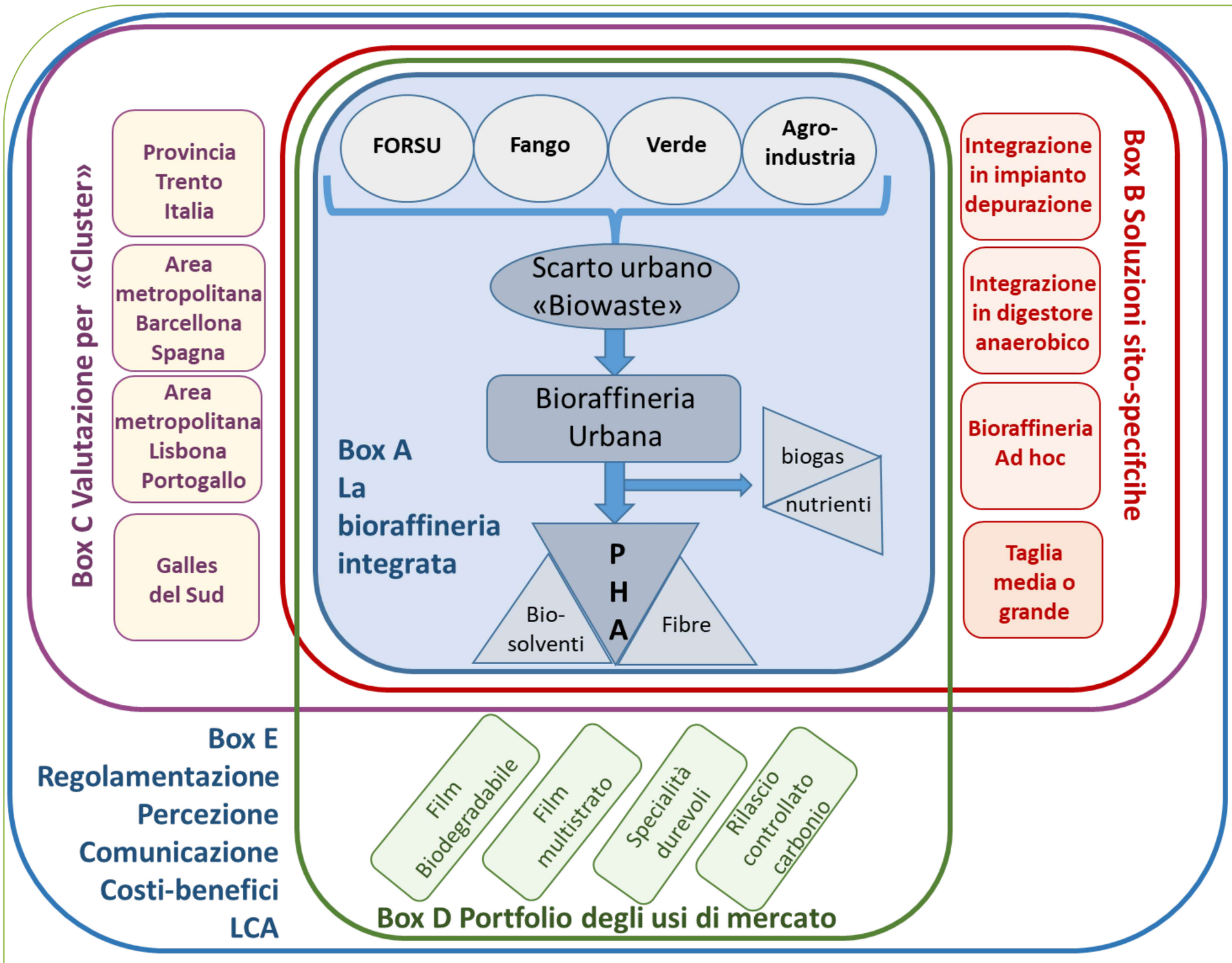
Dal rifiuto urbano alla plastica biodegradabile: il progetto europeo RES URBIS

Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

F. Valentino, L. Lorini, M. Villano, M. Petrangeli Papini, N. Amanat, M.L. Astolfi, S. Canepari, G. Capuani, L. Chronopoulou, C. Palocci, A. Laganà, P. Foglia, C. Cavaliere, A.L. Capriotti, S. Ferrari, A. Martinelli, A. Miccheli, C. Riccardi, M. Majone - *Dipartimento di Chimica*
Email: mauro.majone@uniroma1.it



Il progetto RES URBIS (RESources from URban BIo-waSte) è finanziato dalla Commissione Europea nell'ambito di Horizon 2020 (GA730349) e coinvolge 20 partner provenienti da 8 nazioni europee.

L' obiettivo principale di RES URBIS è lo sviluppo di una bioraffinaria urbana per convertire i rifiuti organici urbani in bioplastiche a valore aggiunto, a base di poliidrossialcanoati (PHA). Questi sono poliesteri particolarmente interessanti perché di origine biologica e completamente biodegradabili nell'ambiente. Due impianti pilota sono stati sviluppati per produrre PHA in continuo a partire dai rifiuti liquidi derivanti dalla lavorazione delle frutta o da una miscela costituita dalla frazione organica dei rifiuti solidi urbani e dal fango in eccesso dal trattamento delle acque reflue municipali. Oltre 20 kg di PHA sono stati prodotti ed estratti dalle cellule microbiche impiegando metodologie prive di agenti inquinanti nonché caratterizzati e testati per varie applicazioni di mercato

European Union

Riferimenti recenti: www.resurbis.eu

Plant Ecology Laboratory – Prof. Loretta Gratani

Research group:

Maria Fiore Crescente
Laura Varone
Maria Pepe
Francesco Bigaran

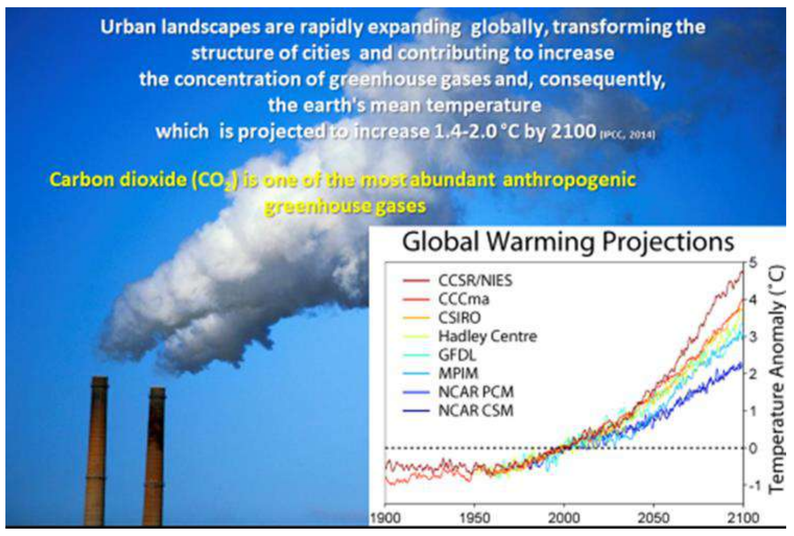
Dipartimento di Biologia Ambientale
Sapienza Università di Roma

Topics: plant ecophysiology; Mediterranean plant adaptative strategies to stress factors; functional plant traits; phenotypic plasticity; metal pollution monitoring by plants; plant CO_2 sequestration

Collaborations:
Department of Biology, University of the Balearic Islands (UIB): Prof. Jaume Flexas
Department of Biology, University of Kiew: Prof. Olena Vasheka
Department of Plant and soil,TexasTech University: Prof. David C. Weindorf

Urban landscapes are rapidly expanding globally contributing to increase the concentration of greenhouse gases and, consequently, the earth's mean temperature, which is projected to increase 1.4 – 2.0°C by 2100. Urban areas account for more than 70% of global greenhouse gases due to artificial surfaces, fossil fuel combustion and traffic density. The problem is emphasized in those urban areas where a high dependence on private transportation contribute to increase gas emission rates.

Urban green areas (i.e. public and private parks, gardens, sport fields, hedges and tree-lined avenues) can generate significant ecosystem services (i.e. those benefits having a direct or indirect impact on the economy). Greening acts as a sink for atmospheric CO_2 by storing carbon through the growth process and lowers air temperature by shading and transpiration (Gratani and Varone, 2007) Moreover, plants contribute to improve air quality by removing particles that are usually associated with metals in airborne dust generated by traffic (Gratani et al., 2000; Gratani et al., 2008). Among the benefits provided by greening, trees are excellent regulators of air temperature, heat and dampness in urban surroundings. In particular, tree structure defines patterns of light-capturing areas and air temperature buffering effects of the canopy, which contribute to mitigate the urban "heat island". Peters et al. (2004) identified the association of traffic-related air pollution and the increase in myocardial infarction events, considering that heart disease and stroke is the most common reasons for premature death attributable to air pollution for 80% of cases (WHO, 2015; 2016).





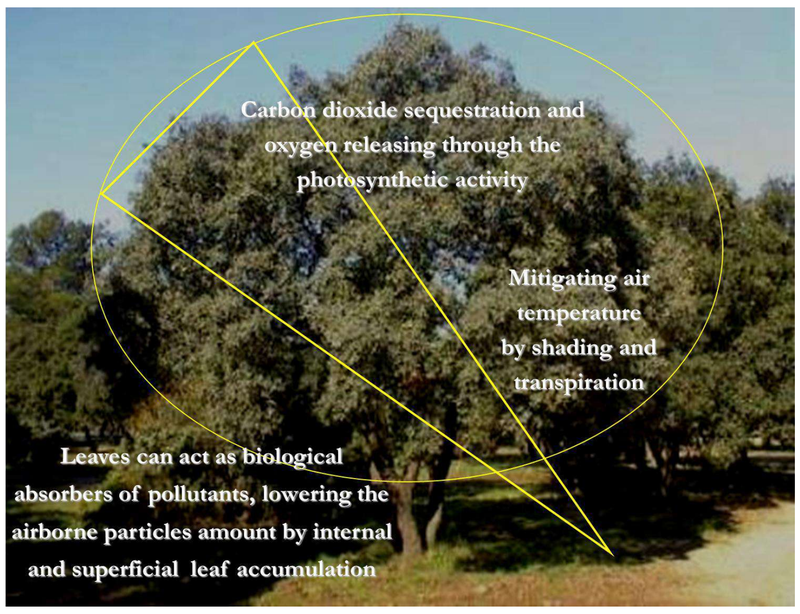






The choice of plant species for urban areas might be set out favoring those species that are largely distributed, and taking into account their own air amelioration capability. Moreover, the analysis of dust deposited on leaves is a good alternative for air pollution monitoring, considering that trees are long living so that a repetition of the investigation is possible over the time.

In such context, our research focuses on the vegetation capability to remove particulate matter from the air and lower CO_2 concentration. Such research is carried out with portable instruments for gas exchange, leaf pigment content, leaf area index (LAI) and microclimate measurements, and laboratory instruments for leaf water potential, leaf area, fresh and dry leaf mass measurements. Metals concentration in leaves was carried out by photon and neutron activation and by atomic absorption spectrometry (Gratani et al., 2000; Gratani et al., 2008; Gratani et al. 2018). Currently, to assess the heavy metals in leaves and soil we are evaluating the portable X-ray Florescence Spectrometry, a non-destructive method applicable on different matrices (Weindolf et al., 2014; Pearson et al., 2017; McGladdery et al., 2018).
This research area has important interactions with medicine, engineering and chemistry.





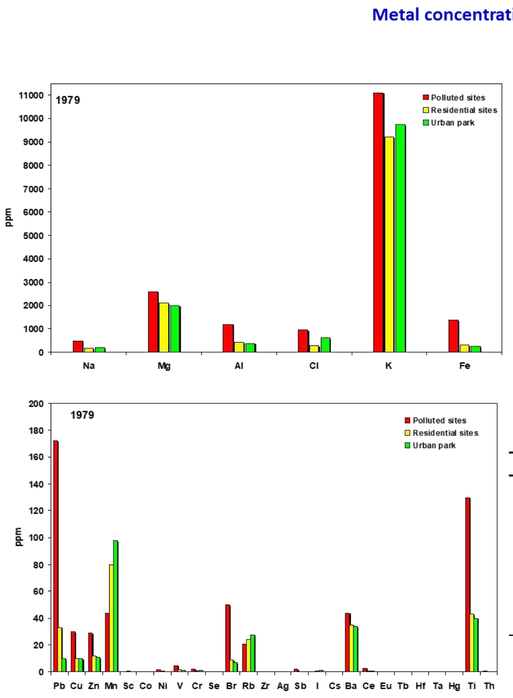
LAI measured by LI-COR LAI 2000



Net photosynthesis was measured by infrared CO_2 gas analyzer (LCA-Pro+, ADC,) and a leaf chamber PLC4



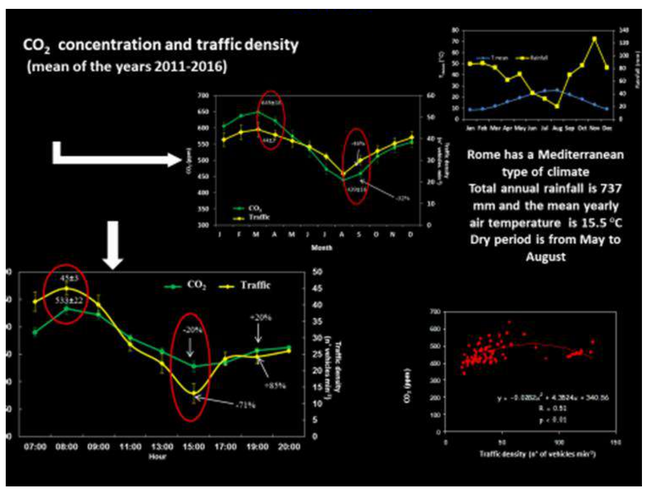
(Portable X-ray Florescence Spectrometer Olympus Vanta M series)





	Crown low layer	Crown high layer
Fe (ppm)	1370	530
Cu (ppm)	30	8
Zn (ppm)	29	16
Br (ppm)	50	12
Rb (ppm)	21	13
Ag (ppm)	0.17	0.09
Pb (ppm)	172	48





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GRATANI L., CRESCENTE M.F., VARONE L., 2008. Long-term monitoring of metal pollution by urban trees. Atmos. Environ., 42: 8273-8277.
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MCGLADDERY C., WEINDORF D. C., CHAKRABORTY S., BIN LI, PAULETTE L., PODAR D., PEARSON D., KUSI N.Y.O., DUDA B., 2018. Elemental assessment of vegetation via portable X-ray fluorescence (PXRF) spectrometry. J. Environ. Manag., 210: 210-225.
PEARSON D., CHAKRABORTY S., DUDA B., LI B., WEINDORF D.C., DEB S., BREVIK E., RAY D.P., 2017. Water analysis via portable X-ray fluorescence spectrometry. J. Hydrol., 544, 172-179.
PETERS A., VON KLOT S, HEIER M, TRENTINAGLIA I, HORMANN A, WICHMANN HE, 2004. Exposure to traffic and the onset of myocardial infarction. N.Engl. J. Med., 51:1721–1730.
WEINDOLF D.C., BAKR N., ZHU Y., 2014. Advances in portable X-ray fluorescence (PXRF) for, environmental, pedological, and agronomic applications. Adv. Agron., 128: 1-45.
WHO, 2015. Global Health Observatory data respiratory. Burden of disease. Lead attributable DALYs. http/apps.who.int/gho/data/node.home .
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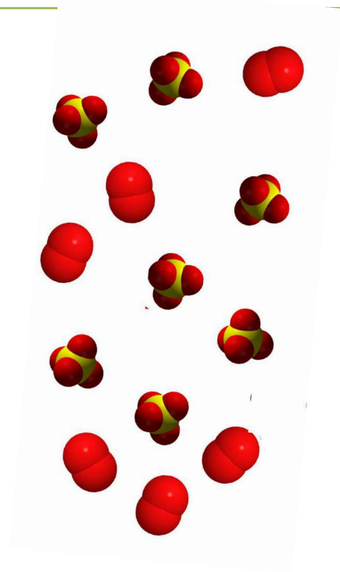
Kinetic models and mixtures

Gabriella Puppo, Marlies Pirner (Vienna), Giuseppe Visconti e Michael Herty (RWTH), Matteo Semplice (Insubria) Andrea Tosin (PoliTo)…
Dipartimento di Matematica, Edificio Castelnuovo, piano primo
Email: gabriella.puppo@uniroma1.it, URL gabriellapuppo.it

Consider a kinetic model for a mixture of particles

$$\partial_t f + v \cdot \nabla f = Q_{11}(f,f) + Q_{12}(f,g)$$
$$\partial_t g + v \cdot \nabla g = Q_{22}(g,g) + Q_{21}(g,f).$$

Q_{ii} describe interactions with particles of the same kind, while Q_{ij} are interactions with particles of the other type



The model contains an evolution towards equilibrium, where the collision kernels are relaxation towards equilibrium

$$M_i(t,x,v) = \frac{n_i(x,t)}{\sqrt{2\pi\frac{T_i(x,t)}{m_i}}^d} \exp\left(-\frac{(v-u_i(x,t))^2}{2T_i(x,t)/m_i}\right).$$

$$M_{ij}(t,x,v) = \frac{n_i(x,t)}{\sqrt{2\pi\frac{T_{ij}(x,t)}{m_i}}^d} \exp\left(-\frac{(v-u_{ij}(x,t))^2}{2T_{ij}(x,t)/m_i}\right),$$

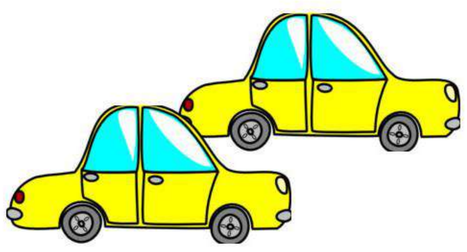


This approach is a bridge between mathematics, physics and scientific computing, but it can also be applied to biology or social sciences.

For instance, it can be used to model mixtures of gases, such as plasmas, but also mixtures of vehicles in traffic flow



In the same way, in traffic flow, we study two particles interactions,



We compute the equilibrium distribution, which provides the closure law necessary to write a macroscopic conservation law for the density of vehicles:

$$\partial_t \rho + \partial_x F(\rho) = 0, \qquad F(\rho) = \rho\, v(\rho)$$

$$v(\rho) = \int_V \xi M_f(\xi;\rho)\, d\xi.$$

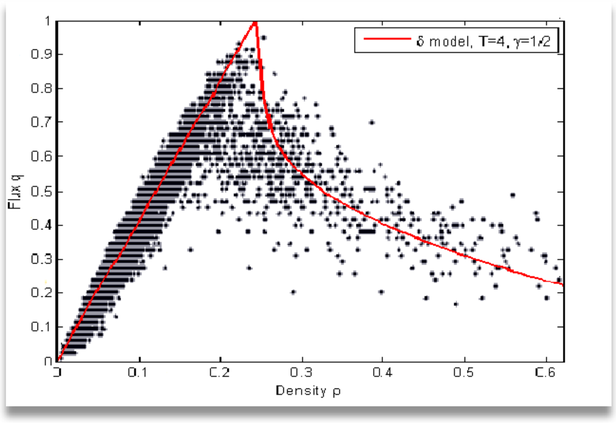
v_* = candidate vehicle (me!); v^* = field vehicle (leading car);

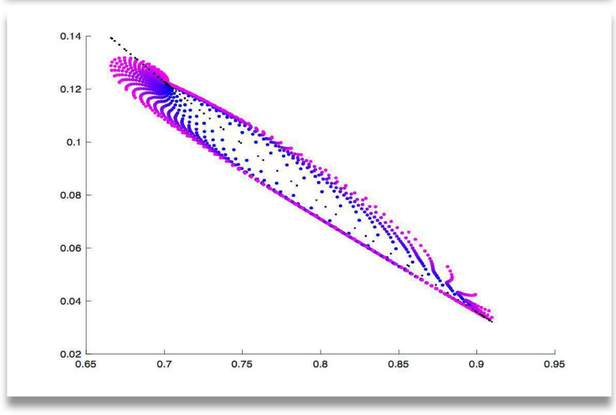
$v_* \le v^*$

$1 - P(\rho)$ v_* $v_* + \Delta v$ $P(\rho)$ v^* $P(0) = 1,\ P(\rho_M) = 0$

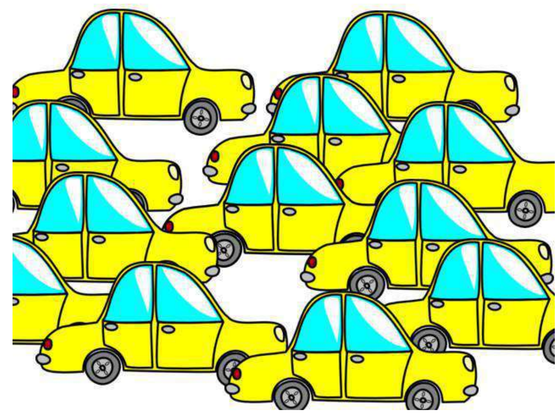
$v_* > v^*$

$P(\rho)$ v_* $1 - P(\rho)$ v^* $P'(\rho) < 0$

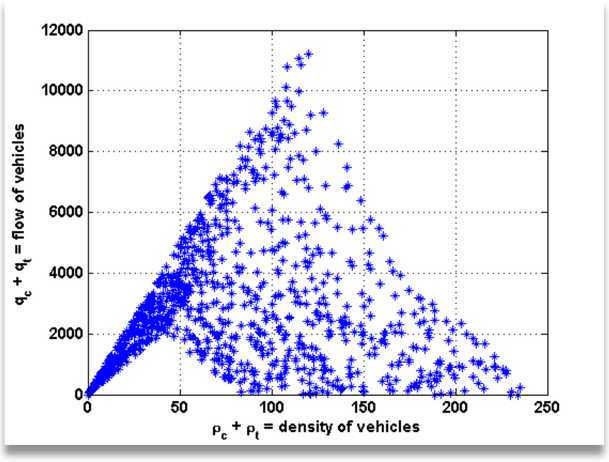




Then we consider the evolution of the statistical distribution



The flux-density diagram we obtain provides a good match with experimental data, except when the vehicles density is high, in a traffic jam, where experimental data appear scattered.



