bank (PDB) is the temple where the structural information collected by X ray crystallographers, NMR spectroscopists and cryo-electron-microscopists is safely stored. More than 90,000 different structures of proteins, DNA and RNA can be now retrieved from PDB.

We have developed a new structural descriptor, the atom depth index (D_i), to analyze protein structures in terms their atom distribution within the reported 3D structure [1]. By using this new tool, protein cores have been systematically investigated and defined, see Fig. 1. Protein core compositions have revealed that specific protein folds require the presence of specific amino acids which might be the basis a specific fold barcoding .

By using D_i analysis on PDB files, protein surface composition has been also investigated, in order to find clues of the mechanisms driving protein-protein interactions [3].

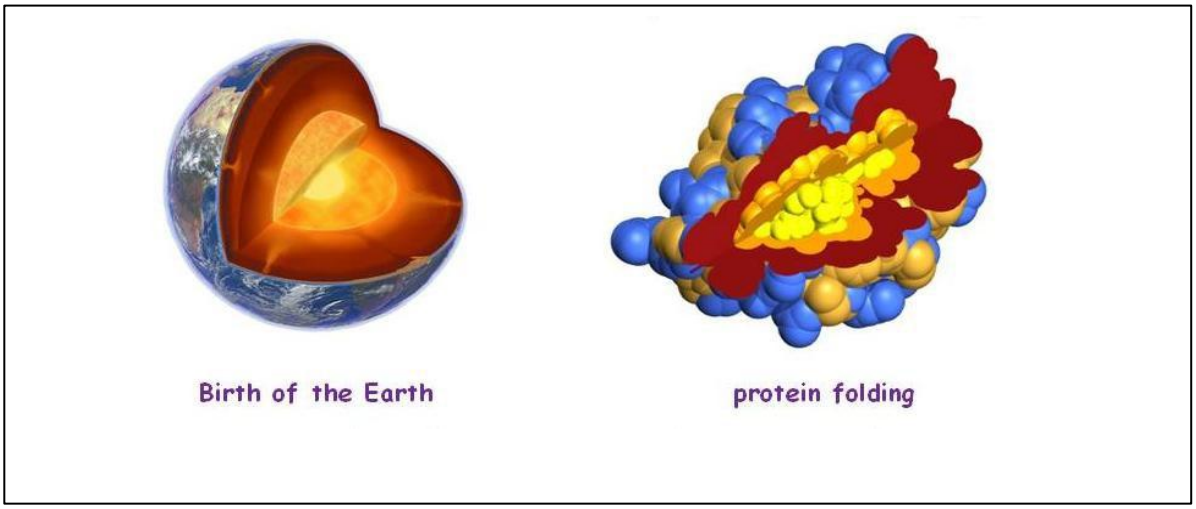

Figure 1. The use of new algorithms to explore new dimensions of protein folding and interactions.

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Cu(I) and Cu(II) binding to the amyloidogenic fragment of the human Prion Protein

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Prion diseases are fatal neurodegenerative disorders characterized by progressive brain degeneration (1). In humans, the group of prion diseases includes Creutzfeldt–Jakob (CJD), Gerstmann–Straussler–Scheinker (GSS), new variant Creutzfeld–Jakob disease and fatal familial insomnia.

These diseases can be transferred between individuals or between the species (2) by several mechanisms, such as blood transfusion, ingestion and iatrogenic transmission (3). The diverse prion diseases share various isoforms of common infectious agent known as PrP^{Sc} (Sc for scrapie), the abnormal form of host-encoded cellular prion protein (PrP^{C}) (4). In fact, these diseases are caused by protein-only infectious agents propagating by inducing protein conformational changes from normal cellular PrP^{C} into the PrP^{Sc} (5). The only differences between them seem to be the monomer conformation and the resulting aggregation properties (6).

PrP^{C} is a 254 amino acid soluble protein: the N-terminal domain is unstructured, while the C-terminal domain contains three α-helices and two β-sheets. PrP^{Sc} form possesses large β-domains and it easily forms protein aggregates (7) because it is insoluble and protease resistant. The formation and accumulation of PrP^{Sc} is a major factor in the development of neurodegeneration and disease (9).