We can account for scattered data, thinking of traffic as a mixture, composed of different types of vehicles, as trucks and cars, and (or) non equilibrium effects.

Riferimenti recenti:
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Puppo, Semplice, Tosin, Visconti, Kinetic and Related Models, 2016, Communications in Math. Scie.2017, 2018.

Ambiente e Territorio

La classificazione ecologica del territorio per la conservazione della biodiversità e il supporto alla definizione di nuove strategie di pianificazione e sviluppo sostenibile

Giulia Capotorti*, Riccardo Copiz, Laura Zavattero, Carlo Blasi
**Dip. di Biologia Ambientale, Edificio di Botanica, CU022, piano 1, stanza 109*
Email: giulia.capotorti@uniroma1.it

Tematica: CLASSIFICAZIONE ECOLOGICA DEL TERRITORIO

settori ERC LS8_4, LS8_6 & LS8_8

Dati di base: rilevamento, analisi, modellizzazione di CARATTERI AMBIENTALI bio-fisici

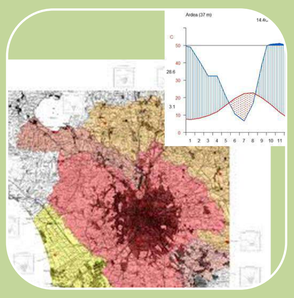
competenze del gruppo di ricerca — *altre competenze disciplinari*



FLORA



VEGETAZIONE



BIOCLIMA



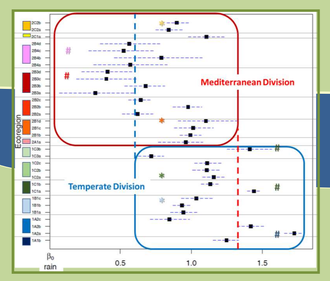
FISIOGRAFIA

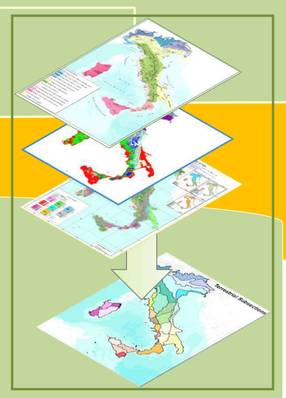


FATTORI ANTROPICI

Approccio metodologico: INTEGRAZIONE MULTIDISCIPLINARE

(analisi statistiche, valutazioni quali-quantitative, elaborazioni cartografiche)





identificazione, delimitazione e caratterizzazione di

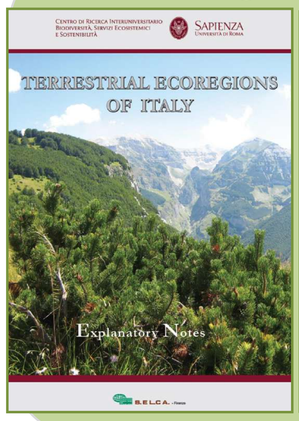
UNITÀ TERRITORIALI ECOLOGICAMENTE OMOGENEE

utili per la conservazione e gestione sostenibile delle risorse naturali

Risultati

LIVELLO NAZIONALE

Le Ecoregioni d'Italia

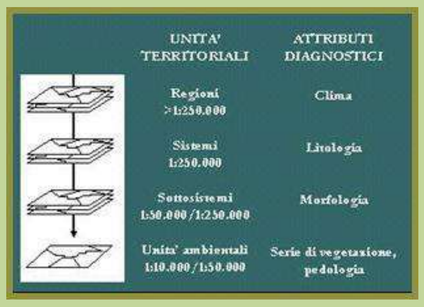




- ✓ Suddivisione del territorio nazionale in unità geografiche ecologicamente distinte e arrangiate gerarchicamente in 2 Divisioni, 7 Province, 12 Sezioni e 33 Sottosezioni
- ✓ Progressiva omogeneità nella combinazione di caratteri climatici, biogeografici, fisiografici, floristici, vegetazionali e faunistici
- ✓ Supporto strategico a livello europeo e nazionale

LIVELLO LOCALE

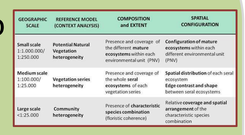
Unità ambientali



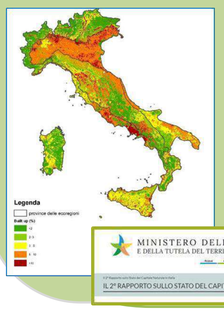
- ✓ Definizione degli ambiti di pertinenza dei diversi tipi di vegetazione naturale potenziale (potenzialità ecologiche del territorio discretizzate in funzione di clima, litologia, morfologia, suoli, vegetazione)
- ✓ Arrangiamento gerarchico in Regioni, Sistemi e Sottosistemi di territorio
- ✓ Supporto alla pianificazione territoriale dal livello regionale a locale (aree metropolitane, comuni, aree protette)

Applicazioni

Valutazione dello stato di conservazione degli ecosistemi
a livello ecoregionale



Capotorti et al., 2015, Plant Biosystems





Consumo di suolo negli ecosistemi
(Rapporti sullo Stato del Capitale Naturale In Italia; in collaborazione con ISPRA, Università del Molise)

Prospettive

Monitoraggio dei flussi di servizi ecosistemici
tramite combinazione di dati ambientali e socio-economici



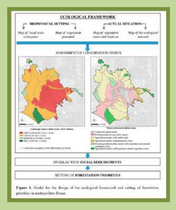
Barò et al., 2016, Land use Policy



Classificazione dei comuni secondo le Ecoregioni d'Italia
(Statistiche sperimentali nazionali e Rapporto Territorio; in collaborazione con ISTAT)

Applicazioni

Piano di forestazione urbana (Roma Capitale)

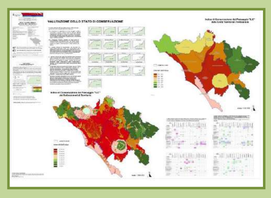


Infrastrutture verdi (Strategie EU/IT)





Rete ecologica provinciale (PTPG Roma)



Sinergie tra biodiversità, servizi ecosistemici, benessere in ecosistemi urbani (EU EnRoute Project)





Prospettive

Approccio multidisciplinare e partecipato alla pianificazione di *Nature-Based Solutions* e ri-naturalizzazione delle città





Valorizzazione dei paesaggi rurali, intesi come *living heritage*, in chiave ecologica, economica e socio-culturale

Riferimenti recenti

Blasi C, Capotorti G, Copiz R, Guida D, Mollo B, Smiraglia D, Zavattero L. 2014 *Classification and mapping of the ecoregions of Italy* Plant Biosyst 148;
Capotorti G, Alós Ortí MM, Anzellotti I, Azzella MM, Copiz R, Mollo B, Zavattero L., 2015 *The MAES process in Italy: Contribution of vegetation science to implementation of European Biodiversity Strategy to 2020* Plant Biosyst 149;
Blasi C, Capotorti G et al. 2017 *Ecosystem mapping for the implementation of the European Biodiversity Strategy at the national level: The case of Italy* Env Sci Policy 78;
Blasi C, Capotorti G, Copiz R., Mollo B. 2018 *A first revision of the Italian Ecoregion map* Plant Biosyst 152;
Mastrantonio G, Lasinio GJ, Pollice A, Capotorti G, Teodonio L, Genova G, Blasi C. 2019. *A hierarchical multivariate spatio-temporal model for clustered climate data with annual cycles* Ann Appl Stat 13

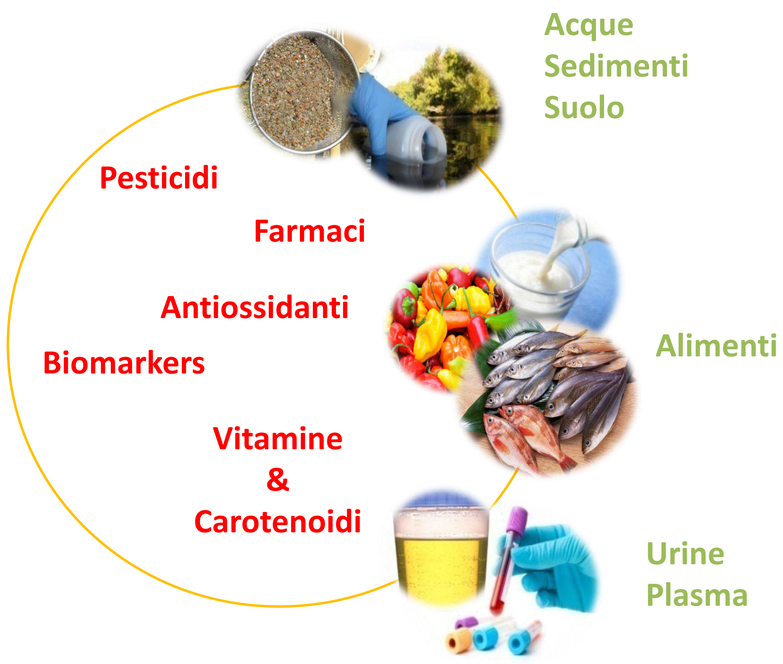
Capotorti G, Mollo B, Zavattero L, Anzellotti I, Celesti-Grapow L. 2015 *Setting Priorities for Urban Forest Planning. A Comprehensive Response to Ecological and Social Needs for the Metropolitan Area of Rome (Italy)* Sustainability 7;
Manes F, Marando F, Capotorti G, Blasi C, Salvatori E, Fusaro L, et al. 2016 *Regulating Ecosystem Services of forests in ten Italian Metropolitan Cities: Air quality improvement by PM 10 and O 3 removal* Ecol Ind 67;
Capotorti G, Del Vico E, Anzellotti I, Celesti-Grapow L. 2017 *Combining the conservation of biodiversity with the provision of ecosystem services in urban green infrastructure planning: critical features arising from a case study in the metropolitan area of Rome* Sustainability 9;
Capotorti G, Alós Ortí MM, Copiz R, Fusaro L, Mollo B, Salvatori E, Zavattero L. 2019 *Biodiversity and ecosystem services in urban green infrastructure planning: A case study from the metropolitan area of Rome (Italy)* Urban For Urban Gree 37

Nuovi materiali e solventi neoterici nelle tecniche di "Sample Preparation"

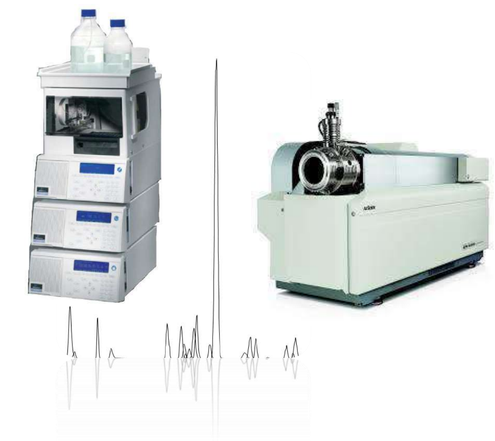
Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

Alessandra Gentili[1]*, Chiara Dal Bosco[1], Pierpaolo Tomai[1],
Co-autori: Andrea Martinelli[1], Valerio Di Lisio[1]
[1]*Dipartimento di Chimica, Edificio Cannizzaro, CU014, piano Terra, stanza 061*
*****Email: alessandra.gentili@uniroma1.it*

Il termine «***Sample Preparation***» si riferisce a tutte le operazioni di pre-trattamento di un campione reale volte a trasferire gli *analiti* dalla matrice reale ad un mezzo idoneo alla successiva analisi strumentale. È un settore della Chimica Analitica in continua evoluzione, che va di pari passo con lo sviluppo tecnologico e che richiede competenze multidisciplinari. In questo contesto, materiali di ultima generazione, come quelli nano-strutturati, rivestono un ruolo fondamentale nelle tecniche «*sorbent-based*». Nell'ambito delle tecniche «*solvent-based*», l'interesse è attualmente focalizzato sui solventi neoterici (*deep eutectic solvents (DES) , low transition temperature mixtures (LTTM), etc.*) come alternativa *low-cost* e *green* ai comuni solventi organici. Le applicazioni coprono diversi settori della Chimica Analitica quali quello ambientale, alimentare e clinico. La sfida è quella di comprendere i meccanismi che regolano l'affinità di questi sistemi nei confronti dei composti chimici di interesse, per mettere a punto metodiche analitiche sempre più performanti in termini di sensibilità, selettività e sostenibilità. Il raggiungimento di tali obiettivi richiede una adeguata progettazione, ottimizzazione e caratterizzazione dei materiali e dei solventi impiegati attraverso la stretta collaborazione con coloro che operano nella Scienza dei Materiali.



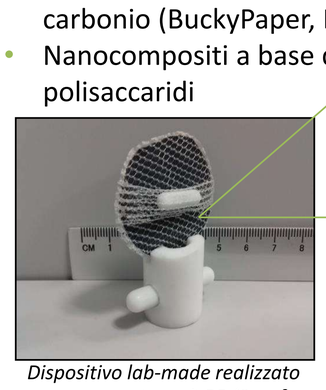
- **Solid-Phase Extraction (SPE)**
- **Dispersive Solid-Phase Extraction (dSPE)**
- **Magnetic Solid-Phase Extraction (MSPE)**
- **Dispersive Liquid-Liquid Extraction (DLLME)**



(nano)LC-(DAD)-MS/MS

Sviluppo di nuovi dispositivi SPE:

- Membrane a base di Nanotubi di carbonio (BuckyPaper, BP)
- Nanocompositi a base di polisaccaridi



Dispositivo lab-made realizzato con una porzione di BP (9 cm²), una rete di polipropilene e un'ancoretta magnetica

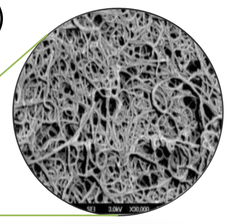
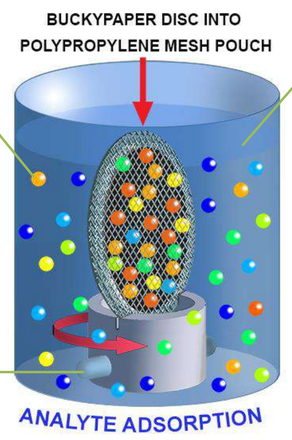


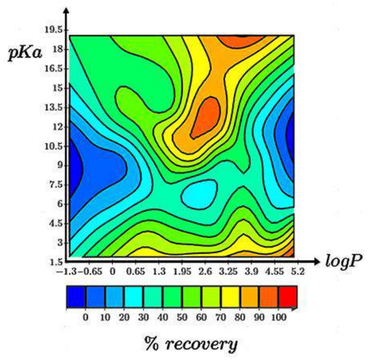
Immagine SEM di una porzione di BP

Rimozione di 76 contaminanti organici

Acqua ambientale contaminata

Barra magnetica





Per studiare la capacità estrattiva della BP, sono stati selezionati 76 composti modello caratterizzati da diverse proprietà chimico-fisiche. L'adsorbimento è risultato essere governato da due parametri fondamentali: logP e pKa. Le **curve di livello** mostrano il loro effetto combinato sulle rese estrattive**.**
Si può notare come solo composti con logP > 1 esibiscano recuperi (R%) tra il 50% e il 100% in funzione del loro pKa

$R\% = f(pK_a, logP)$, $y = 25.74 + 0.52x$, $r^2 = 0.69$

Il coefficiente di correlazione ($\mathbf{r^2}$) è buono ma non ottimale: ulteriori parametri dovrebbero essere considerati.

Preparazione e caratterizzazione di solventi neoterici:

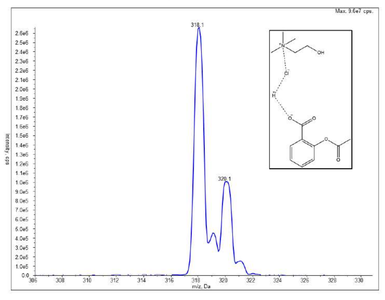
- DES e LTTM a base di Cloruro di Colina (ChCl)
- Impiego come solventi estraenti in tecniche DLLME



ChCl-Acido Acetilsalicilico (1:2)
Liquido viscoso a temperatura ambiente più denso dell'acqua
d = 1.20 ±0.01 g mL⁻¹

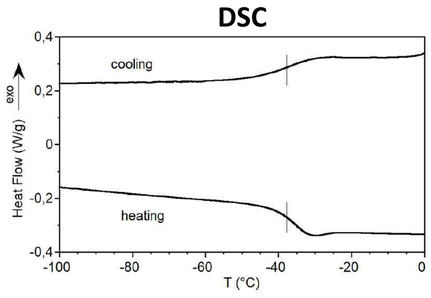
CARATTERIZZAZIONE:

ESI-MS



Lo spettro di massa rivela la presenza del complesso ChCl-ASA (1:1) ma non quella del complesso 1:2

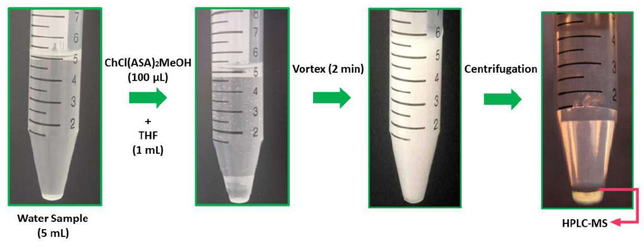
DSC



Il termogramma mostra una intensa transizione vetrosa che identifica il solvente come LTTM e non come DES

APPLICAZIONE:

Estrazione di diverse classi di pesticidi da campioni di acqua di fiume mediante ***DLLME***



Efficienza estrattiva (ER%) 20 – 96 % paragonabile ai solventi clorurati tipicamente impiegati in DLLME

Riferimenti recenti

P. Tomai, A. Martinelli, S. Morosetti, R. Curini, S. Fanali, A. Gentili, Oxidized Buckypaper for Stir-Disc Solid Phase Extraction: Evaluation of Several Classes of Environmental Pollutants Recovered from Surface Water Samples, Anal. Chem. 90 (2018) 6827–6834. doi:10.1021/acs.analchem.8b00927
P. Tomai, A. Lippiello, P. D'Angelo, I. Persson, A. Martinelli, V. Di Lisio, R. Curini, C. Fanali, A. Gentili, A low transition temperature mixture for the dispersive liquid-liquid microextraction of pesticides from surface waters, J. Chromatogr. A. (2019) 360329. doi:https://doi.org/10.1016/j.chroma.2019.06.050.

Scienze della Vita

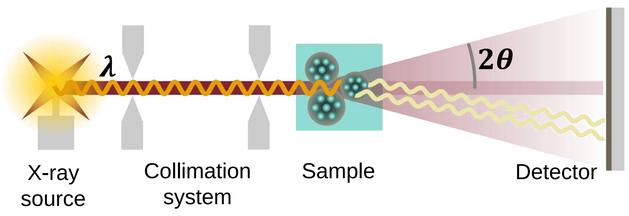
Dipartimento di Chimica
SAPIENZA Università di Roma
SAXSLab Sapienza

SAXSLab Sapienza - A University facility for the structural characterization of matter at the nano- and meso-scale

Alessandra Del Giudice*, Luciano Galantini, Nicolae Viorel Pavel
Dipartimento di Chimica, Edificio Cannizzaro, CU014, piano terra, stanza 058
Email: alessandra.delgiudice@uniroma1.it

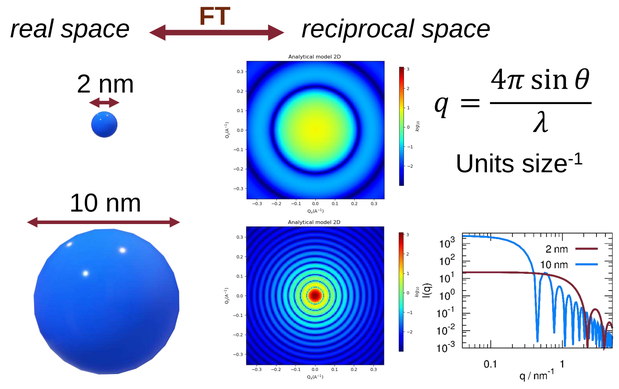
Small angle X-ray scattering

Electrons in the sample scatter monochromatic X-rays and a pattern is generated by the interference of the scattered waves which contains information about the relative positions among scatterers.



Every technique based on scattering follows a reciprocity law: at fixed λ, the **larger the dimensions** of the inhomogeneities, the **smaller the angles** from the incident beam at which the scattered intensity can be seen.

real space ⟷ FT ⟷ reciprocal space

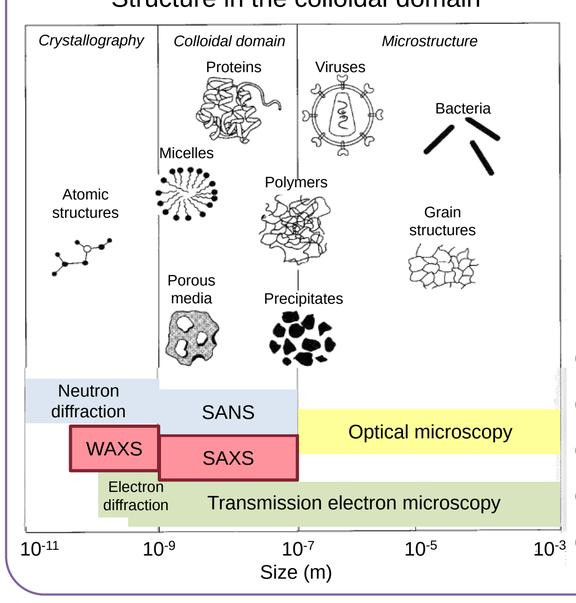


$$q = \frac{4\pi \sin\theta}{\lambda}$$

Units size^{-1}

Why small angles?

Structure in the colloidal domain



Advantages

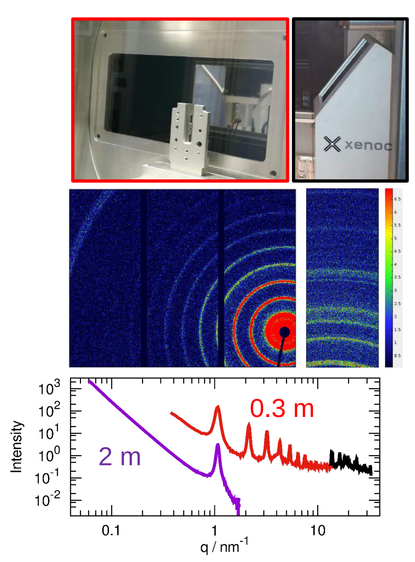
- Average information
- Non-destructive
- Minimal sample preparation («in-situ»)
- Large range of sizes probed (0.2-100 nm)
- Variable sample states (solution, powder, gel,…)

Experimental system

Xeuss 2.0-QXoom in operation since November 2018



- Microfocus Cu kα X ray source (λ=0.154 nm)
- Single reflection multilayer optics monochromator
- «Scatterless» slits collimation



Features

- Flexible motorized sample stage
- Possibility of reflection geometry for surfaces (GISAXS and GIWAXS)
- Evacuated chamber (p~0.2 mbar), possibility of in-air setup
- Pilatus single-photon counting detector (high dynamic range)
- SAXS detector variable distance (overall q-range 0.04-16 nm^{-1})
- Simultaneous WAXS detector
- Intensity on absolute scale



Thermalized capillary cells — Solids holders



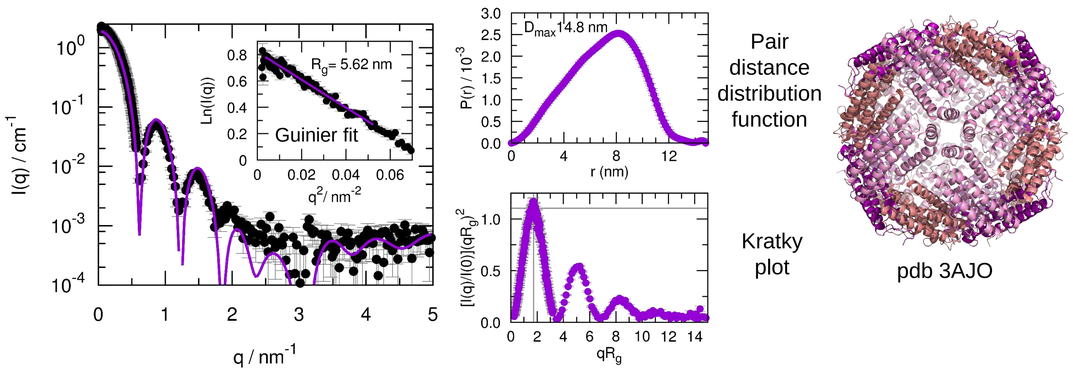
Disposable capillaries — Gels/powders/ slurries capsules — GISAXS stage for flat surfaces

Examples

Proteins in solution

thanks to A. Fiorillo (Dept. of Biochemical Sciences @ Sapienza)

Recombinant Human Ferritin self-assembles in the expected 24-mer «hollow sphere» form and the scattering profile is in agreement with the crystal structure.



pdb 3AJO

In solution the structural information is averaged over all possible orientations

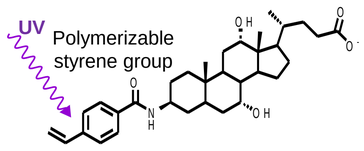
SAXS can help in the characterization of purified samples of biological macromolecules:

- average size and shape
- oligomeric state
- quality assessment
- degree of flexibility
- conformational changes
- oligomerization equilibria and complex formation

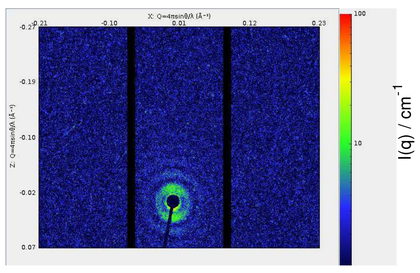
Self-assembled nanotubes

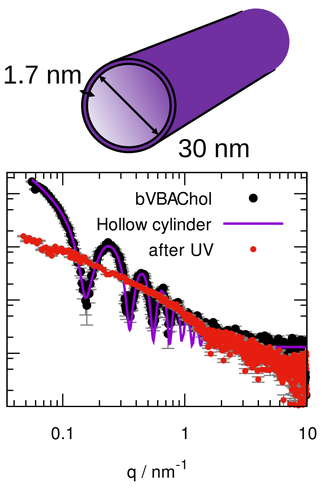
thanks to M. Alfonsini (Dept. of Chemistry @ Sapienza)

A bile salt derivative bearing a styrene moyety self-assembles in long hollow cylinders. The polymerization by UV-light irradiation destroys the nanotube structure.



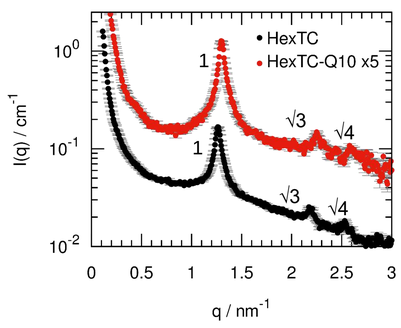
β-Vinylbenzamide cholate





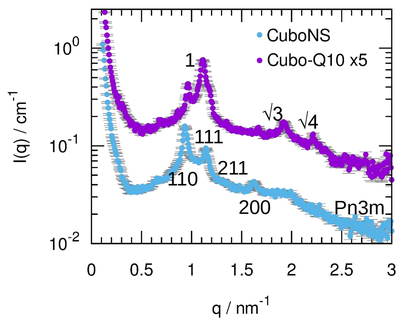
Liquid-crystalline phase formulations

thanks to M. Fornasier (Dept. of Chemistry @ Università di Cagliari)



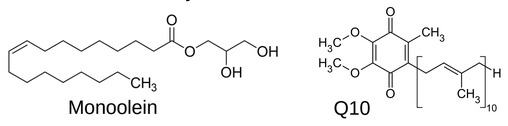
The hexagonal phase of the hexosomes formulation is retained when encapsulating the Q10 coenzyme

Lattice parameter: 5.74(1) nm
5.59(2) nm

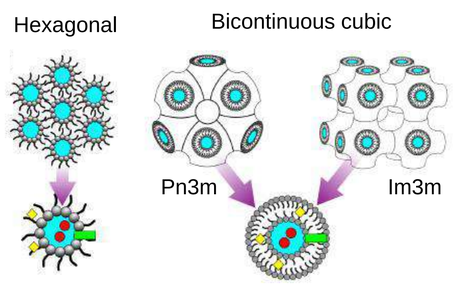


For another formulation in which a cubic phase was aimed at (Cubo-Q10) the SAXS suggests the presence of a hexagonal phase too.

Cubosomes and hexosomes are systems in which liquid crystalline phases (usually based on monoolein) are dispersed in the form of nanoparticles, and can be used for the delivery of active molecules

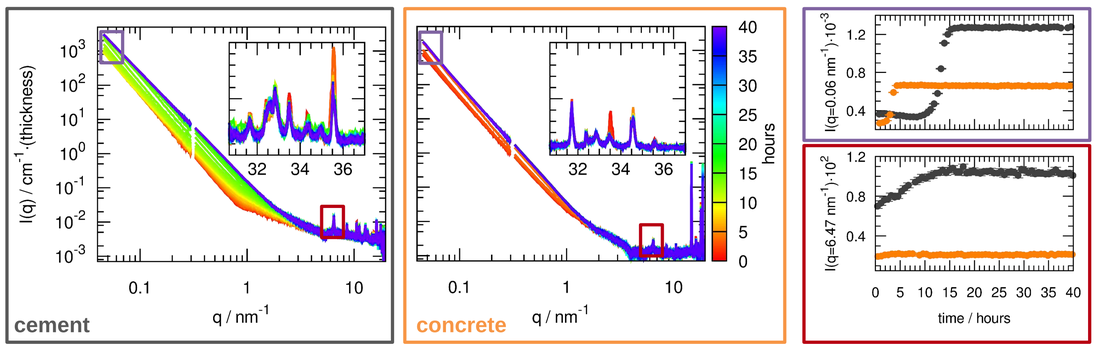


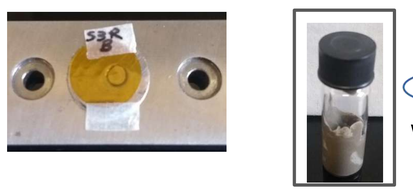
The SAXS peaks allow for phase identification and measure of the lattice parameter, from which the size of water channels can be inferred.

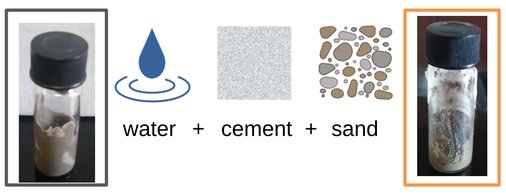


Cement vs. concrete setting

thanks to G. Chass (Dept. of Chemistry @ Queen Mary University of London)









Hydration-driven setting promotion of nano- through meso-scale particle growths are inhibited in concretes, due to inflated surface area: volume ratios; representative of industrial and bulk deliveries of concretes to form in infrastructures.

Dipartimento di Fisica
SAPIENZA Università di Roma

A CVD-chamber for aligned carbon nanotubes synthesis

I. Rago, F. Pandolfi, M. G. Betti, C. Mariani, A.D.Polosa, G. Cavoto.
*Dipartimento di **Fisica**, Edificio **Marconi CU013** piano **terzo** stanza **329***
Email: gianluca.cavoto@uniroma1.it, francesco.pandolfi@roma1.infn.it, ilaria.rago@roma1.infn.it

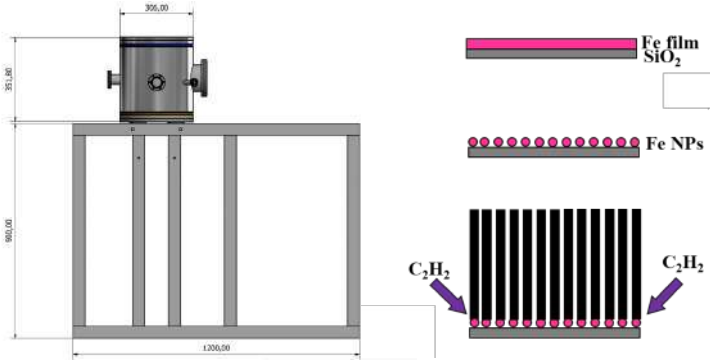
OBJECTIVES

A facility to synthesize Vertically Aligned Carbon Nanotubes (**VA-CNTs**) via a Chemical Vapour Deposition (**CVD**) technique is being realized at the Department of Physics in collaboration with INFN Roma. This CVD chamber will be able to grow high-quality VA-CNTs on any surface (even transparent to light) covered by nanoparticles of a catalytic element (eg. iron). Our primary goal is to build high-efficiency **UV light** detectors, and we envision longer term applications to **dark matter** searches.[1,2] At the same time, we believe that our facility can also disclose new perspectives in life sciences. In fact, CNT-modified surfaces unequivocally show *in-vitro* and *in-vivo* cellular **biocompatibility** as well as their ability to boost the electrical activity of neuronal cells cultured on them. [3,4]

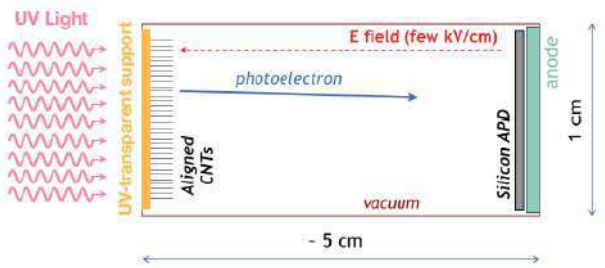
ERC sectors: *PE2, PE5, LS3, LS5.*

METHODS

✓ **CVD chamber and synthesis of CNTs**

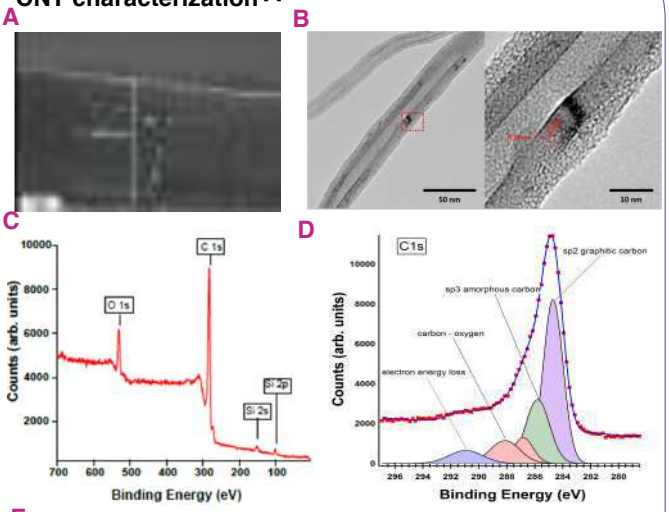


✓ **The 'NanoUV' detector concept[5] (EU ATTRACT project)**



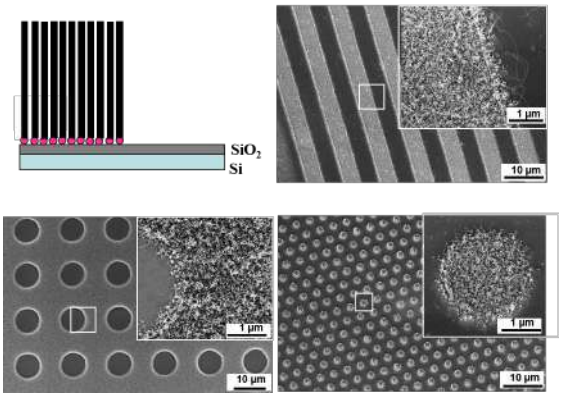
RESULTS

✓ **CNT characterization** [4]



- FE-SEM (**A**) and TEM (**B**) micrographs of CVD-grown CNTs
- XPS survey (**C**), C1s core level (**D**) and Raman (**E**) spectra with MWCNTs characteristic bands

✓ **CVD assisted growth of patterned CNT substrates**[6]



OUTLOOK

Our study paves the road to adopt VA-CNTs as potential targets in novel sensors, possibly extending their application to biology

Recent references:
[1] G. Cavoto, F.Luchetta, A.D.Polosa, **Phys.Lett. B** 776 (2018) 338-344
[2] D'Acunto et al., **Carbon** 139, 768 (2018)
[3] I. Rago et al., **Advanced Biosystems** (2019)1800286
[4] N.Pampaloni, I.Rago, et al., **Development Neurobiology** (2019) 00 1-16
[5] Also in collaboration with A.Ruocco (Roma Tre)
[6] Also in collaboration with L.Casalis and A.Goldoni (Elettra Sincrotrone Trieste)

Dipartimento di Biologia
e Biotecnologie
Charles Darwin

SAPIENZA
UNIVERSITÀ DI ROMA

Effetto della temperatura ambientale sul proteoma dell'encefalo e sulle capacità cognitive in individui adulti di pesce zebra (*Danio rerio*)

Mattia Toni *, Elisa Angiulli, Carla Cioni

Dipartimento di Biologia e Biotecnologie "C. Darwin", Edificio Anatomia Comparata RM057, piano 3 stanza 11

Email: mattia.toni@uniroma1.it

Il gruppo di ricerca si occupa dello studio degli effetti delle variazioni della temperatura ambientale utilizzando come animale modello individui adulti di pesce zebra wild type e mutanti per il gene BDNF (KO e eterozigoti). [Settori ERC LS2_3, LS8_7]

Per studiare gli effetti della variazione termica vengono effettuate due tipologie di esposizione a breve termine (4 giorni) in grado di simulare uno stress acuto e a lungo termine (21 giorni) che permette di studiare la risposta adattativa alla variazione dell'ambiente.

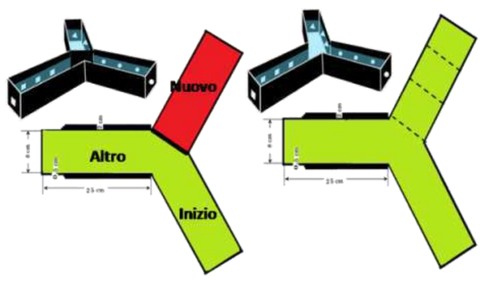
L'approccio è multidisciplinare e prevede l'analisi del proteoma dell'intero encefalo mediante la tecnica shotgun label free, analisi dell'espressione genica delle neurotrofine mediante Real-Time PCR e l'analisi del comportamento utilizzando differenti paradigmi comportamentali.

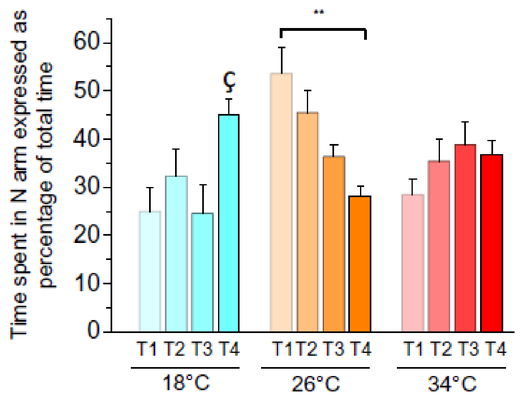
DISEGNO SPERIMENTALE

Adattamento alle condizioni di laboratorio (26°C) → **Trattamento termico**: ↑ 34°C; ↓ 18°C; 4/21 giorni → **Analisi comportamentale**: Batteria di test (novel tank, dark & light, social preference, Y-maze) ANY-maze software; **Analisi molecolare**: Proteomica, Real-Time PCR

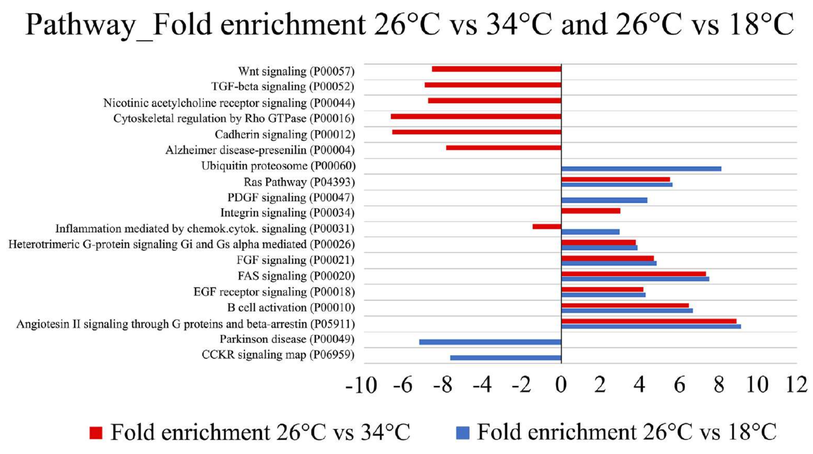


CASO STUDIO 1



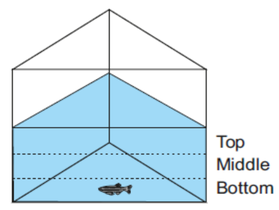


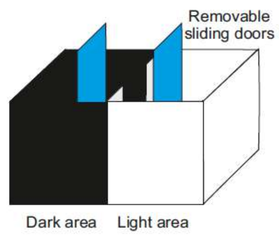
Pesci wild-type adattati ad alte e basse temperature mostrano un'alterazione delle funzioni cognitive nel test del labirinto a Y.

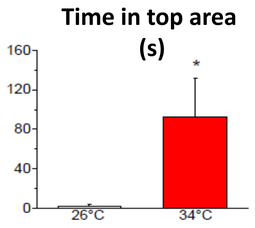


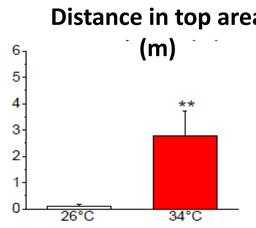
L'analisi del proteoma dell'encefalo ha rivelato che diverse proteine coinvolte nell'organizzazione del citoscheletro, nella regolazione mitocondriale e nel metabolismo energetico sono regolate in modo diverso alle temperature estreme. In oltre l'espressione delle proteine associate alle sinapsi e al rilascio di neurotrasmettitori risulta down-regolata a 18°C e 34°C.

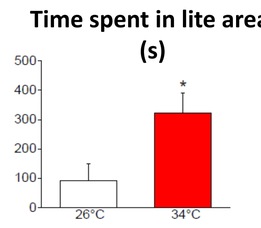
CASO STUDIO 2

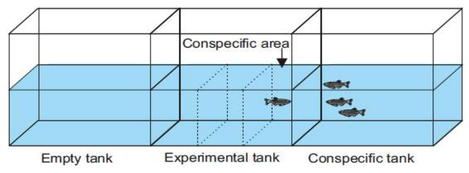




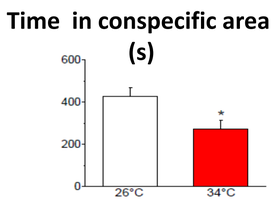


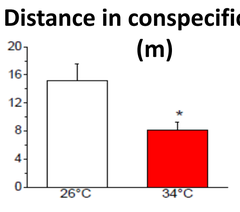




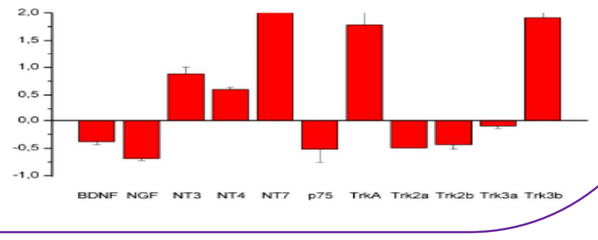


Pesci wild-type adattati a lungo termine alle alte temperature modificano il comportamento esplorativo, la naturale preferenza per luoghi in ombra e per il branco.





Dai dati di espressione genica si osserva una modulazione dell'espressione delle neurotrofine e dei loro recettori nei soggetti mantenuti a 34°C rispetto ai controlli .



Questi studi indicano che le variazioni di temperatura possono provocare alterazioni neurochimiche in grado di influenzare il comportamento animale. L'approccio combinato permetterà di accrescere le conoscenze circa i meccanismi di risposta a fattori di stress ambientale e di adattamento.