The cellular form of prion protein is also widely known as a copper binding protein, that is possibly necessary for its normal cellular function (10). In mammals, the PrP^{C} 60-91 region is formed by the octapeptide PHGGGWGQ, repeated four times, and have the peculiarity to bind Cu^{2+} by the His, in a way which is dependent on pH and metal availability (11). One or even two additional Cu^{2+} ions can be tethered to PrP at the so-called "fifth binding-site", located in the amyloidogenic PrP region of (90–126), where two His residues (96 and 111) are present (12). Met109 and/or Met112 residues are also involved in complexation at the site centered at His111 (13). The aim of this study is to investigate the role played by His96, His111, Met109 and Met 112 on Cu^{2+}/Cu^{+} binding through several experimental techniques, such as NMR, IR, CD and Cyclic Voltammetry.

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The Mysterious Fungi: The Good, the Bad and the Ugly

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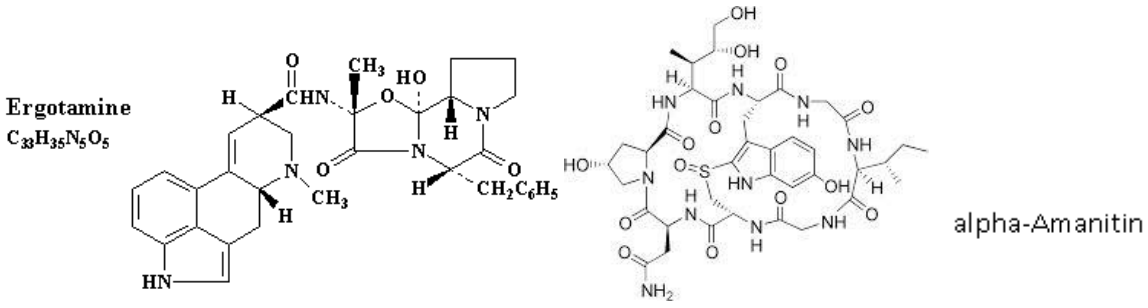
Since the 16th century the Sienese Doctor Valenti Serini tried to teach the people about the mysterious organisms called the fungi that could be edible and good tasting food, have medicinal properties to treat various illnesses or be a terrible enemy of human life. He tried through clay models and paintings to show the high fungal diversity and characteristics of edible and poisonous mushrooms to educate people. Even today, with all of the research that has been done on this topic, people are hospitalized because of fungal toxins/poisoning, directly because of eating wrongly identified fungal species (macromycetes) or indirectly because of the unknown presence of dangerous fungal plant pathogens (micromycetes) that can contaminate food. The toxins that these organisms produce are among the most toxic compounds known on the planet. For instance a study is still underway on the group of white Amanita, particularly on *Amanita ovoidea,* considered by some as a good edilble mushroom. The phytochemical screening showed that compound contents depends on the part of the fruiting body considered and through the cell viability analysis a high mortality was found in cold extraction of pileus and volva. On the other hand there is no effects of pollution by heavy metals (1).

Numerous fungi (micromycetes) that secrete highly toxic substance, secondary metabolites known as mycotoxins, are known to infect plants that humans and animals consume as food. These fungi include species of *Claviceps*, *Fusarium*, *Aspergillus* and *Penicillium* and produce the extremely toxic substances ergotin alkaloids, fumonisins, aflatoxins, and patulin, respectively. In particular, *Claviceps purpurea* and the disorder it produces commonly known as Ergotism has caused harm to and kill untold numbers of people over the centuries (2).



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From *P. eryngii* Versatile Peroxidase to *A. AURicula-Judae* Dye-decolorizing Peroxidase: an EPR work in progress