Riferimenti recenti

1. Toni M, Angiulli E, Miccoli G, Cioni C, E Alleva, Frabetti F, Pizzetti F, Grassi Scalvini F, Nonnis S, Negri A, Tedeschi G, Maffioli, E (2019) Environmental temperature variation affects brain protein expression and cognitive abilities in adult zebrafish (*Danio rerio*): A proteomic and behavioural study. Journal of proteomics 204, 103396.
2. Angiulli E, Pagliara V, Cioni C, Frabetti F, Pizzetti F, Alleva E, Toni M (2019) Behavioural response to the increase of environmental temperature in adult zebrafish (*Danio rerio*) 2019 in Proceedings of the 65th Congress of the GEI-Italian Society of Development and Cell Biology (GEI-SIBSC) 38th Congress of the Italian Society of Histochemistry (SII), European Journal of Histochemistry 63(2) :2
3. Toni M, Manciocco A, Angiulli E, Alleva E, Cioni C, Malavasi S (2018). Assessing welfare in research and aquaculture contexts, with a particular focus on European directives. Animal 13:161-170

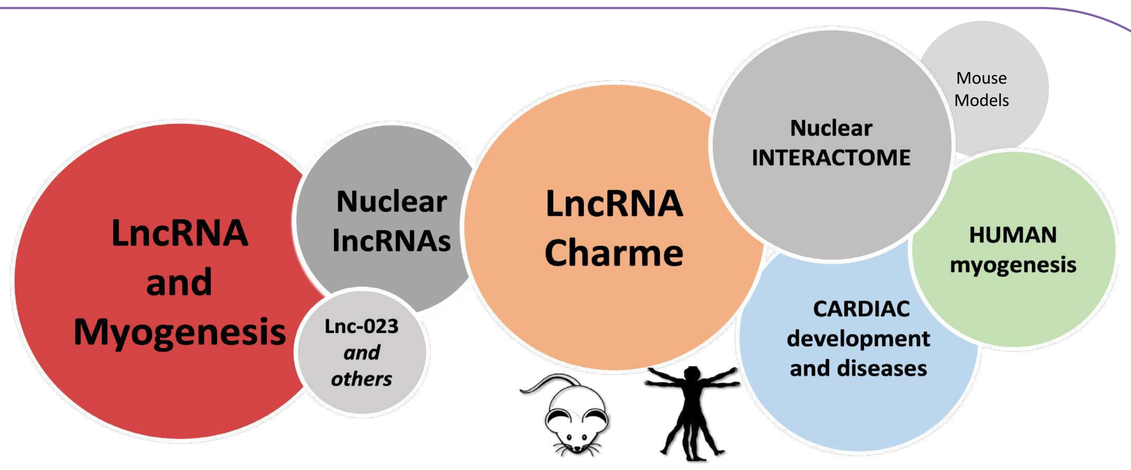
Deciphering the long noncoding RNAs language in myogenesis: a comprehensive glimpse on *Charme*

Dipartimento di Biologia e Biotecnologie Charles Darwin
SAPIENZA UNIVERSITÀ DI ROMA

Giulia Buonaiuto, **Fabio Desideri, Valeria Taliani, Tiziana Santini, Alessio Colantoni, Emerald Perlas, Carmine Nicoletti, Antonio Musarò, Irene Bozzoni, Monica Ballarino**
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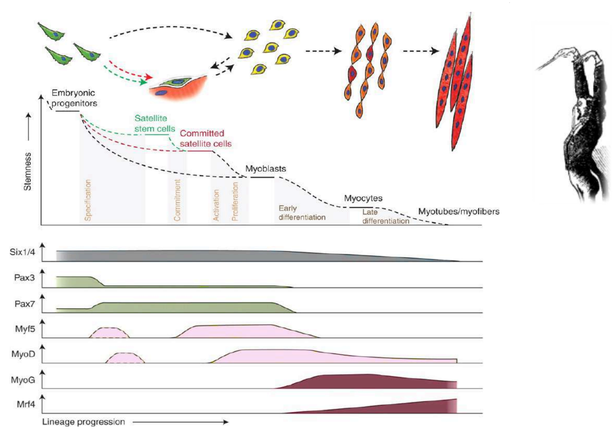
SCIENCE RAH — Strumentazioni e Tecniche

The mammalian genome contains thousands of long noncoding RNAs (lncRNAs), which have been proposed to be fundamental in the regulation of many biological processes. Through an high-throughput transcriptome screening, we identified a subset of new polyadenylated and multi-exonic lncRNAs which result differentially expressed during murine skeletal muscle *in vitro* differentiation. In particular one candidate, *Charme* (for Chromatin architect of muscle expression) is an abundant and highly conserved noncoding transcript specifically required for *in vitro* myogenesis. Mechanistically, *Charme* acts in the nucleus as a structural RNA, contributing to the formation of chromosome territories where coordinated expression of pro-myogenic genes occurs. Interestingly, *Charme* ablation *in vivo* resulted in a very distinct cardiac pathological phenotype in which the morphology of the murine heart is deeply remodelled (Ballarino et al., 2018). We are now working to understand the molecular determinants of this phenotype as well as deepening our knowledge on the human syntenic transcript (*hsCharme*).

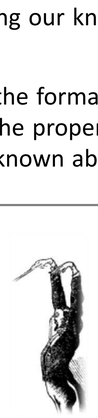


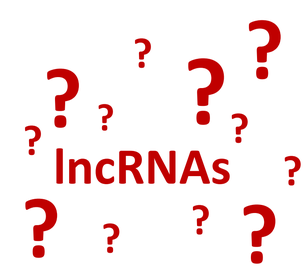
Myogenesis is an orderly orchestrated process that leads to the formation of functional myofibers from staminal precursors. This process needs to be tightly regulated in time and space by the coordinated expression of a specific network of transcription factors (MRF) controlling the proper induction of appropriate developmental stage-specific transcripts. In the past few years many other molecules were demonstrated to be crucial for that process, including noncoding RNAs but still very little is known about lncRNAs role in this process.

Model systems

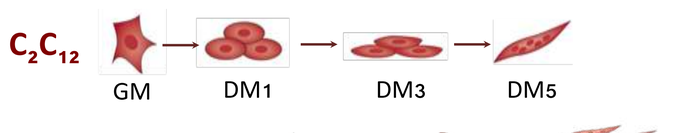


Adapted from Bentzinger et al. Cold Spring Harb Perspect Biol 2012

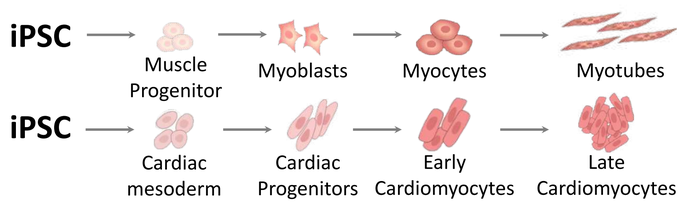




Murine cell line



Human cell line



Mouse Model



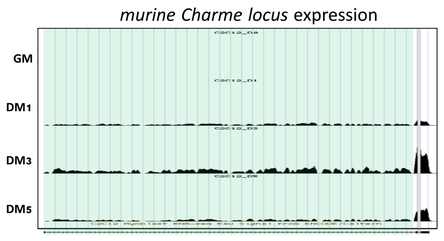
Next Generation Sequencing

An RNA-Seq experiment in proliferating and differentiating myoblast (C2C12), revealed the existence of several previously unidentified lncRNAs. Among them, we focused our attention on *Charme*.

LncRNA	FPKM GM	FPKM D1	FPKM D3	FPKM D5	FPKM (D5-D0)
lnc-405	0	10,18	51,15	42,09	42,09
lnc-666	0	0,34	30,56	22,87	22,87
lnc-182	0,43	1,85	16,73	17,03	16,60
lnc-389	0	5,31	14,50	14,65	14,65
lnc-214	0	0,34	16,09	13,48	13,48
lnc-058	1,81	4,56	10,54	14,63	12,83
lnc-082	0,00	4,83	3,49	11,44	11,44
lnc-165	0,13	0,40	11,67	11,44	11,31
lnc-267	0	0,54	8,65	7,79	7,79
lnc-460	0	0,17	2,90	7,50	7,50
lnc-803	0,01	0,22	11,38	7,11	7,10
lnc-049	0	1,34	17,25	6,89	6,89
lnc-861	0	0	2,93	5,95	5,95
lnc-613	0	0,53	7,63	5,94	5,94
lnc-312	0,00	0,40	1,91	4,86	4,85
lnc-962	0	1,71	13,45	4,42	4,42
lnc-509	0	0,00	0,90	3,68	3,68
lnc-994	0,05	0,09	4,49	3,57	3,52
lnc-776	0	0,03	1,37	3,12	3,12
lnc-561	1,22	8,54	2,74	3,32	2,09
lnc-149	0	0,07	2,44	1,81	1,81
lnc-996	0	0,26	2,68	1,77	1,77
lnc-023	0,57	1,45	0,42	0,05	-0,52
lnc-083	3,18	1,64	0,17	0,02	-3,17
lnc-793	3,61	1,74	0,01	0	-3,61
lnc-456	6,41	0,98	0,16	0,21	-6,20
lnc-31	22,11	19,64	7,38	12,91	-9,20
lnc-686	13,98	10,70	3,19	4,37	-9,62
lnc-254	23,50	14,55	3,03	4,77	-18,73

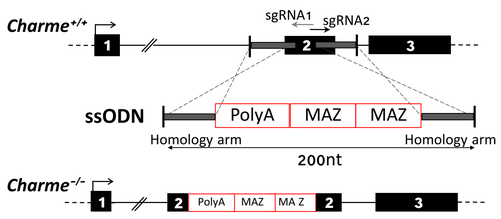
22 up-regulated
7 down-regulated

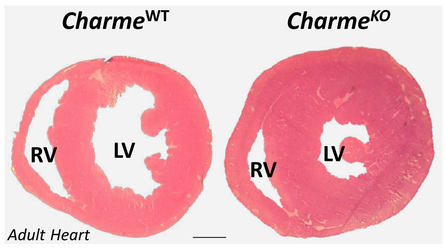
murine Charme locus expression



Charme is expressed during differentiation and is characterized by the presence of a highly expressed and retained intron.

Genome editing

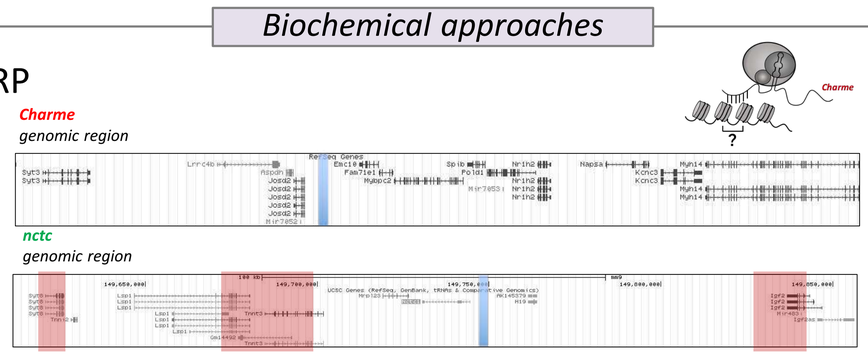




CRISPR/Cas9 methodology was used to generate a *Charme* null allele in mice. A very strong phenotype was detected in both newborn and adult mice when analysing heart morphology.

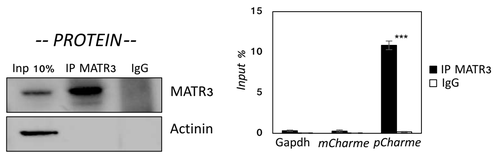
Biochemical approaches

❖ ChIRP

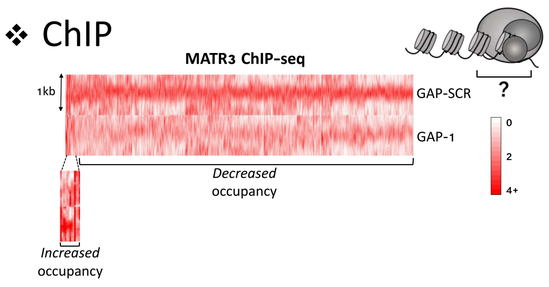


❖ RAP
❖ CLIP





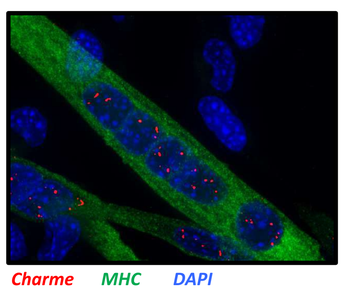
❖ ChIP



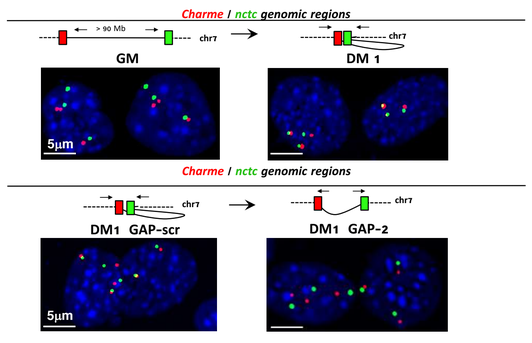
ChIRP analysis revealed a direct interaction between *Charme* and a specific chromosomal region (nctc). RNA Antisense Purification (RAP) followed by masspectrometry analysis revealed the interaction of *Charme* with MATRIN3 and PTBP1, two proteins involved in splicing regulation and nuclear structure. ChIP-seq analysis of MATR3 after *Charme* depletion showed a severe impairment of its binding capability to the genome.

Imaging

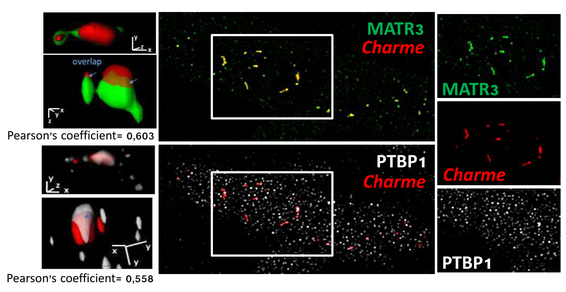
❖ RNA FISH



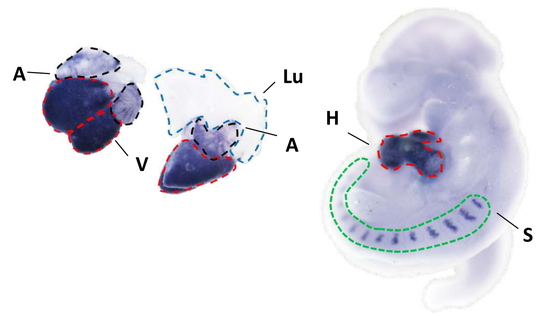
❖ DNA/DNA FISH



❖ IF/RNA FISH



❖ Whole Mount *in situ* hybridization



FISH analyses were used to verify *Charme* subcellular localization in mature myotubes and confirm its interaction with nctc genomic region and Matr3 and PTBP1 while Whole-mount *in situ* hybridization (WISH) to confirm *Charme* expression in heart and somites (skeletal muscle precursors).

Ballarino M, Morlando M, Fatica A & Bozzoni I (2016) Non-coding RNAs in muscle differentiation and musculoskeletal disease. *Journal of Clinical Investigation* **126:** 2021–2030
Ballarino, M., Cazzella, V., D'Andrea, D., Grassi, L., Bisceglie, L., Cipriano, A., Santini, T., Pinnarò, C., Morlando, M., Tramontano, A., Bozzoni, I., 2015. Novel long noncoding RNAs (lncRNAs) in myogenesis: a miR-31 overlapping lncRNA transcript controls myoblast differentiation. Mol. Cell. Biol. 35, 728–736. doi:10.1128/MCB.01394-14
Ballarino, M., Cipriano, A., Tita, R., Santini, T., Desideri, F., Morlando, M., Colantoni, A., Carrieri, C., Nicoletti, C., Musarò, A., Carroll, D.O., Bozzoni, I., 2018. Deficiency in the nuclear long noncoding RNA Charme causes myogenic defects and heart remodeling in mice. EMBO J. 37, e99697. doi:10.15252/embj.201899697
Santini T, Martone J and **Ballarino M. 2019** "Visualization Of Nuclear And Cytoplasmic Long Noncoding RNAs At Single-Cell Level By RNA-FISH", *Methods in Molecular Biology*, *in press*

Scienze della Vita

Dipartimento di Biologia
e Biotecnologie
Charles Darwin

SAPIENZA
UNIVERSITÀ DI ROMA

Risposta del lievito agli stress ambientali (#42)

Michele M. Bianchi, Ilaria Camponeschi

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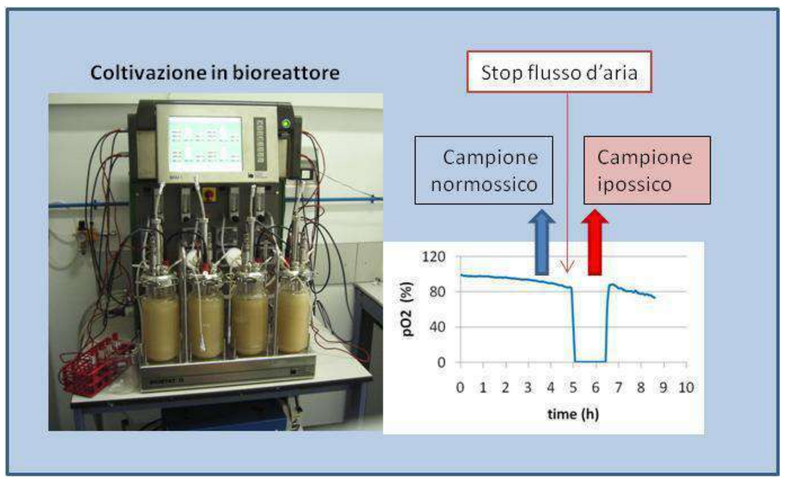
Nel gruppo di ricerca di Biologia e Biotecnologie Microbiche (Dip. BBCD, Sez. CU026) sono in atto studi sugli effetti ambientali - luce, temperatura, ossigeno e composizione del terreno - sulla fisiologia dei microrganismi e sul ruolo di specifici fattori di regolazione sul metabolismo cellulare e sullo stato cellulare. Gli organismi studiati sono lieviti modello e lieviti con applicazioni industriali.

Vengono utilizzate metodologie inerenti a vari settori Bio: biologia molecolare, biochimica, microbiologia, genetica.

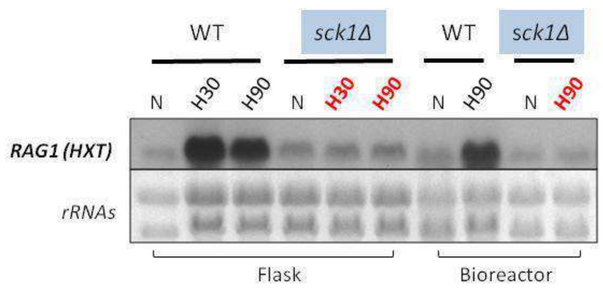
Il settore ERC attinente è LS9_1 - Applied biotechnology (including, transgenic organisms, applied genetics and genomics, biosensors, bioreactors, microbiology, bioactive compounds).

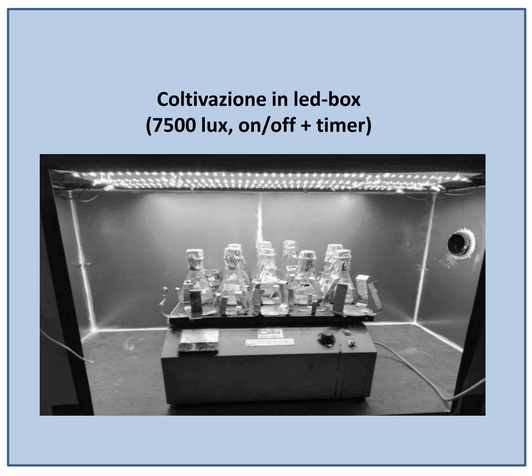
Le competenze dei ricercatori includono coltivazione e manipolazione dei microrganismi, estrazione e manipolazione di acidi nucleici e proteine, ingegneria genetica e metabolica, analisi qualitativa e quantitativa degli acidi nucleici e delle proteine, microscopia ottica e fluorescenza e altro.

Come strumentazione, il gruppo ha a disposizione un Laboratorio delle Fermentazioni con un bioreattore da 4x1L, uno da 2L, uno da 30L, cappa sterile, autoclave da pavimento e centrifuga fino a 6L, un micromanipolatore, un lettore di micropiastre, camere termostatate, chemidoc. I laboratori di ricerca contengono la piccola strumentazione: termocilatori, centrifughe da bancone, sistemi di elettroforesi, cappe sterili, elettroporatore, incubatori, microscopi ottici, spettrofotometro, etc.

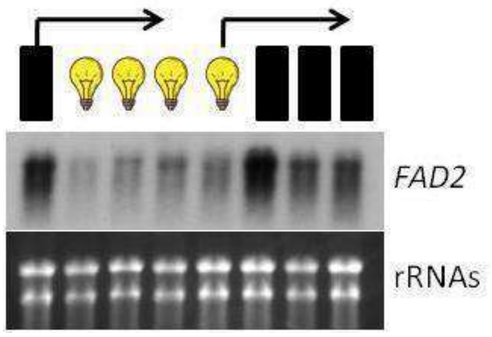


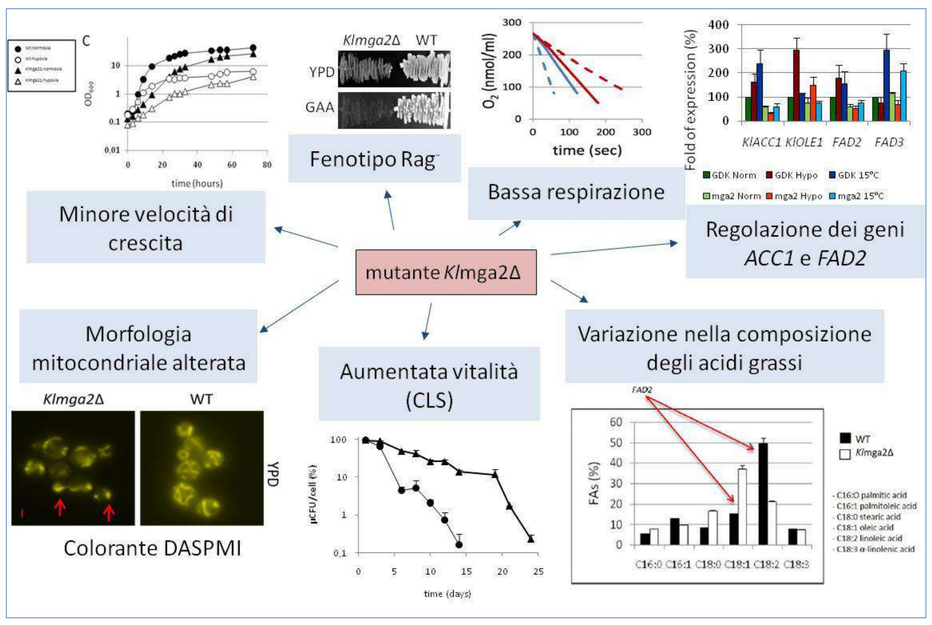
Geni indotti in ipossia



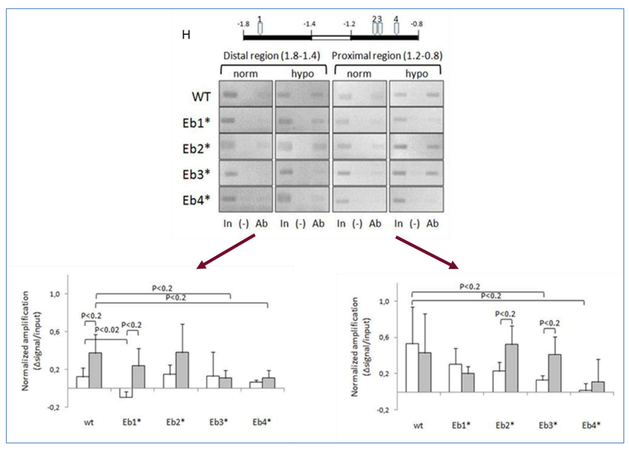


Geni regolati dalla luce



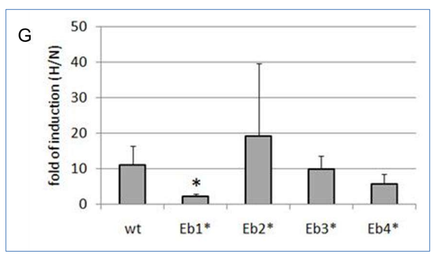


Analisi fenotipica di mutanti



Immunoprecipitazione della cromatina

Realtime PCR



Riferimenti recenti

1. **Ottaviano D. et al. FEMS YEAST RES. doi: 10.1093/femsyr/fov028 2015.**
2. **Proietto M. et al. INT. J. MOL. SCI. doi:10.3390/ijms160715347 2015.**
3. **De Angelis L. et al. MICROBIOLOGY doi: 10.1099/mic.0.000315 2016.**
4. **Santomartino R. et al. WORLD J. MICROBIOL. BIOTECHNOL. doi: 10.1007/s11274-017-2257-y 2017.**
5. **Santomartino R. et al. FEMS YEAST RES. doi: 10.1093/femsyr/foz020 2019.**
6. **Santomartino R. et al. FEMS YEAST RES. doi: 10.1093/femsyr/foz041 2019.**

Remediation of Cr(VI) contaminated water by iron nanoparticles and impact of reused water on tomato plant growth

ERC LS9_8

Elisa Brasili*,Irene Bavasso, Valerio Petruccelli, Alessio Valletta, Giorgio Vilardi, Chiara Dal Bosco, Alessandra Gentili, Luca Di Palma, Gabriella Pasqua*

Dipartimento di Biologia Ambientale, CU022, piano terra, stanza 33

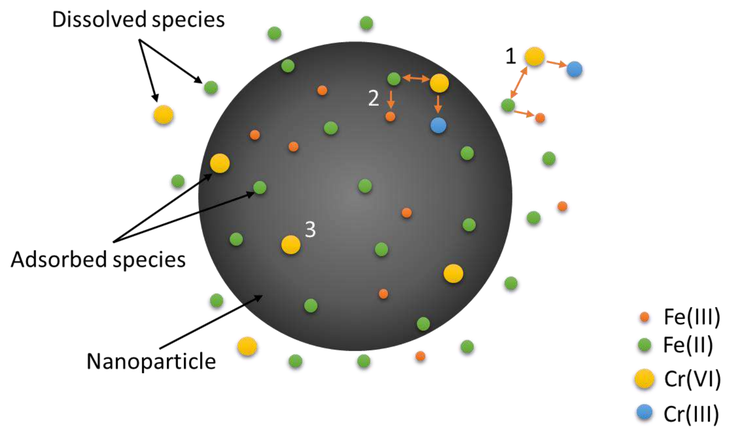
Email: elisa.brasili@uniroma1.it

INTRODUCTION

Water pollution by heavy metals is a very common and serious environmental problem. Anthropogenic **Cr(VI) (hexavalent chromium)** contamination is generally related to industrial applications such as metallurgical, refractories and chemicals. Cr(VI) has been shown as possible **carcinogenic compound**. Several technologies for Cr(VI) removal from industrial wastewater have been successfully proposed. In recent years, **nZVI (zero valent iron nanoparticles)** have attracted a great attention due to their efficiency in removal of different types of contaminants from aqueous solutions, including Cr(VI).

AIMS

A comprehensive study of Cr(VI) removal from wastewater by zero valent iron nanoparticles (nZVI) was carried out. nZVI particles, were continuously synthetized in a Spinning Disk Reactor (SDR) by borohydride reduction method, without the addition of any stabilizer. The reuse of the reclaimed wastewater on tomato plant growth, in terms of seed germination, length of hypocotyl and roots, levels of carotenoids and chlorophylls, was investigated, in a wide range of Cr(VI) and nZVI concentrations. Carotenoid, fat-soluble vitamin and nicotianamine levels were analyzed by LC-MS/MS.



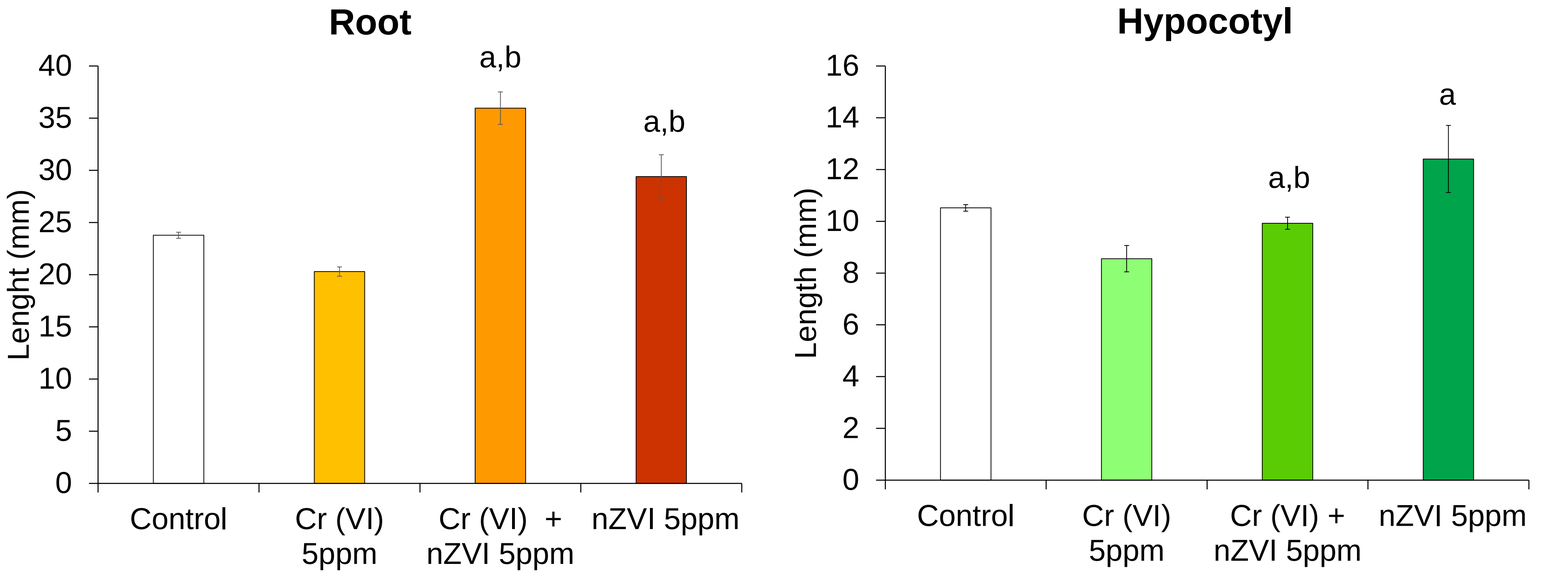
Mechanisms proposed for reduction of Cr(VI) to Cr(III) by ZVI nanoparticles.

RESULTS

Germination

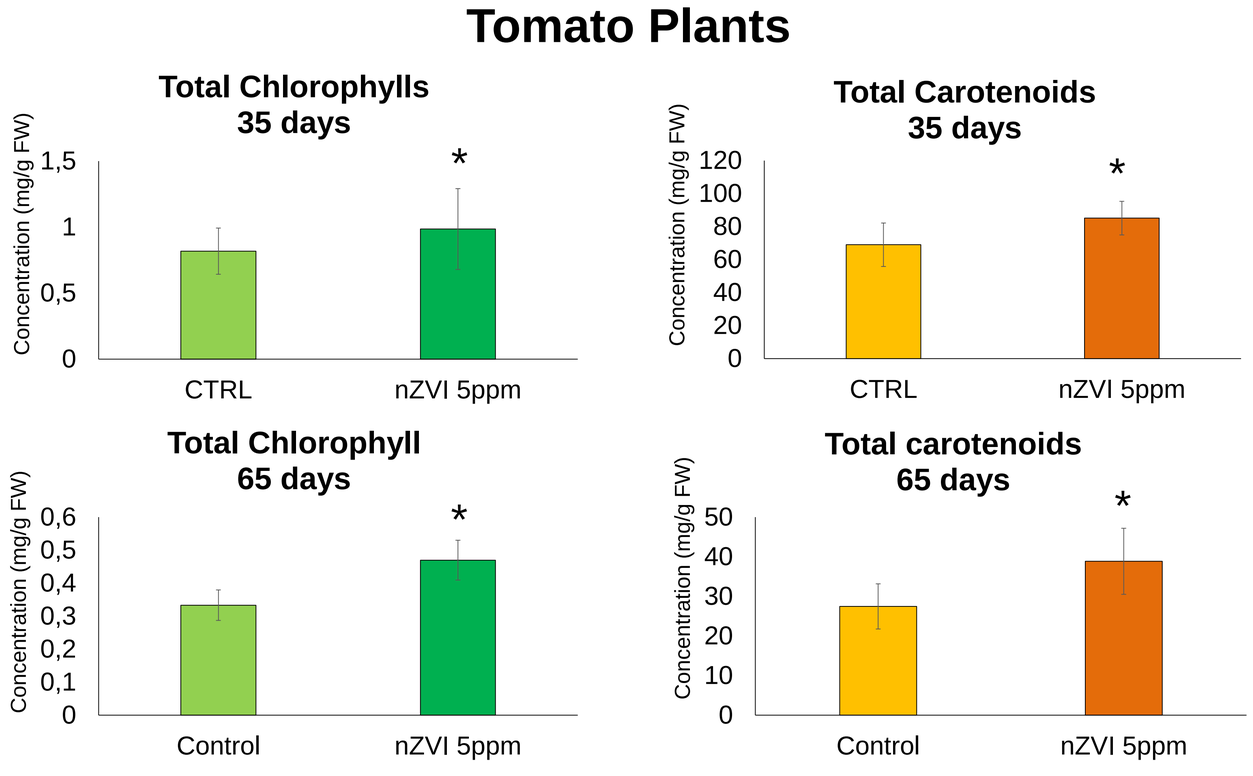
Time (days)			
Treatment	**3**	**6**	**10**
Control	82%	94%	100%
Cr(VI) 5 ppm	56%	78%	82%
Cr(VI) + nZVI 5 ppm	82%	92%	100%
nZVI 5 ppm	100%	100%	100%
Cr(VI) 50 ppm	46%	74%	78%
Cr(VI) + nZVI 50 ppm	76%	96%	100%
nZVI 50 ppm	88%	100%	100%
Cr(VI) 100 ppm	40%	70%	76%
Cr(VI) + nZVI 100 ppm	56%	80%	96%
nZVI 100 ppm	72%	88%	96%
Cr(VI) 1000 ppm	6%	20%	26%
Cr(VI) + nZVI 1000 ppm	0%	4%	4%
nZVI 1000 ppm	0%	4%	4%

Seedlings



Seed germination percentage was higher after nZVI treatment compared to Cr(VI) + nZVI and Cr(VI) at all tested concentrations. After treatment with Cr(VI) + nZVI, seed germination was significantly higher compared to Cr(VI) treatment at all tested concentrations. The combined treatment with Cr(VI) and nZVI 5 ppm particles induced a significant increase of both hypocotyl and root length compared to Cr(VI) 5ppm treatment.

Tomato Plants



Carotenoid content by LC-MS/MS in tomato fruits after 180 days of nZVI 5 ppm treatment

Metabolite	Control (µg/g)	Treated (µg/g)	test.T p-value
α-tocopherol	4.37 ± 0.43	3.99 ± 0.23	NS
β-carotene	1.88 ± 0.22	2.79 ± 0.43	<0.05
phytoene	86.00 ± 4.04	94.36 ± 3.94	NS
phytofluene	43.21 ± 2.97	50.01 ± 3.43	NS
lutein	0.82 ± 0.04	0.97 ± 0.11	NS
zeaxanthin	9.66 ± 0.61	11.21 ± 1.15	NS
ζ-carotene	0.50 ± 0.14	0.50 ± 0.04	NS
β+γ tocopherol	7.01 ± 2.69	5.91 ± 0.81	NS
γ-carotene	0.88 ± 0.49	1.48 ± 0.22	NS
licopene	43.59 ± 14.74	57.08 ± 7.44	NS
nicotianamine	22.44 ± 1.96	25.00 ± 2.89	NS

Plants grown in pots treated with nZVI 5 ppm showed a significant increase of leaf total chlorophyll and total carotenoid levels at 35 and 65 days of growth compared to the control. At 180 days, no differences were observed in carotenoid content of fruits.

Reference: Gueye, M. T., Petrucci, E., & Di Palma, L. (2015). Chemical reduction of hexavalent chromium (VI) in soil slurry by nano zero valent iron. Chemical Engineering Transactions, 43.

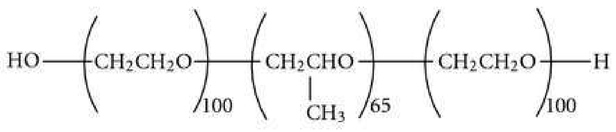
Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

Doxorubicin hydrochloride hosted in bile salt/pluronic mixed micelles

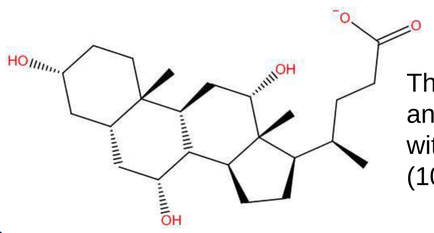
Mauro Giustini, Luciano Galantini, Alessandra Del Giudice, Elisamaria Tasca
Dipartimento di Chimica, Edificio Caglioti CU032, piano V - stanza 11
Email: mauro.giustini@uniroma1.it

- Doxorubicin hydrochloride (DX) is a powerful anticancer drug, but its use is impaired by its intrinsic cardiotoxicity.
- To increase its latency time in the organism, suitable drug delivery system are necessary.
- The self-assembly ability and their intrinsic stealth nature let the pluronics in general, and F127 in particular, promising candidates.
- The catanionic mixture of the DX (positively charged) and bile salts (sodium cholate, NaC, for example, anionic) should drive the drug solubilization in the inner compartment of F127/NaC mixed micelles.

The Host

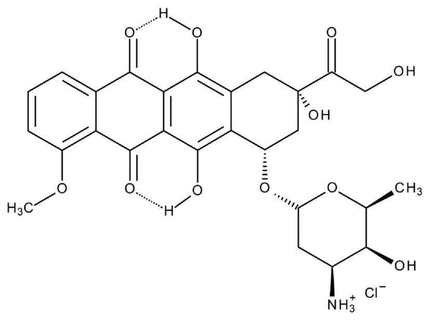


Pluronic F127 is a triblock copolymer composed of hydrophobic poly(propylene oxide) (PPO) block and two units of a hydrophilic poly(ethylene oxide) (PEO) block. It has surfactant properties and above cmc and cmt self-assembles into micelle with a core-shell structure.

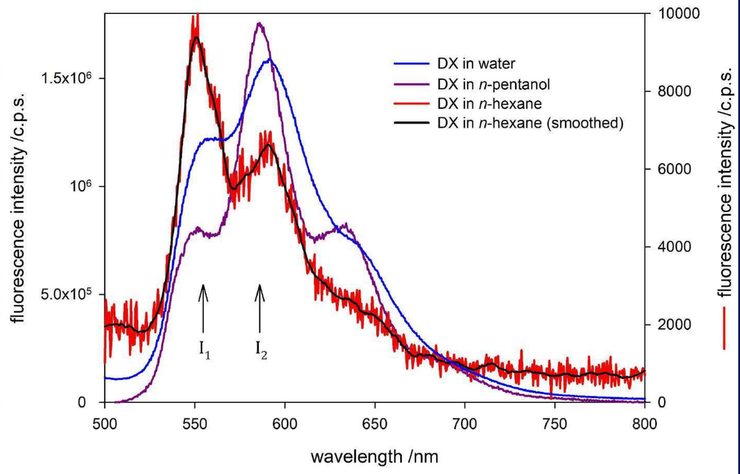


The bile salt NaC is an anionic natural surfactant with a relatively high cmc (10-18mM).

The Guest

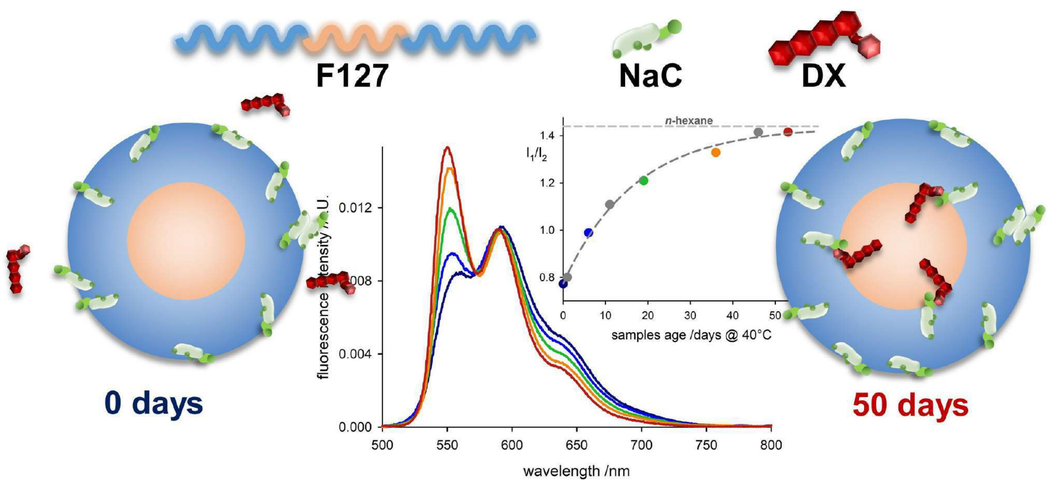


The anthracycline DX is an antibiotic used in cancer chemotherapy. It was isolated from a strain of *Streptomyces peucetius* in 1960.

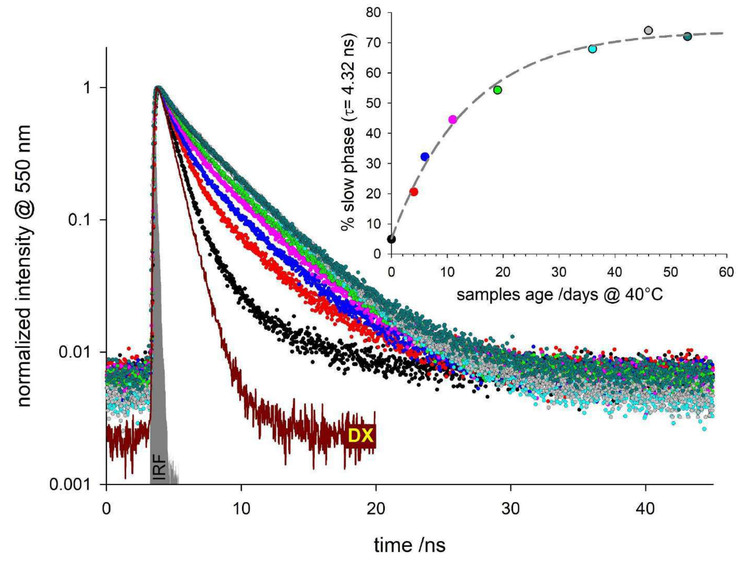


Emission spectra of DX in different solvents (λ_{exc}= 410nm).

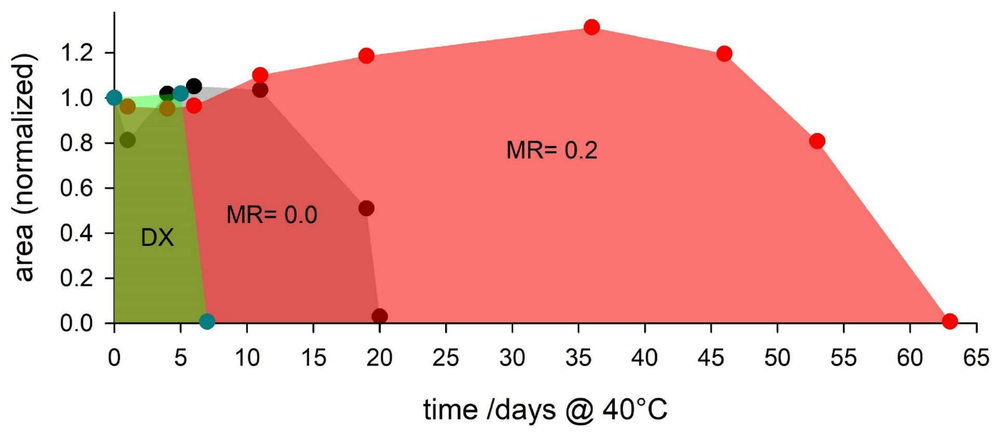
Host-Guest system characterization



Emission spectra of DX in NaC/F127 mixed micelles as a function of the incubation time at 40 °C. Inset: the evolution of the I_1/I_2 ratio with time (same colours as in the main graph – dashed line is a mere guide for the eye).