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Amino acid radicals are found as redox active reaction intermediates in an increasing number of enzymes [1]. It has been demonstrated that EPR and its related techniques are important tools for identification, e.g. discrimination of tyrosyl and tryptophan radicals, investigation of structure and protein interactions, and even site selective assignment of freeze-trapped protein-based radicals.
Heme peroxidases are two electron oxidized by H_2O_2 and converted into Compound I (with oxo-ferryl, Fe^{4+}=O, heme containing a porphyrin π-cation radical). The activated enzyme subsequently performs one electron oxidations of two substrate molecules, coming back to the resting state via Compound II (the one-electron oxidized intermediate Fe^{4+}=O heme).
Versatile peroxidases are ligninolytic enzymes capable of oxidizing large molecular size aromatic compounds. The proposed catalytic mechanism involves formation of the Fe^{4+}=O-porphyrin radical (Cpd I), and a long range electron transfer to form a tryptophan radical at the protein surface [2]. High-Field EPR and ENDOR studies, on a freeze-trapped radical intermediate in the reaction of VP from *P.eryngii* with hydrogen peroxide, clearly identified a neutral tryptophan radical [3].
Quantum-mechanics/molecular-mechanics (QM/MM) calculations have allowed a detailed characterization of the tryptophan radical within the protein matrix of VP. The applied computational strategy made it possible to obtain a mechanistic description of the proton-coupled electron transfer process leading to the radical formation and provided additional details on the role played by the nearby protein residues and solvent water molecules in affecting the EPR spectral properties and the geometrical structure of the radical intermediates [4].
In some members of the peroxidase superfamilies, like the more recently discovered, dye-decolorizing peroxidases (DyPs), the catalytic mechanism is still to be defined. Recently a protein radical catalytic site has been identified and assigned to a Tyr337 residue as an additional substrate interaction site in the jelly fungus *Auricularia auricula-judae* (AauDyPI) [5].
Starting from the EPR data of *P. eryngii* VP and its variants, newly collected EPR data combined with a QM/MM investigation on AauDyPI (native and variants) will be presented to shed light on the catalytic mechanism through the identification of surface-exposed protein radical sites for the oxidation of large molecular size substrates.

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Laccase-mediated Synthesis of new dyes for applications in textile industry

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Biocatalysis has become a common applied "industrial technology" alternative to traditional chemical synthesis. The discovery and improvement of biocatalysts suitable for industrial uses and their immobilisation will address to increase stability and efficiency of enzymes. Bioprocesses will allow expanding the type of chemical transformations at large scale with the optimisation and improvement of novel bioreactors. The feasibility of new bioprocesses has been demonstrated during the EU BISCOL project (ECO/09/256112/SI2.567273).

The objective of the European project BISCOL was to propose a new dyeing process as global alternative for the bioconversion of raw materials into competitive eco-viable final products through:

- textile plasma pre-treatments aiming to increase dyeability of textiles
- synthesis of bio-dyes using new safe and environmental friendly routes (enzymatic processes)
- synthesis of new auxiliaries at lower environmental impact
- optimisation of dyeing process reducing energy and water demand.

In this frame, the synthesis of new bio-dyes by laccase, at medium/large scale, has been investigated starting from the previous results on the laccase-mediated synthesis of dyes like LAR-1 and CURIE-22 in the SOPHIED project (FP6-NMP2-CT-2004-505899) [1-3]. Different routes of synthesis have been investigated by laccase-mediated homocoupling and heterocoupling reactions using natural (i.e. ferulic acid) and chemical precursors (i.e. 4-amino-1-naphthalenesulfonic acid). A tri-colour set (yellow, red and blue) of acid biodyes for woollen fabrics has been selected and their scale up has been performed by a new developed bioreactor at production site. The synthesized bio-dyes showed a lower or similar toxicity and light fastness/washing properties comparable to the industrial ones.

Life Cycle Assessment (LCA) analysis has been used for the comparison between the conventional dye synthesis and that proposed by the BISCOL project [4].

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Confocal microscopy and mass spectrometry: two important methodologies in biotechnology

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The Toscana Life Sciences (TLS) Foundation is a non-profit organization that has been active in the regional panorama since 2005 with the objective of supporting research activities in the Life Sciences and, in particular, of sustaining the development of projects from basic research to industrial application.
To reach these objectives, TLS has created a modern Science Park where it provides technological platforms and expertise and experience networks within the regional scientific community – starting from universities, research centers and private laboratories that work in the biomedical sector – offering their support in the industrial, scientific, and business development contexts.

Today the TLS Science Park, is one of the few single-theme parks in Italy for the Life Sciences. It is located in the historic "Torre Fiorentina" area, hosts 22 subjects among incubated companies, non-profit research groups and service companies that operate in the research and development of new drugs, diagnostics and medical devices, and gives access to a wide range of qualified services and advanced technological platforms.