The fluorescence decay of DX in NaC/F127 mixed micelles (MR= 0.2) is biexponential. Experimental traces have been analysed as the convolution of the Instrument Response Function (IRF) with the sum of two exponentials, whose lifetimes were fixed at 1.00 ns (that of DX in water) and 4.32 ns, respectively. The weight of the slow phase as a function of the incubation time at 40°C is reported in the inset (same colours as the main graph – dashed line is a mere guide for the eye). Also shown is the decay of a DX water solution at the same concentration, but at 25 °C.



The solubilization of DX in the NaC/F127 mixed micellar system confers to DX a surprising stability. In water DX is readily decomposed in a few days, while in the NaC/F127 mixed micelles it is stable for almost two months.

The results here presented point to the successful solubilization of DX in the apolar domain of the NaC/F127 mixed micellar aggregates. At this moment, in-vitro drug-delivery capacity and toxicity toward three different DX-sensitive cancer cell lines (A549, 4T1, Hela) of the DX/NaC/F127 systems are under scrutiny.

Recent bibliography

- E. Tasca, M. D'Abramo, L. Galantini, A.M. Giuliani, N.V. Pavel, G. Palazzo, M. Giustini, Chem. Eur. J. 24 (2018) 8195-8204.
- E. Tasca, A. Del Giudice, L. Galantini, K. Schillén, A.M. Giuliani, M. Giustini, J. Colloid Interf. Sci. 540 (2019) 593-601.
- E. Tasca, J. Alba, L. Galantini, M. D'Abramo, A.M. Giuliani, A. Amadei, G. Palazzo, M. Giustini, Colloids and Surfaces A 577 (2019), 517-522.

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Supramolecular systems

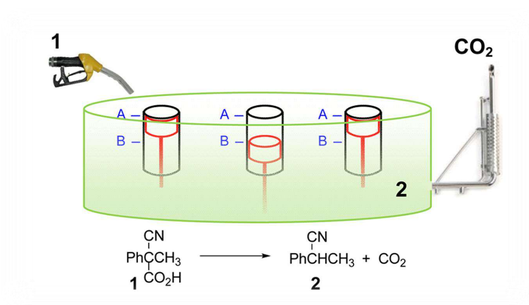
G. Capocasa*, C. Biagini, A. Barbieri, O. Lanzalunga, S. Di Stefano
Dipartimento di Chimica, Edificio S. Cannizzaro, CU014, piano 3 stanza 324
Email: giorgio.capocasa@uniroma1.it

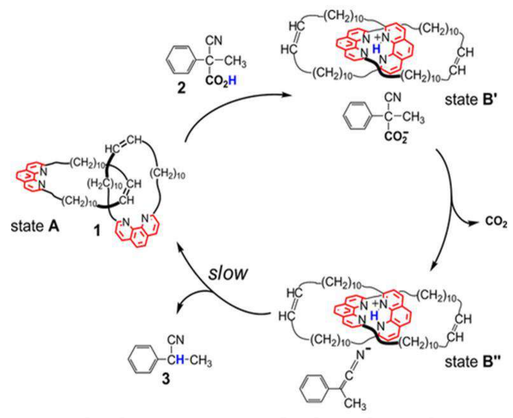
Supramolecular chemistry focuses on the weak interaction between distinct molecules which can be regarded as building blocks for larger structures or *supramolecules.*
Multiple hydrogen bonds, π-π stacking, metal-ligand interactions, ion-π bonding and electrostatic effects can all be involved in the formation of supramolecular systems.
Exploitation of host-guest recognition, dynamic covalent bond formation and production of mechanically-interlocked architectures allow supramolecular systems to display exciting emergent properties such as self-healing of polymers, multistimuli-responsive phase transitions, (directed) mechanical movement or enzyme-like catalysis.

Decarbossilative fuels for molecular machines

Coupling of the Decarboxylation of 2-Cyano-2-phenylpropanoic Acid to Large-Amplitude Motions: A Convenient Fuel for an Acid–Base-Operated Molecular Switch

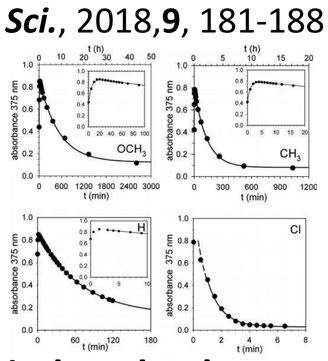
J. A. Berrocal, C. Biagini, L. Mandolini, S. Di Stefano, ***Angew. Chem. Int. Ed.***, 2016, **55**, 6997-7001





Variations in the fuel structure control the rate of the back and forth motions of a chemically fuelled molecular switch

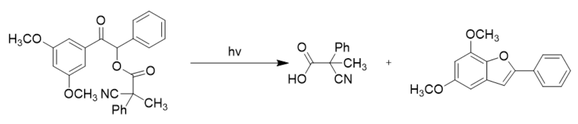
C. Biagini, S. Albano, R. Caruso, L. Mandolini, J. A. Berrocal , S. Di Stefano, ***Chem. Sci.***, 2018,**9**, 181-188

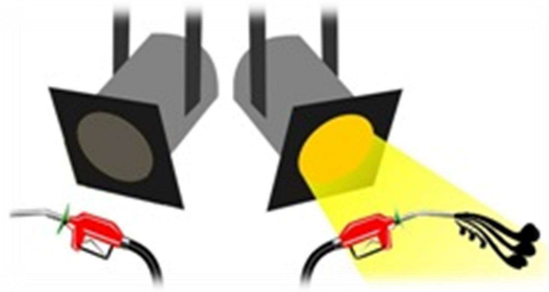




Photoinduced Release of a Chemical Fuel for Acid–Base-Operated Molecular Machines

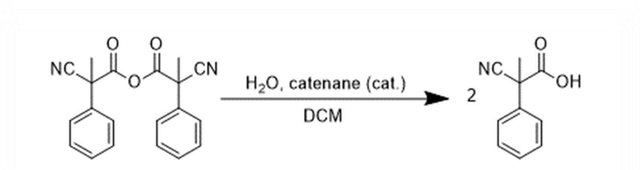
C. Biagini, F. Di Pietri, L. Mandolini, O. Lanzalunga, S. Di Stefano, ***Chem. Eur. J.***, 2018, **40**, 10122-10127

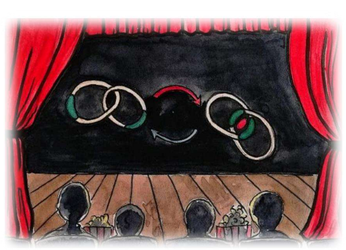




The Hydrolysis of the Anhydride of 2-Cyano-2-phenylpropanoic Acid Triggers the Repeated Back and Forth Motions of an Acid-Base Operated Molecular Switch

C. Biagini, G. Capocasa, V. Cataldi, D. Del Giudice, L. Mandolini, S. Di Stefano, ***Chem. Eur. J.,*** accepted article

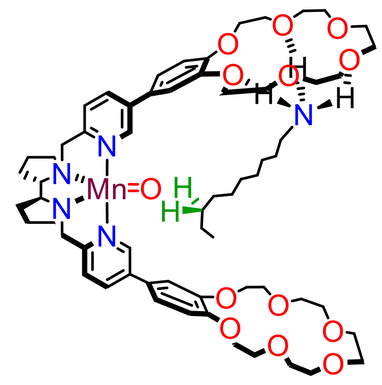




Enzyme-like selectivity in C-H oxidation

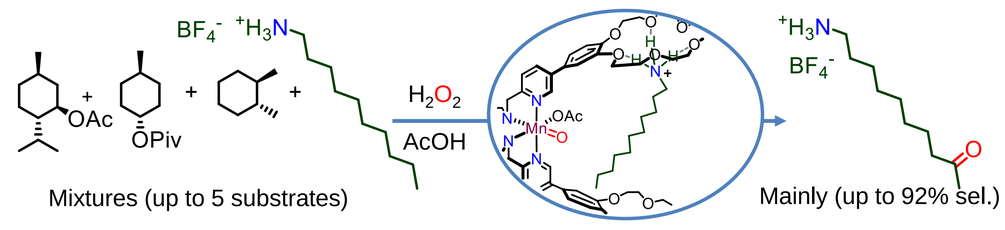
Supramolecular Recognition Allows Remote, Site-Selective C-H Oxidation of Methylenic Sites in Linear Amines

G. Olivo, G. Farinelli, A. Barbieri, O. Lanzalunga, S. Di Stefano, M. Costas, ***Angew. Chem. Int. Ed.***, 2017, **56**, 16347 –16351



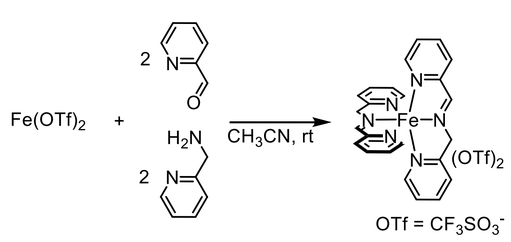
Enzyme-like Substrate-Selectivity in C-H Oxidation Enabled by Recognition

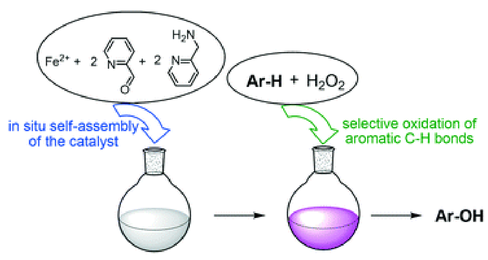
G. Olivo, G. Capocasa, O. Lanzalunga, S. Di Stefano, M. Costas, ***Chem. Commun.***, 2019,**55**, 917-920



Direct hydroxylation of benzene and aromatics with H_2O_2 catalyzed by a self-assembled iron complex: evidence for a metal-based mechanism

G. Capocasa, G. Olivo, A. Barbieri, O. Lanzalunga, S. Di Stefano, ***Catal. Sci. Technol.***, 2017,**7**, 5677-5686





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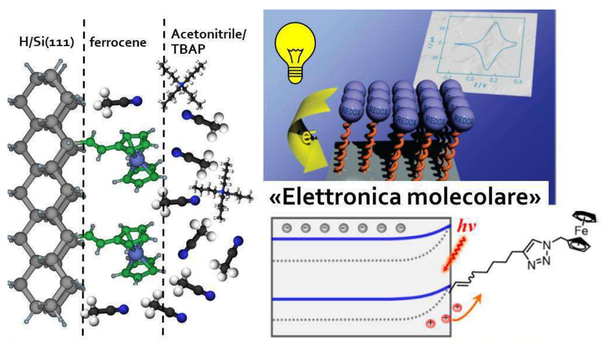
Surface Science of Electrified Interfaces

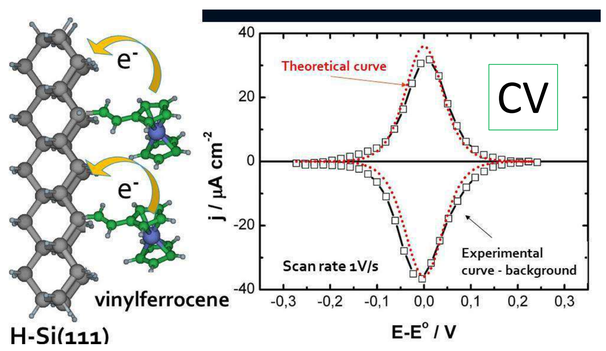
Andrea Giacomo Marrani*, Robertino Zanoni, Alessandro Motta, Valeria Lanzilotto
Dipartimento di Chimica, Edificio «V. Caglioti», CU032, piano 5 stanza 8.
Email: andrea.marrani@uniroma1.it

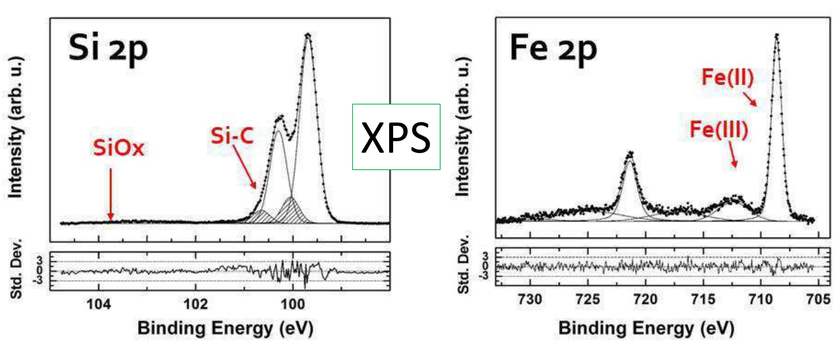
In our group we investigate the chemical properties and electronic structure of surfaces, with particular attention to the interactions established between surface atoms and external species, such as covalently bound organic molecules, weakly bound electrolyte molecules and adsorbed degradation products from electro/chemical reactions. Our attention is devoted to semiconductor and metal surfaces, as components of materials for applications in electronic devices, where the surface is actually an "electrified" interface. Our competences range from use of surface-sensitive spectroscopies, such as photoemission and photoabsorption related techniques, to basic electrochemical characterization of the materials, and theoretical modelling based computations.

ERC sectors: *PE4_4 - Surface science and nanostructures; PE5_3 - Surface modification PE5_6 - New materials: oxides, alloys, composite, organic-inorganic hybrid, nanoparticles*

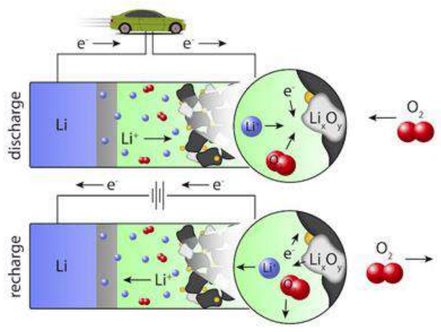
The semiconductor/ molecule/ electrolyte interface



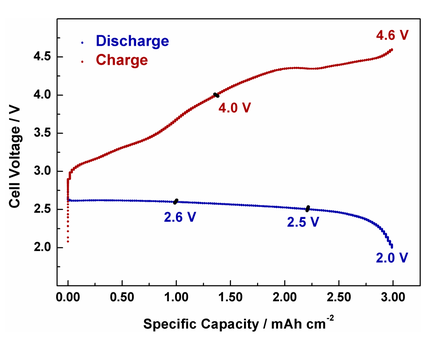




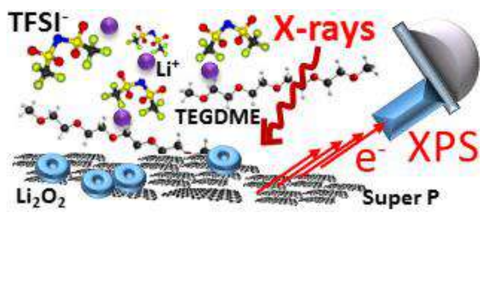
The electrode/ molecule/ gas/ electrolyte interface

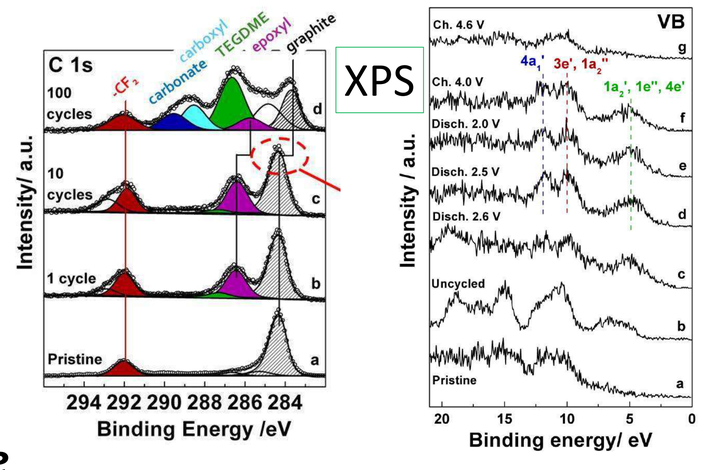


Li-O_2 batteries

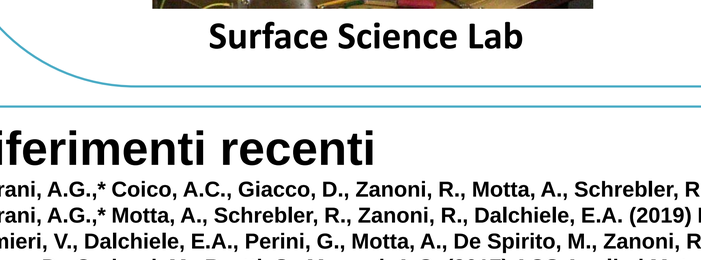


Galvanostatic cyclation

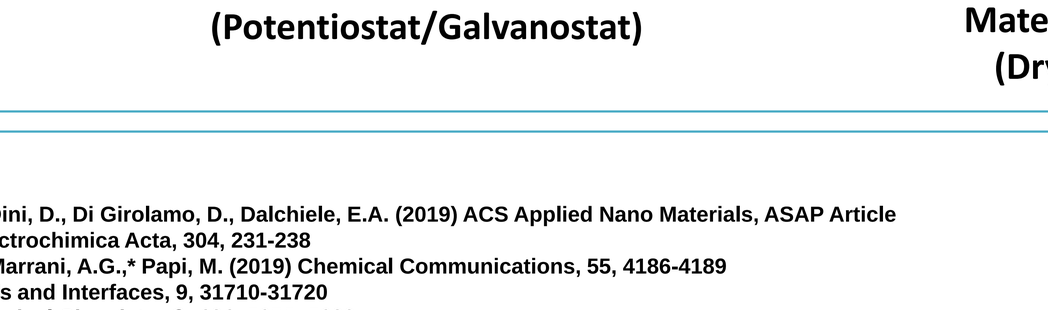


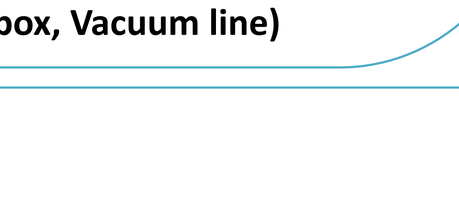


The graphene/ silicon interface



Electrochemical reduction of graphene oxide on silicon





Flexible substrates

Multidisciplinarity: Our research skills and facilities nicely apply to all those fields involving the presence of «reactive» surfaces: electronics, optoelectronics, sensors, catalysis, biomaterials, cultural heritage

Surface Science Lab

XPS
UPS
PEEM

MAIN INSTRUMENTATION AND FACILITIES:

Electrochemical Lab
(Potentiostat/Galvanostat)

Materials Preparation Lab
(Drybox, Vacuum line)

Riferimenti recenti

Marrani, A.G.,* Coico, A.C., Giacco, D., Zanoni, R., Motta, A., Schrebler, R., Dini, D., Di Girolamo, D., Dalchiele, E.A. (2019) ACS Applied Nano Materials, ASAP Article
Marrani, A.G.,* Motta, A., Schrebler, R., Zanoni, R., Dalchiele, E.A. (2019) Electrochimica Acta, 304, 231-238
Palmieri, V., Dalchiele, E.A., Perini, G., Motta, A., De Spirito, M., Zanoni, R., Marrani, A.G.,* Papi, M. (2019) Chemical Communications, 55, 4186-4189
Giacco, D., Carboni, M., Brutti, S., Marrani, A.G. (2017) ACS Applied Materials and Interfaces, 9, 31710-31720
Marrani, A.G., Zanoni, R., Schrebler, R., Dalchiele, E.A. (2017) Journal of Physical Chemistry C, 121, 5675−5683
Marrani,* A.G., Carboni, M., Boccia, A., Galloni, P., Morpurgo, S., Zanoni, R. (2014) Journal of Physical Chemistry C, 118 (39), pp. 22509-22521

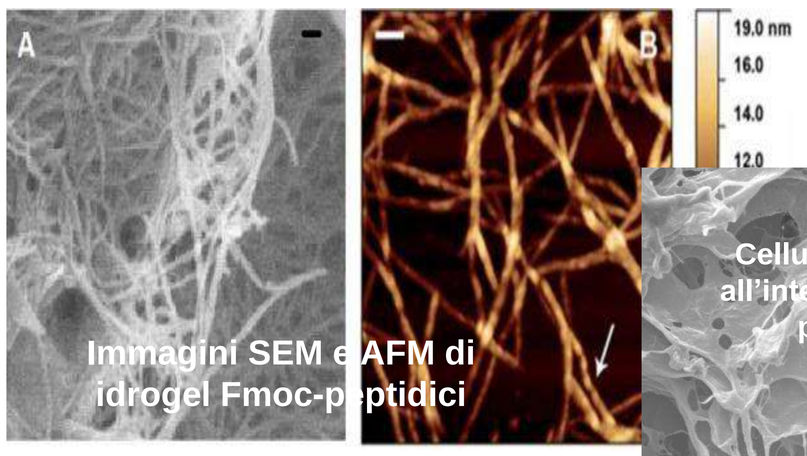
Dipartimento di Chimica
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Bio e nanotecnologie per una chimica industriale sostenibile

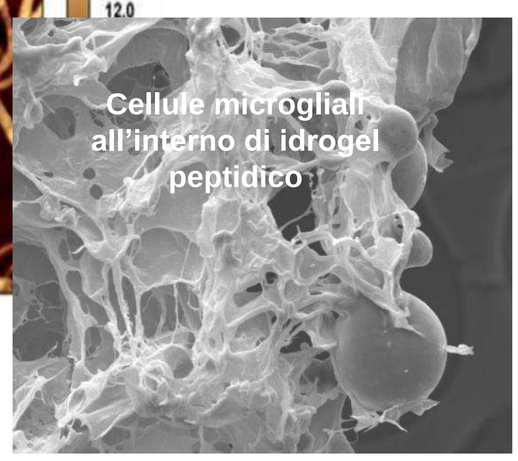
Cleofe Palocci*, Laura Chronopoulou, Antonio Di Nitto
Dipartimento di Chimica, Edificio Caglioti, CU032, piano IV stanza 5a
Email: cleofe.palocci@uniroma1.it

Biofabbricazione

L'attività di ricerca riguarda la biosintesi di sistemi iniettabili, biocompatibili e biodegradabili a base di peptidi autoassemblanti, utilizzati come scaffolds per la crescita e il differenziamento cellulare e nel drug delivery.