Since its establishment TLS Foundation supports also research in the orphan disease field.

Until today TLS has moved in this field with three initiatives:

- Aggregation of research groups active in the field
- Orphan-1 project, co-financing of research already underway at Tuscan public laboratories
- Orphan-2 project, management and coordination of development activities in the sector of protein (enzyme) replacement therapy

In the ambit of Orphan-2 project, during the last few years TLS is working on the production, characterization of a recombinant enzyme and development of an appropriate delivery system to cell cultures.

During the visit, a short presentation of TLS research activities will be given. After that a mass spectrometry experiment will be performed, starting from the sample preparation, the analysis and the elaboration of the data.

Laccase immobilization onto nanofibers and mesoporous materials

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Enzyme immobilization is advantageous for industrial application due to convenience in handling, ease of separation of enzymes from the reaction mixture and reuse, low product cost and a possible increase in thermal and pH stability. An important requirement for protein immobilization is that the matrix should provide a biocompatible and inert environment [1,2]. The result of immobilization, including the performance of immobilized enzymes, strongly depend on the properties of support. Improvements of biocatalytic efficiency can be achieved by manipulating the structure of carriers for enzyme immobilization. In recent decades, nanostructured and mesoporous materials have attracted much attention because of their unique properties and interesting applications [3,4]. They stand out of other supports because of their extremely high surface area-to-volume ratios, which can provide large specific areas for an efficient immobilization as well as stabilization of enzymes.
In this context, nanofibers represent excellent supports as: (i) a great variety of polymers can be electrospunned and meet different requirements for support applications, (ii) the high porosity and the interconnectivity endow them with a low hindrance for mass transfer and (iii) the nanofiber surface can be modified accordingly to the functional groups present on the enzyme surface to enhance the amount of supported enzyme.
The SBA family of mesoporous silicates have a narrow pore size distribution, high surface area, high pore volumes and well-ordered pore structures with uniform mesopores ranging in size from 2 to 50 nm. The regular repeating pore structures of these materials offer the possibility of adsorbing or entrapping large molecules within their pores. Covalent binding sites for enzymes can be also introduced by post or direct synthesis modification. After modification, sufficient space is preserved for the introduction of enzymes leaving a path for substrate diffusion to the catalytically active sites.

In this work Laccase from *Trametes versicolor* was immobilized onto nylon 6 nanofibers prepared by electrospinning method and synthetized SBA-15 ordered mesoporous material. Carriers have been functionalized by glutaraldehyde as crosslinker for enzyme immobilization. TEM and SEM microscopy, and infra red spectroscopy (IR) have been used to monitor the effect of surface functionalization on the structural features of the carriers. The enzyme immobilization efficiency for nylon nanofibers and SBA-15 carriers were 71% and 45%, respectively. The operational and thermal stabilities of the immobilized laccase were improved compared to free counterpart. Based on their properties, the resultant biocatalytic materials would enable novel applications of enzymes for industrial purposes.

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Analysis of top quality Chianti wines from the years 2010-2013 grape harvests. The content of polyphenols and selected metal ions

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The content of anti-oxidants like certain polyphenols and selected metal analytes play a key role in wine quality, and grape extracts [1,2]. Furthermore, grape extracts are used as sources of natural compounds in the pharmaceutical, food and nutraceutical industries [3]. On another side certain other phenols, particularly volatile phenols like 4-ethylphenol and 4-ethylguaicol play a deleterious effect on wines especially the aged ones, because the undesired smell and flavors of horse saddle that they might cause even at very low concentration [2].
As a continuation for previous researches on wines, we wish to report here on the highlights from a project on top quality Chianti red wines produced from the grape harvests of the years 2010 and 2013 from vineyards located at an average altitude by 450 m on the sea level, 100% Sangiovese vine variety in the Comune di Gaiole in Chianti. The selected data are reported in Table 1.

Table 1. Selected parameters obtained from (a) Sangiovese grape and wine from harvest 2013 and (b) wine from harvest 2010. A, overall acidity (g lactic acid/L); VA, volatile acidity (mg acetic acid/L); SO_2 (mg/L); Ph, total phenols (mg gallic acid/L); R, resveratrol (mg/L), selected metals (mg/L).

Product	**Parameter**						
	A	**VA**	**SO_2**	**Ph**	**R**	**K**	**Cu**
Juice[a]	7.5(1)	279(3)	22.3(1)	420(10)	0.024	191(7)	-
Novello[a]	6.9(1)	398(4)	66(1)	3033(20)	1.2(1)	643(7)	0.25(1)
Wine[a]	5.7(5)	515(10)	41(1)	2982(52)	1.0(1)	722(13)	0.26(1)
Wine[b]	5.7(2)	460(10)	84(1)	3220(30)	2.6(3)	592(12)	0.36(1)

Resveratrol analysis has been carried out via chromatographic method (HPLC-UV detector) on the sample previously extracted, whereas the total phenols content has been analyzed by using the Folin-Chacolteau reaction and a photometric detector in the visible region.
The overall Ph and R in grape juice is 420(1) mg/L and 0.024(3) mg/L expressed as wet mass, whereas the content of R in grape skin and seeds is 10.5(1) and 0.32(1) mg/kg dry mass. The data confirm that Resveratrol is present at a high level in the skin of the berries and the values are in agreement or somewhat higher than those from other Sangiovese grape skin reported after a wide analytical investigation by others [4]. The high anti-oxidant potential of the Chianti wines from this work are evidenced by the high overall Phenol (Ph, ca 2980-3220 mg/L) and Resveratrol (R, 1.0-2.6 mg/L) contents.
The analysis of selected metals has been carried out via Atomic Absorption Spectrophotometry using both flame (FAAS) and graphite furnace (GFAAS) atomization and in the second case the instrument was equipped by Zeeman effect correction. It has to be noted that the content of Cu is below 400 µg/L a value that is in agreement with the selection of high quality grape that did not need heavy treatments before harvest neither at vinification/aging steps. The analysis of the selected toxic heavy metals like Cr, Ni, Cd, Pb revealed values of order of ppt, thus confirming the high quality of the products.

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The depositional and tectonic history of ridges and basins of Southern Tuscany: geological controls on the quality of wines and food produced in Val d'Orcia and in the Chianti mts

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Tuscany is traditionally regarded as a not-to-be-missed stop when visiting Italy, not only for its early human history dating back to the Etruscan age, and for the consequent richness in arts and architecture that have flourished ever since, but also for the quality of its renowned wines and for the taste of its food products, whose combination makes the traditional tuscan cuisine worldwide known and appreciated. Tuscan food and wine owe their specific character and taste to the variety of the landscape and climate, combined with a great diversity of bedrock and soils, that collectively make the unicity of this terroir. But which are the relationships between geology and wine? And between geology and food? How do the composition of the substratum, weathering, soil development, climate and landscape evolution influence the character of wine and the quality of food? These questions, once considered solely as matters to be treated in nice convivial events, are now receiving increasing attention amongst the geological community, to the point that thematic sessions and disciplinal conferences are organized on these topics, with a consequent impact in the scientific literature at the highest international level.

Italy has a long tradition in promoting its cuisine, which reflects a high vocation in quality assessment for its agricultural production. Yet there are to date relatively few studies on the geological factors that control the quality of Italian food and wine [1]. The Apennines are a mountain range that represents the backbone of the italian peninsula. These mountains are made of a stack of tectonic slices, consisting of Mesozoic and Tertiary mainly marine sedimentary rocks; these were detached from a Palaeozoic basement and piled northeastwards since Upper Cretaceous time largely during the Alpine orogeny. The structurally highest units are unconformably covered by younger sediments, that were deposited in fluvial-lacustrine and marine basins whose formation began in Late Tertiary time, following the orogenic climax [2].

The Mesozoic-Tertiary sequence differs greatly from younger sediments, thus reflecting a significantly different depositional environment. This lecture, conceived as an introduction to the reader who is little familiar with the geological history of Italy, outlines the main sedimentary and tectonic events that led to the development of the Apennine belt. The lecture aims at providing a framework for the study of the relationships between geology and food/wine in Southern Tuscany. Emphasis is given to the history of the Mesozoic-tertiary sedimentary sequence, whose deformation gave rise to the Chianti Mountain Range famous for its wine production. The development of younger sedimentary basins, whose fill extensively crops out in the Val d'Orcia, will also be illustrated, with the aim at providing a clue for the understanding why the cereal production of this province is greatly appreciated by food experts and gourmets alike worldwide.