Immagini SEM e AFM di idrogel Fmoc-peptidici



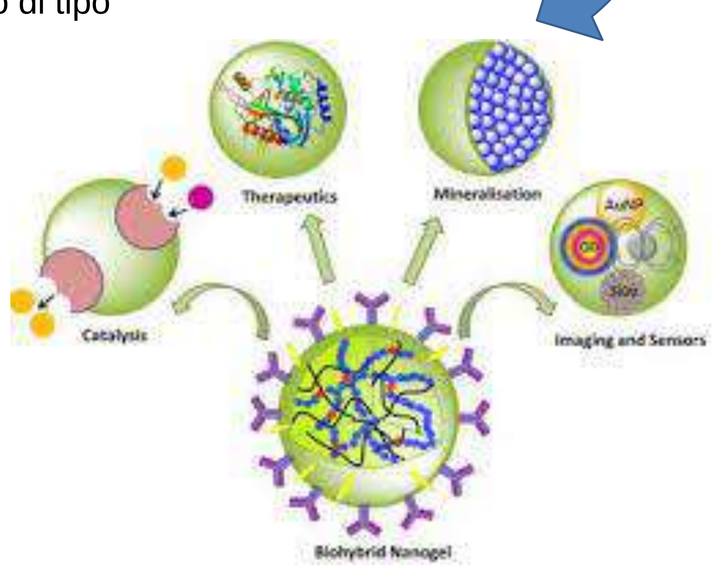
Cellule microgliali all'interno di idrogel peptidico

Nanofabbricazione

Il gruppo ha expertise nella sintesi di nanomateriali biopolimerici per veicolare molecole bioattive e acidi nucleici in cellule animali e vegetali o come carriers di enzimi industriali. La preparazione di tali materiali è realizzata tramite tecniche innovative brevettate nell'ambito del gruppo di ricerca e reattori microfluidici.

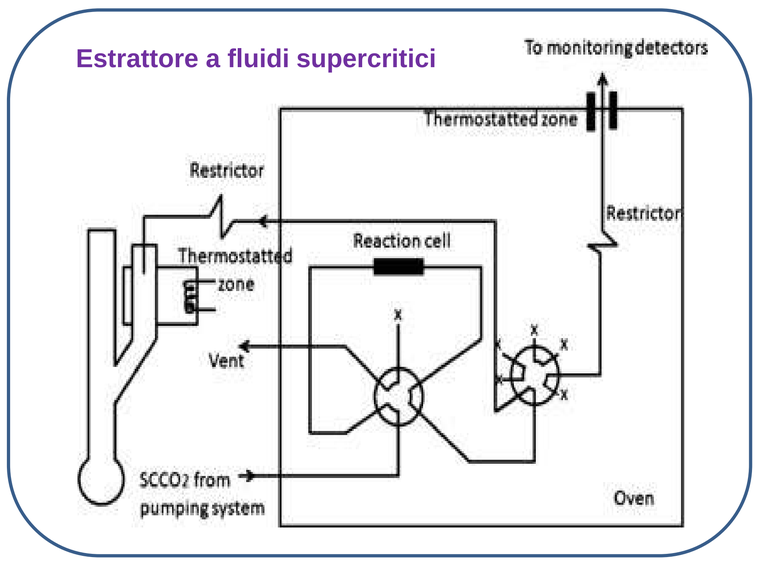


Reattore microfluidico di tipo flow-focusing

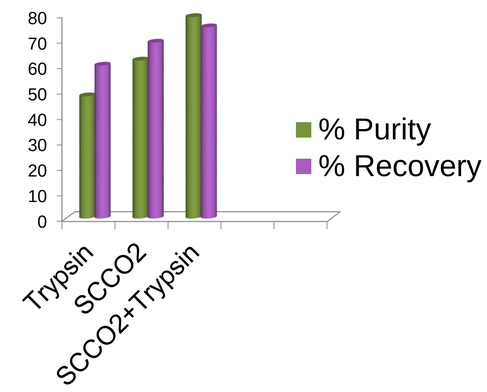


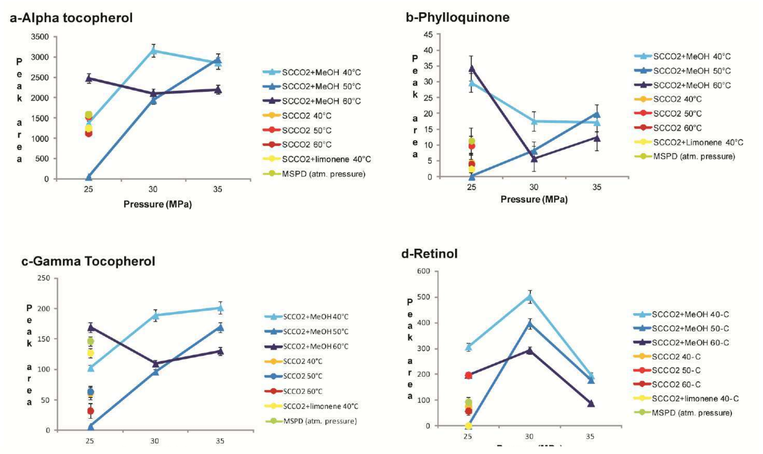
Green solvents e fluidi supercritici

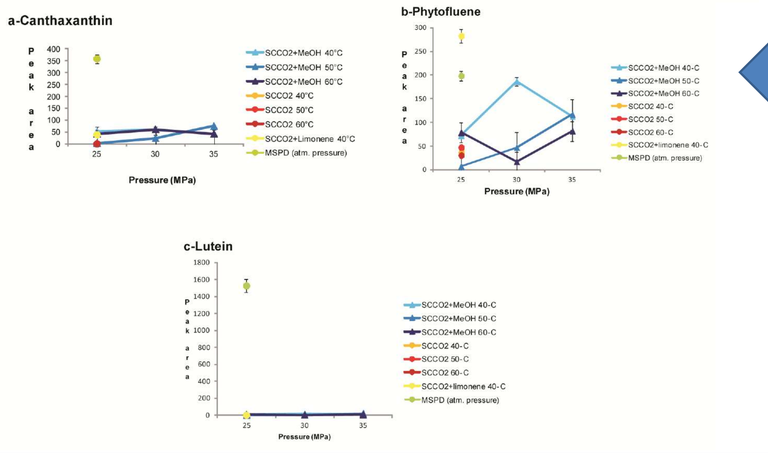
I fluidi supercritici e in particolare la CO_2 supercritica sono impiegati come alternativa ecosostenibile per l'estrazione di polimeri biodegradabili (es. poliidrossialcanoati) nonché di sostanze ad elevato valore aggiunto quali sostanze ad attività antiossidante da biomasse vegetali (es. microalghe) e da scarti di lavorazioni industriali (es. industria olearia). Il gruppo dispone di un estrattore da banco su scala di laboratorio (Carlo Erba).



Purificazione di PHA da colture microbiche miste







Estrazione di carotenoidi e vitamine liposolubili da microalghe

Riferimenti recenti

Chronopoulou et al. Extraction of Carotenoids and Fat-Soluble Vitamins from Tetradesmus Obliquus Microalgae: An Optimized Approach by Using Supercritical CO_2. *Molecules* 2019, 24, 2581-2594.
Chronopoulou et al. PLGA based particles as "drug reservoir" for antitumor drug delivery: characterization and cytotoxicity studies. *Colloids and Surfaces B: Biointerfaces* 2019, 180, 495-502.
Cacciotti et al. Controlled release of 18-β-Glycyrrhetic Acid by nanodelivery systems increases cytotoxicity on oral carcinoma cell line. *Nanotechnology* 2018, 29, 285101-285112.
Chronopoulou et al. A physico-chemical approach to the study of genipin crosslinking of biofabricated peptide hydrogels. *Process Biochemistry* 2018, 70, 110-116.
Fusco et al. Evaluation of novel Fmoc-tripeptide based hydrogels as immobilization supports for electrochemical biosensors. *Microchemical Journal* 2018, 137, 105-110.

Artificial Intelligence in Medicine

A. Ciardiello*, R. Faccini, S. Giagu, C. Mancini Terracciano, A. Russomando, A. Sbandi, C. Voena
Dipartimento di Fisica, Edificio Marconi; INFN Sezione di Roma
Email: andrea.ciardiello@roma1.infn.it

NEPTUNE

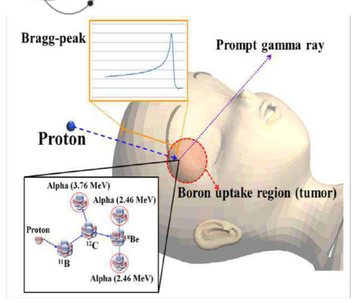
PE2_2
LS7_2

Improvement of Proton Therapy

The goal is the enhancement of proton therapy effectiveness using nuclear reactions with boron and fluorine used as chemical radio-sensitizing agents.
Technique: administration of borated and fluorinated compounds, that accumulate in tumor, to patients before irradiation.

$p + {}^{11}B \longrightarrow 3\ alpha\ (up\ to\ 4\ MeV)$

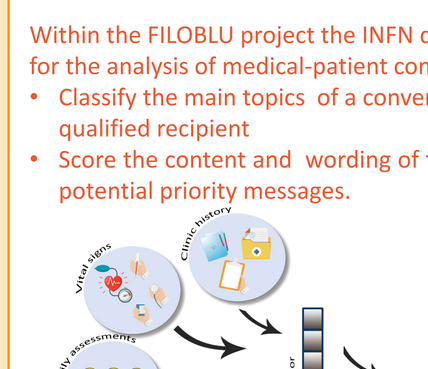
$p + {}^{19}F \longrightarrow {}^{16}O + alpha\ (up\ to\ 13\ MeV)$



Imaging with ^{19}F

To evaluate the effectiveness of these compounds it is necessary to measure the bio-distribution of tracers and the clinical application of the treatment will need the development of a reliable imaging technique optimized for the tracer of interest.
The isotope 19F is characterized by excellent nuclear magnetic properties and it is almost non-existent in the human body so its target-non-target signal ratio is very high while the limiting factor in the application is its small signal-to-noise ratio due to the low concentration of molecules.

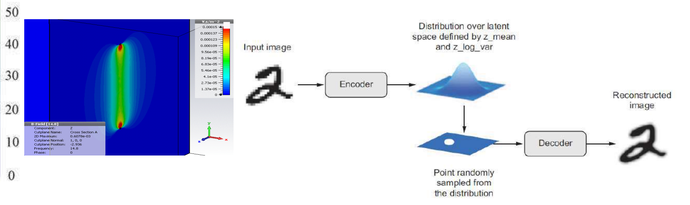
^{1}H-MRI + ^{19}F-MRI Imaging

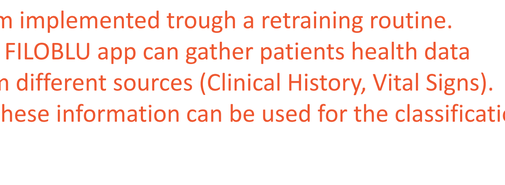


P. Porcari, S. Capuani, E. D'Amore *et al.* 2008 *Phys. Med.* Biol.

Prospectives

- Choice of new fluorinated tracers to extend the technique.
- Improve the NMR RF coil design and electronics.
- Use Deep Learning based denoisers to improve SNR .





FILOBLU

PE6_11

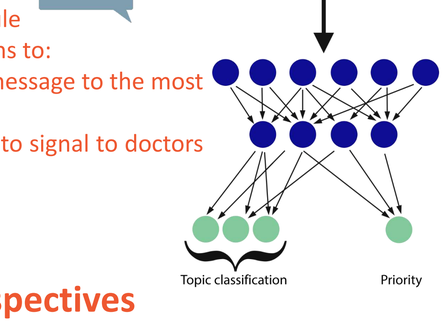
Machine Learning Application to Doctor – Patient Interactions

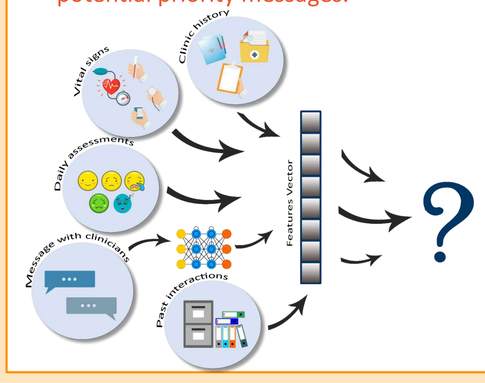
FILOBLU is a software application that aims to improve the communication in the doctor-patient relationship by acting on the monitoring of domiciliary care for oncological patients.

Status

Within the FILOBLU project the INFN developed an AI module for the analysis of medical-patient communications that aims to:

- Classify the main topics of a conversation to direct the message to the most qualified recipient
- Score the content and wording of the message in order to signal to doctors potential priority messages.





Prospectives

- Customization of the AI module for each medical team implemented trough a retraining routine.
- The FILOBLU app can gather patients health data from different sources (Clinical History, Vital Signs). All these information can be used for the classification.

Artificial Intelligence in MRI analysis

PE6_11

Tumor Stadiation

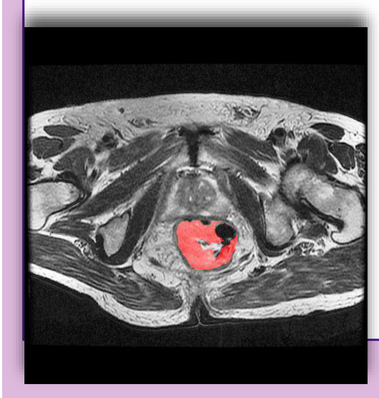
Tumor stadiation is crucial to define and personalize therapeutic strategies and different medical imaging modalities are used for the various types of cancer. Images are usually evaluated "by eye" by the radiologist: the perspective of creating an automatic tool with quantitative data could be a significant improvement in this field. Radiomics, which involves the extraction of high-dimensional data from digital images, can provide non-visual information relating to tumor characteristics. Radiomic features can be then combined in Artificial Intelligence models that can learn to classify the images. Moreover, deep learning neural network techniques can be directly applied to images without the intermediate feature extraction step.

Results

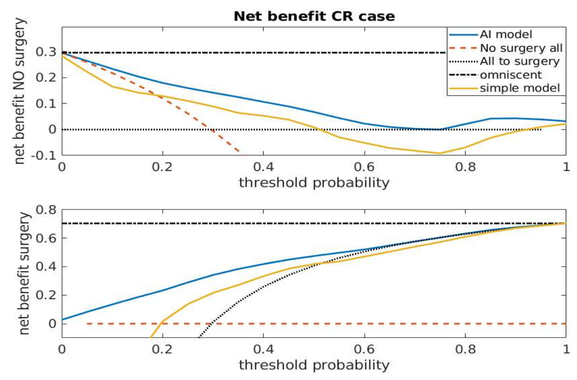
- An Artificial Intelligence model (Random Forest) has been developed to magnetic resonance images to assess the response to chemo-radiotherapy in local advanced rectal cancer.
- The model is intended to give the radiologists and clinicians solid answers to individuate rapidly patients that completely respond to therapy. The correct stratification of complete responders will help the affirmation of less invasive therapeutic strategies.
- Good classification accuracy and clinical utility has been obtained.

Prospectives

- Artificial intelligence can be also used for automatic segmentation of Region-Of-Interest (tumor, red area in the image).
- The main limit of this kind of applications is the small patient populations.
- Advanced learning techniques, such as transfer learning, can be used to reduce the number of patients needed to train the artificial intelligence algorithms.



Clinical Benefit

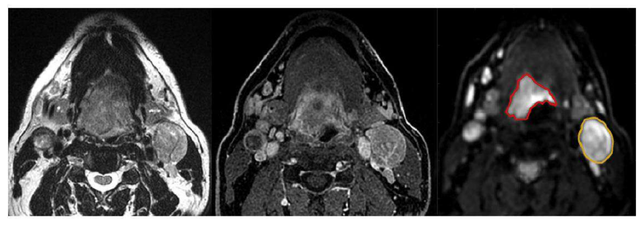


Prediction of HPV Status in Tumors

Purpose: To investigate the relationships between imaging parameters derived from intravoxel incoherent motion diffusion-weighted imaging (IVIM-DWI) and HPV status in oropharyngeal squamous cell carcinoma (OPSCC). HPV status portends a better prognosis and is recognized as an important independent prognostic factor.

Proposed methods

- We are developing an analysis method for composite images of high resolution T2 images with diffusion / perfusion maps derived from IVIM imaging.
- Diffusion imaging parameters in composite images are treated as "colours" channels.
- Different acquisition protocols gives complementary information that can be easily integrated with a deep learning approach.



Recent references : R.Ferrari et al. , MR-based artificial intelligence model to assess response to therapy in locally advanced rectal cancer, European Journal of Radiology 118, (2019), 1-9

ERC (sub sectors): PE6_11, LS7_2, LS7_3

Lab-on-chip Systems for in-situ Determination of Mycotoxins and Fungi

F. Costantini[1,2], N. Lovecchio[1], M. Nandimandalam[2], L. Iannascoli[3], M.Reverberi[2], C. Manetti[2], G. de Cesare[1], A. Nascetti[3], D. Caputo[1]

[1]Department of Information, Electronic and Telecommunication Engineering, Sapienza University of Rome, Via Eudossiana 18, 00184 Roma, Italy
[2]Department of Environmental Biology, Sapienza University of Rome, p.le Aldo Moro 5, 00185, Rome, Italy
[3]School of Aerospace Engineering, Sapienza University of Rome, Via Salaria 851/881, 00138 Roma, Italy

Motivation

What is a Lab-on-chip system:

Microfluidic Channel

Micro/Nanofabrication

Microfluidic Chip

Integration of heating detection systems, temperature control and samples pretreatment

Lab-on-Chip











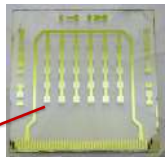
Advantages/Disadvantages of Lab-on-chip:

- Low fluid volume consumption (less waste, low reagents costs and less sample volume to analyze);
- Compactness of the system due to integration of many functionalities ensuring analysis directly in the field (portability);
- Massive parallelization due to compactness, which allows high through-put analysis;
- Novel technology not fully developed: less sensitive detection systems;

Developed Lab-on-Chip Systems

On-Chip Aptamer Assay for OTA Detection

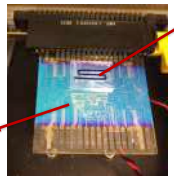




The array is connected to a home-made electronic board and to a computer. The functionalized microfluidic chip is aligned with the photosensors. The entire system is contained in a small metallic box (picture on the right).

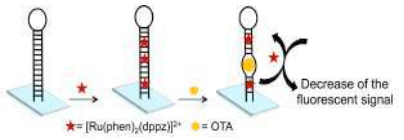
On-Chip Isothermal Amplification of Bacteria/Fungi DNA



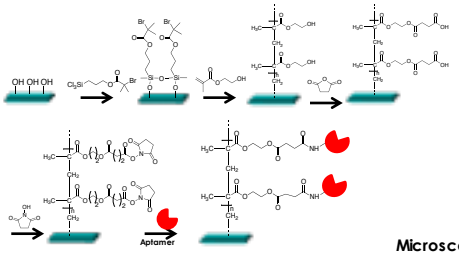


A12 x 8 x10 cm^3 metal box shields electromagnetic interferences.
The excitation source is a LED Roithner Lasertechnik APG2C1-450, whose exitation spectra is centered at 450nm.

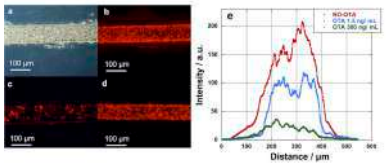
OTA Detection



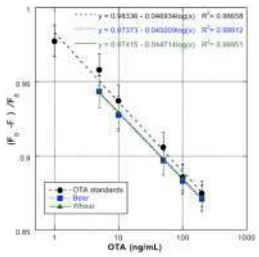
Label-free aptamer assay is based on the binding displacement, of the fluorescent switching complex $[Ru(phen)_2(dpz)]^{2+}$, upon the interaction of OTA with the aptamer causing a decrease of the fluorescent signal detected by the photosensors.



Fabrication of the aptasensor nanomaterial on a glass substrate: immobilization of **aptamer 1.12.2**, labelled with an amino functional group, via peptide bond formation (PHEMA-Aptamer)

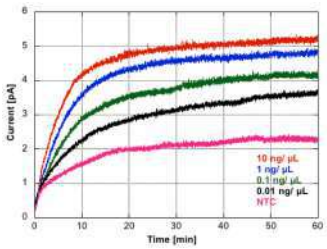


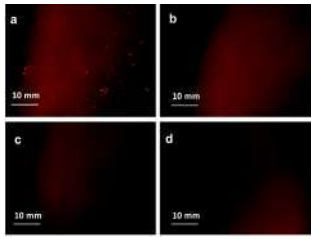
Microscope images of PHEMA-aptamer patterned lines and their fluorescent profile:
a) transmission mode and after incubation, b) with $[Ru(phen)_2(dppz)]^{2+}$, c) with $[Ru(phen)_2(dppz)]^{2+}$and OTA 300 ng/ mL, d) $Ru(phen)_2(dppz)]^{2+}$ and OTA 1.5 ng/ m and e) graphic of the fluorescent profile along the cross section of a 100 µm wide patterned line.



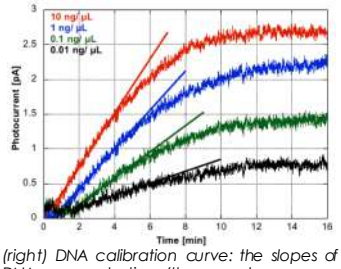
Calibration curves obtained by using the Lab-on-Chip: for OTA in HEPES 1-200 ng/ ml (circle), and in beer (square) and wheat (triangle) extracts spiked with OTA 5-200 ng/ ml (error bars are the standard deviation different measurements using three different functionalized microfluidic networks).