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FIELD TRIPS

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VISIT TO NOVARTIS VACCINES ITALIA

20 JUNE 2014
VISIT TO BARONE RICASOLI VINEYARD AND CELLAR

25 JUNE 2014
VISIT TO VILCA

VISIT TO SOVESTRO IN POGGIO

Note - The abstracts reported in the following pages related to the companies/factories are downloaded from the respective websites or from previous editions.

11 JUNE 2014

VISIT TO NOVARTIS VACCINES ITALIA

http://novartisvaccines.com/about-vaccines/index.shtml
(See also http://www.novartisvaccines.it/index.shtml; in Italian)

The Novartis Vaccines division is a leader in providing products to fight more than 20 vaccine-preventable viral and bacterial diseases.
The only thing better than finding a cure for a disease is preventing illness in the first place.
Novartis Vaccines—the world's fifth largest manufacturer of vaccines and the second largest producer of influenza vaccine—is committed to the fulfillment of this highest of medical ideals.
By our very function, we play a key role in the Novartis core mission: keeping healthy people healthy by alleviating suffering and enhancing quality of life. At Novartis Vaccines, caring begins with prevention.

Nothing prevents viral or bacterial infections quite as well as a vaccine, which trains the human immune system to attack invading microbes before they can establish themselves in the body and cause diseases that can lead to death or a lifetime of disability.
Vaccines can be composed of dead or inactivated pathogens, but are increasingly made from purified antigens—proteins or other biomolecules found on the pathogen being targeted.
Once the immune system is exposed to these antigens, it learns to recognize and attack the pathogen that bears them before the infectious agent has a chance to cause disease. But the protective power of a vaccine can reach beyond those who have received it. Vaccinating even one person in a community against an infectious disease can impede the transmission of that disease to other people. In this way, vaccines protect not only the people who have received the immunization, but others as well.
This is one of the reasons the World Health Organization (WHO) considers vaccines the most cost-effective healthcare intervention available today; the only measure that has done more to improve global health in the past century is access to clean drinking water.
In the US, according to a recent study by the Centers for Disease Control and Prevention (CDC), a dozen often deadly diseases targeted by childhood vaccinations—from polio to diphtheria—have been either eliminated or have declined in incidence by more than 90 percent over the past century. The WHO estimates that vaccines saved the lives of more than two million people in 2003 alone by preventing the onset of a host of preventable diseases.
While vaccines have eradicated devastating diseases such as smallpox, the battle against infectious disease is far from over. Novartis continues to strive to develop and deliver innovative vaccines against pathogens that have long proved intractable, as well as those that are only now emerging as threats to global health; one such threat is the H5N1 avian influenza virus, thought most likely to cause the next influenza pandemic.

20 JUNE 2014

VISIT TO BARONE RICASOLI VINEYARD AND CELLAR

http://www.ricasoli.it/

Ricasoli is the oldest winery in Italy, the second oldest in the world according to the leading American magazine Family Business. Today it is the largest winery in the Chianti Classico area: Brolio Castle, where Baron Bettino Ricasoli invented the Chianti formula in 1872, is surrounded by 1,200 hectares in the communes of Gaiole and Castelnuovo Berardino. Valleys, hills, woods of oak and chestnut trees, 240 hectares of vineyards and 26 hectares of olive groves, all enjoying the beauty and the wide variety of soils and climate in this central Chianti area.

In the middle of the 1990s, Barone Ricasoli started a huge project to renew the vineyards in its Chianti Classico land. They were old vineyards (all planted at the end of the 1960s and the beginning of the 1970s), ripped apart by Esca, with low densities per hectare and containing all the varieties belonging to Chianti Classico, but distributed randomly. So an excellent opportunity arose to renew and improve the vineyards, while introducing international varieties, such as merlot and cabernet, at the same time.

Considering that most of the land was made up of rock and that the breaking up of the land had to be done using ploughs and explosives, the problem of reclamation proved to be complicated and hard right from the start.

So far 204 hectares have been replaced in Brolio, using modern preparation techniques and genetically selected material, all aimed at obtaining long-lived vineyards capable of producing high-quality grapes.

Plant spacing was based on high density and the number of vines varies from 5500 to 6600 per hectare. The training system is spurred cordon, 50 cm from the ground. There are 8 buds per plant and crop thinning enables a yield of about 1 kg of grapes per vine (65-70 quintals/ha).The white grape varieties, on the other hand, are guyot trained so as to exploit bud fertility to the full.

The attention paid to the *terroir*, which influences Barone Ricasoli's decisions, is at the base of the zoning study.

The harvest is done separately for every vineyard plot. The grapes are taken to the vat room in containers with a maximum capacity of 200 kg; vinification takes place in small steel vats, enabling us to carefully control the fermentation process and to keep all the characteristics of every single vineyard plot separate. Experiments and a thorough knowledge of the land have led us to vinify separately also within the same plot and according to the morphological similarities of the subsoil. The structure of the vinification vat room was devised so that the vats can be filled by means of gravity, which allows a gentle punching down so as to extract the noblest substances from the skins. At the end of the fermentation process the wines are transferred to barrels and oak barriques. The frequent organoleptic and laboratory controls accompany Ricasoli wines throughout their development right up to the long (sometimes very long) bottle maturation, in appropriate heat-controlled rooms, before being sent off to the four corners of the earth.

Brolio has always been a prime place for innovation and experimentation. It was here that Bettino Ricasoli, in search of a "sublime wine", invented the Chianti formula in 1872, after three decades of patient research and meticulous experiments, a compromise between art, passion and science: "...meanwhile, we beat our path to you, science and a little bit of art; to me more art than science" (Bettino Ricasoli, 1873).

25 JUNE 2014

VISIT TO COLLEVILCA GLASS FACTORY

http://www.collevilca.it/

Nowadays, the main production of Colle Val d'Elsa is made up of several companies that produce crystal glass objects applying an automatic or semi automatic manufacturing technique. Among those, only one company still produces handcrafted items, that is ColleVilca srl, which keeps to the old and traditional art of manufacturing crystal. A visit to the ColleVilca factory is planned, to show how the crystal is manufactured. The crystal, 'crystal glass' or 'lead crystal', is a form of glass with high concentrations of Pb. The lead crystal industry produces high-quality drinking glasses, stemware, cups, goblets, vases and similar articles made of glass that contain up to 35 wt% of lead oxide. According to an EU directive (69/493/EEC, Council Directive of 15 December 1969 on the approximation of the laws of the Member States relating to crystal glass. OJ, 1969. L326, 599-602), which explains the definitions and rules for its composition, glass traded within the EU must contain at least the 24% of PbO to be called 'crystal'. Moderate additions of PbO to the glass increase its chemical resistance. High lead content lowers the melting temperature and results in decreased hardness, but an increased refractive index of the glass, which is important for its 'brilliance'. At ColleVilca, each crystal glass product is manufactured in full, from the mixing of its raw materials to the final package, for successive distribution and usage processes. Visiting ColleVilca will allow everyone to observe in detail each step of the manufacturing process. Melting of the raw materials in furnaces, crystal forming, tempering, cutting and acid polishing are the most traditional steps of the manufacturing process that could be seen. Much attention will be paid to the traditional step of blowing and modelling of the pieces, which demonstrates the ceremonial magic of the masters. In fact, the magic touch of ColleVilca glass masters has never been surpassed, as they transform a shapeless glowing mass into a piece of art with their keen skill. The results are unique, highly artistic objects. The principal steps and techniques in making and decorating fine crystal glass objects at the plant will be shown and explained in English by an expert.

25 JUNE 2014

SOVESTRO IN POGGIO VINEYARD AND CELLAR

http://www.sovestroinpoggio.it/
http://www.siena.coldiretti.it/

Sovestro in Poggio is a farm located on the hills of Chianti near San Gimignano. We are a small farm and we produce wine, olive oil, grappa and sweet wine. We delight our self in receiving people from all over the word and we are pleased to involve everybody in our activities.
The visit to our farm consists in explanation of viticulture, visit to the cellars, vinification, technical wine tasting with typical Tuscan foods.
We love what we are doing, we love nature and what nature gives us: our wines and the simplicity of our life.
Mostly we love people, particularly when people appreciate the products from this land.
We are waiting you.