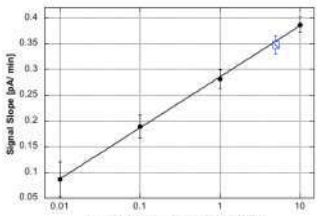
DNA Amplification



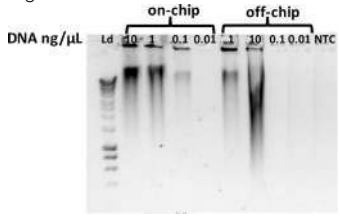


(**a**) On-chip real-time monitoring of the MDA reaction (amplification curves) showing the increase of the photocurrent as function of time for different initial dsDNA concentrations. (**b**) Fluorescent images of samples with an initial dsDNA concentration of a) 500 pg/µL, b) 50 pg/µL, c) 5 pg/µL and d) the NTC.





(right) DNA calibration curve: the slopes of the linear trend lines as a function of the initial DNA concentration (the error bars are an average of three measurements reported as standard deviation, error was below 10%). (left) determination of unknown DNA sample by using the calibration curve.



Gel-electrophoresis of isothermal amplification products performed using off- chip and on-chip procedures (Ld = ladder).

Conclusions

In this work, an aptasensor material based on the immobilization of an OTA-aptamer on PHEMA polymer brushes was achieved. A **DNA intercalating dye, $[Ru(phen)_2(dpz)]^{2+}$** was used. Upon OTA binding to the aptamer, the dye is displaced from the DNA causing a decrease of the fluorescent signal. **The LoC is able to quantify OTA down to 1.56 ng/ mL**
With the integrated heater and sensors on one device in combination with a COC chip, **the DNA isothermal amplicafon** could be monitored in real-time by the use of the fluorophore [Ru(phen)2(dppz)]2+. After 60 minutes the photocurrent values are linearly dependent on the initial DNA concentration. Unknown DNA sample quantification using this LoC system was achieved.

Acknowledgements

Authors thanks the center for Life Nano Scienze @Sapienza, Istituto Italiano di Tecnologia, the Italian Space Agency (ASI) through PLEIADES project and Sapienza university of Rome for the financial support.

aSiDaS
amorphous Silicon Devices and Systems

Nuove metodologie analitiche nella conservazione dei beni culturali

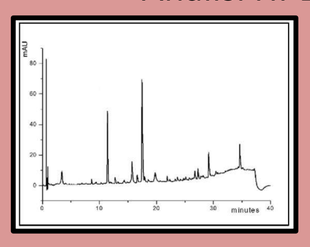
Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

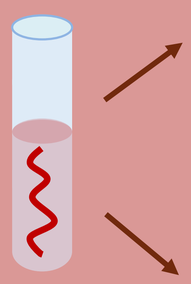
Ilaria Serafini*, Alessandro Ciccola, Flaminia Vincenti, Camilla Montesano, Roberta Curini
Dipartimento di Chimica, Edificio Cannizzaro, Laboratorio 062
Email: ilaria.serafini@uniroma1.it

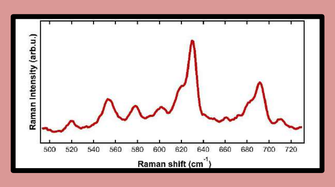
Il gruppo di ricerca per la messa a punto di metodi analitici per la diagnostica dei beni culturali è guidato dalla prof.ssa Curini ed è finalizzato allo sviluppo di nuove soluzioni per l'analisi e la conservazione di materiali organici di interesse nei beni culturali, che rappresentano il nucleo principale della ricerca. L'approccio multianalitico risulta fondamentale per la completa caratterizzazione delle matrici, spesso fortemente composite e degradate, e vede la combinazione di tecniche di cromatografia liquida, spettrometria di massa e, in collaborazione con il Dipartimento di Fisica (Prof. Paolo Postorino, Prof. Alessandro Nucara), di spettroscopia Raman e FTIR. In particolare, i principali argomenti di ricerca riguardano la caratterizzazione di coloranti naturali da lacche pigmento e matrici tessili attraverso spettrometria di massa in alta risoluzione e spettroscopia SERS (*Surface Enhanced Raman Spectroscopy*), l'identificazione di fibre tessili in campioni archeologici e lo studio di materiali nell'arte contemporanea. L'attività di ricerca è inoltre dedicata allo sviluppo di nanomateriali per la conservazione di manufatti tessili, cellulosici e in pelle e ha portato a un brevetto, depositato presso Sapienza. Diversi progetti sono svolti in collaborazione con enti museali e Istituti di Restauro (Galleria Nazionale di Arte Moderna e Contemporanea, Istituto Centrale per il Restauro e la Conservazione).

Analisi di coloranti da matrici tessili e pittoriche

Analisi HPLC-MS





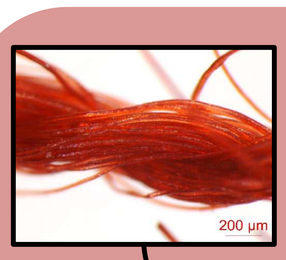


Estrazione *mild* del colorante

Analisi SERS

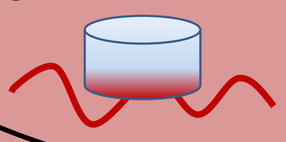
- Nuove metodologie di estrazione
- Preservazione del *pattern* molecolare del colorante
- Alta sensibilità

Tecniche di campionamento micro-invasive



Prima

Campionamento su gel da matrice tessile



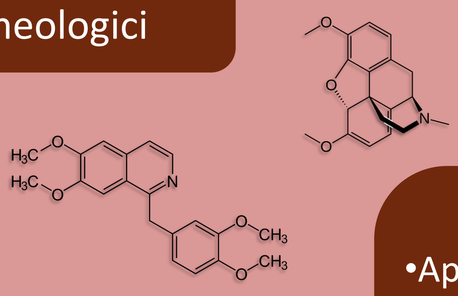
Dopo

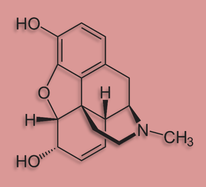


- Versatilità della tecnica estrattiva
- Micro-invasività
- Analisi su substrato e/o post riestrazione

Sostanze stupefacenti in residui archeologici

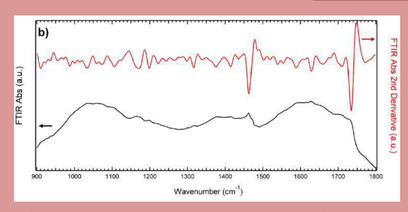


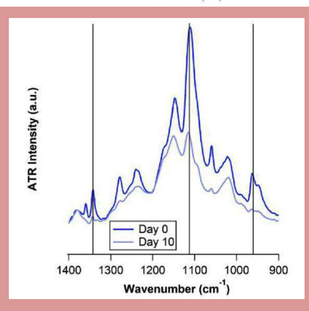




- Applicazione di metodologie forensi a campioni archeologici
- Estrazione ASE e dMLLE per identificazione di oppiacei e cannabinoidi in vasi antichi

Studio di processi di degrado





- Identificazione di materiali degradati
- Caratterizzazione di processi di invecchiamento in materiali contemporanei

[1] A. Ciccola et al., "Spectroscopy for Contemporary Art: discovering the effect of Synthetic Organic Pigments on UVB degradation of acrylic binder", Polymer Degradation and Stability, 159 (2019), 224-228
[2] I. Serafini et al., "New advanced extraction and analytical methods applied to discrimination of different lichen species used for orcein dyed yarns: Preliminary results", Microchemical Journal, 138 (2018), 447-456
[3] I. Serafini et al., "How the extraction method could be crucial in the characterization of natural dyes from dyed yarns and lake pigments: The case of American and Armenian cochineal dyes, extracted through the new ammonia-EDTA method", Microchemical Journal, 134 (2017), 237-245
[4] A. Ciccola et al., "Azo-pigments effect on UV degradation of contemporary art pictorial film: A FTIR-NMR combination study", Polymer Degradation and Stability, 140 (2017), 74-83
[5] I. Serafini et al., " A new multi analytical approach for the identification of synthetic and natural dyes mixtures. The case of orcein-mauveine mixture in a historical dress of a Sicilian noblewoman of nineteenth century", Natural Products Research, 33 (2019), 1040-1051

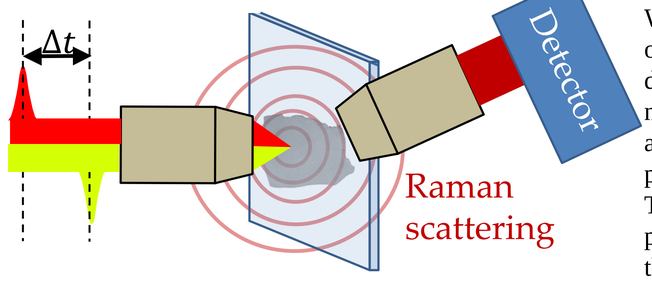
A pulsed laser-based facility for time resolved and fast imaging studies

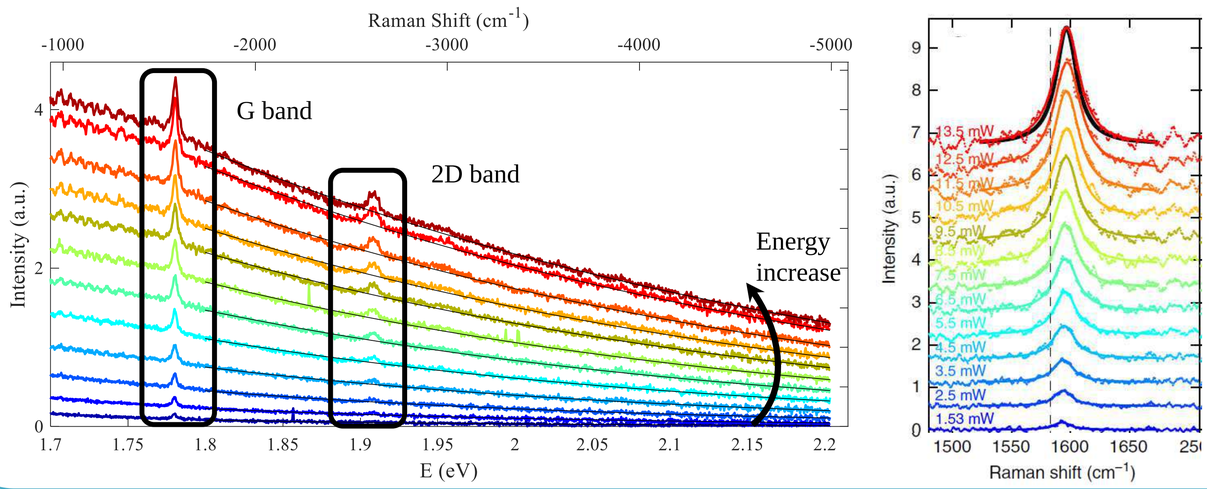
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SAPIENZA UNIVERSITÀ DI ROMA

G. Batignani 1, C. Ferrante 1, T. Scopigno 1*
Dipartimento di Fisica, Edificio Fermi, CU033, piano -1 stanza S01, S02, S03
Email: tullio.scopigno@uniroma1.it

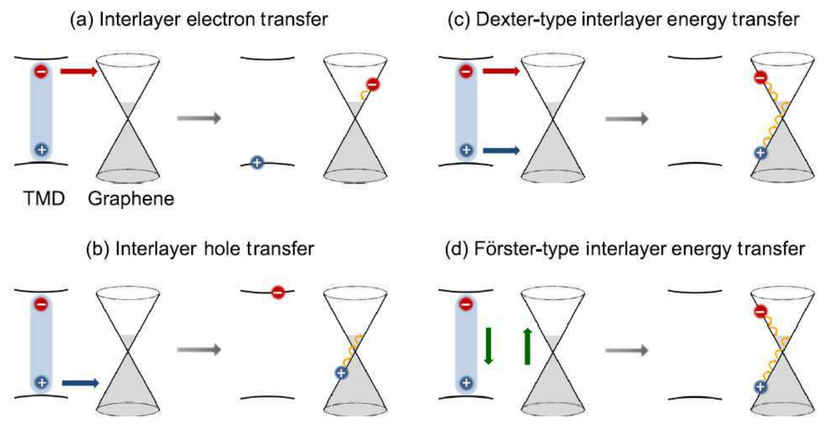
Raman spectroscopy with pulsed excitation

The rise of graphene, followed by the more recent (re)discovery of the vast family of transition-metal dichalcogenides (TMDCs), has fuelled an unprecedented cross-disciplinary research effort. In our laboratory we detect the out-equilibrium Raman signature of graphene, using Spontaneous Raman with pulsed laser excitation [1].
The observation of electron-phonon modification from the point of view of phonon allows to quantify the ps blurring of the Dirac cone surface.





Recent demonstrations of hybrid photodetectors, based on graphene-TMDC van der Waals heterostructures (vdWH), is boosting a rapid progress of this field towards optoelectronic applications. The operation and intrinsic performance of vdWH-based devices are governed by band alignment, interactions with the underlying substrate, and near-field quantum phenomena, such as photoinduced-interlayer charge transfer (ICT) and energy transfer (IET). To discriminate between ICT and IET effects, we perform pump-probe imaging with two pulses. The first photoexcites (pump) the vdWHs above TMDC (donor) energy gap and the second probes at different time delays upon photoexcitation the response on graphene, which represents the acceptor component in the ICT and IET process.



PHYS. REV. X 8, 011007 (2018)

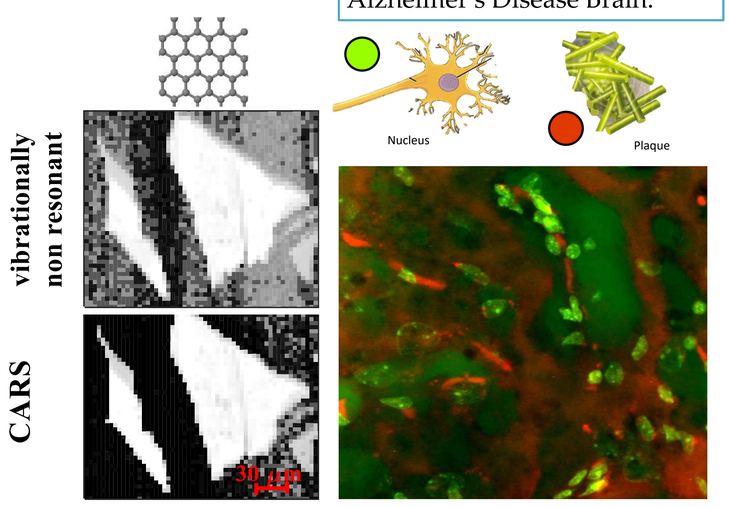
Coherent Raman micro-spectroscopy

Imaging

Performing Raman spectroscopy through a confocal microscope is a powerful method to spatially resolve cells, tissues and two dimensional materials. But, **acquisition time is long (~1 s per pixel).**
Such limitation can be overcomed by Coherent Raman (CR) spectroscopy:
INGREDIENTS - the simultaneous excitation of the sample by two picosecond beams at frequencies ω_P and ω_S, which match the frequency of a particular molecular vibration, results in the coherent stimulation of the system vibrations, greatly enhancing the Raman signals.
RESULTS - dramatically reduce acquisition time **~10^{-6} s per pixel**

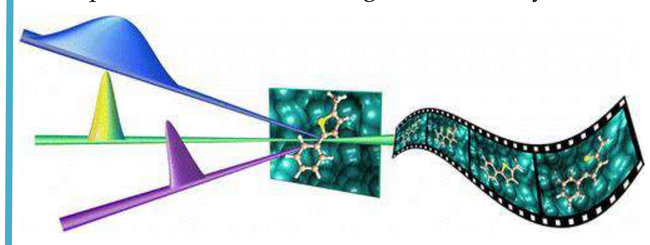
We rationalize CR of Graphene, enabling a real-time structural characterization [2].

We observe with our imaging system simultaneously the two photon fluorescence from nuclei and CR signal of CH bond of Amyloid-β Plaques in Alzheimer's Disease Brain.

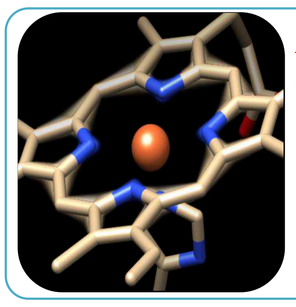


Time resolved spectroscopy

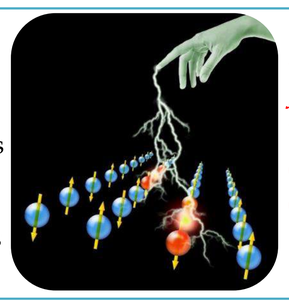
By means of a three pulses sequence it becomes possible to study out of equilibrium states tracking vibrational dynamics



A first ultrashort pulse excites the sample and then the combination of a narrowband ps pulse and an ultrashort white light continuum is used to detect transient vibrational frequencies [3-4]

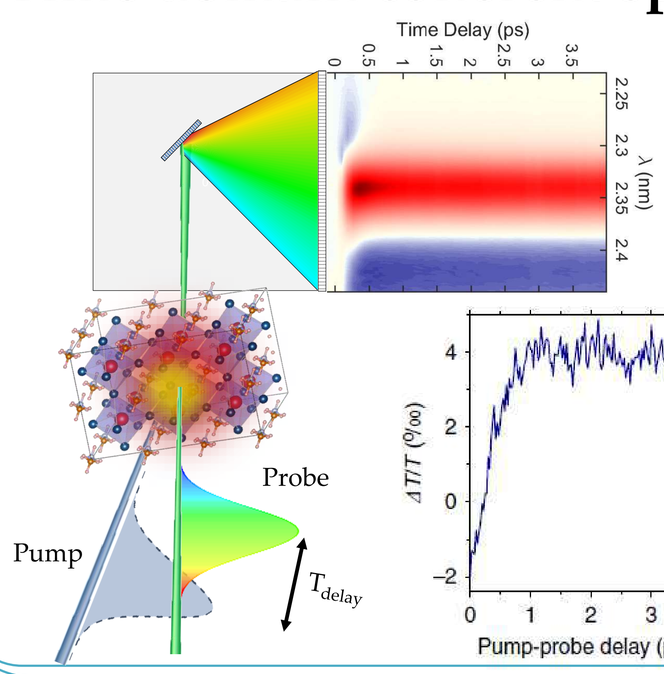


Molecular movie of heme-proteins femtosecond and picosecond dynamics of Myoglobin is unveiled observing the Raman hot bands [5]

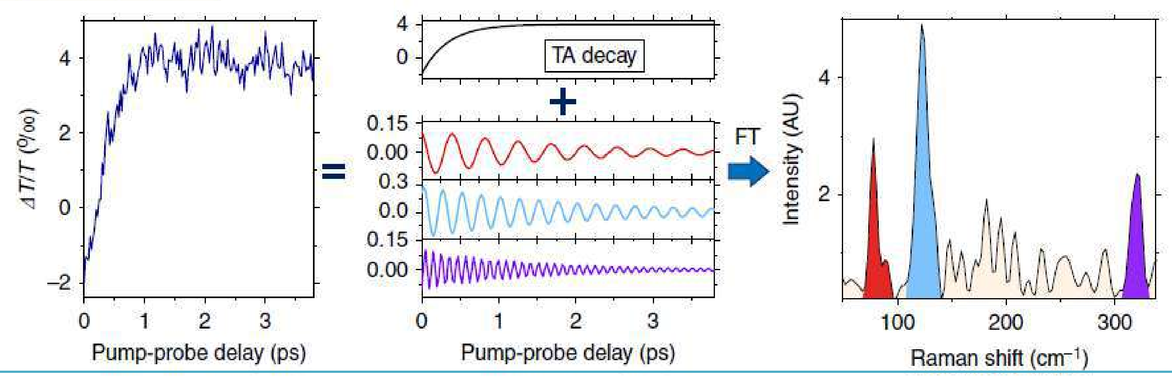


Light induced femtosecond modification of antiferromagn etic interaction [6]

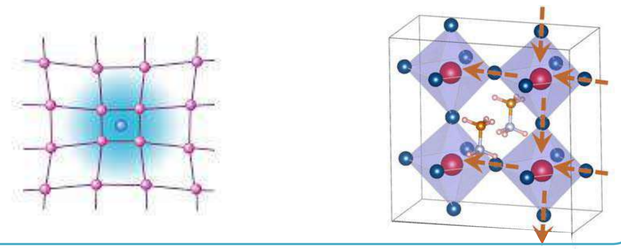
Time domain coherent spectroscopy



Impulsive Stimulated Raman Spectroscopy (ISRS) exploit a time-domain probe protocol consisting of two temporally separated laser fields: a ~ 10 fs pump pulse impulsively excites the Raman active modes of a system, and, then, a femtosecond broadband probe measures at variable time delays the optical transmission, which is temporally modulated by the coherently stimulated vibrations. By Fourier transforming the signal to the frequency domain, the transient Raman spectrum can be retrieved.



A novel class of hybrid semiconducting materials, composed by an inorganic lattice and an organic matrix, has emerged as the prototypical candidates for the next-generation of photovoltaic devices. The key property for their high energy conversion efficiency is represented by the long lifetime of the photo-carriers, enabling long diffusion lengths. By using ISRS setup for the simultaneous injecting of photo-carriers and monitoring the subsequent coherent lattice motions, we have unveiled the physical mechanism responsible for the high carriers mobility. Specifically, we observe the role of polaron, that can be represented as an electron surrounded by a cloud of phonons, in the charge dynamics [7].



[1] Ferrante, C. et al., Nat. Commun., 9, 308 (2018).
[2] A. Virga et al., Nat. Commun., 10, 3658 (2019)
[3] G. Batignani et al, J. Phys. Chem. Lett., 7, 15, 2981-2988(2016)
[4] G. Batignani et al., ACS Photonics, 6, 492−500 (2019)
[5] C. Ferrante et al., Nat. Chemistry, 8, 1137–1143 (2016)
[6] G. Batignani et al., Nat. Photonics, 9, 506, (2015)
[7] G. Batignani et al., Nat. Comm., 9, 1971 (2018).

Molecular Modelling of complex systems

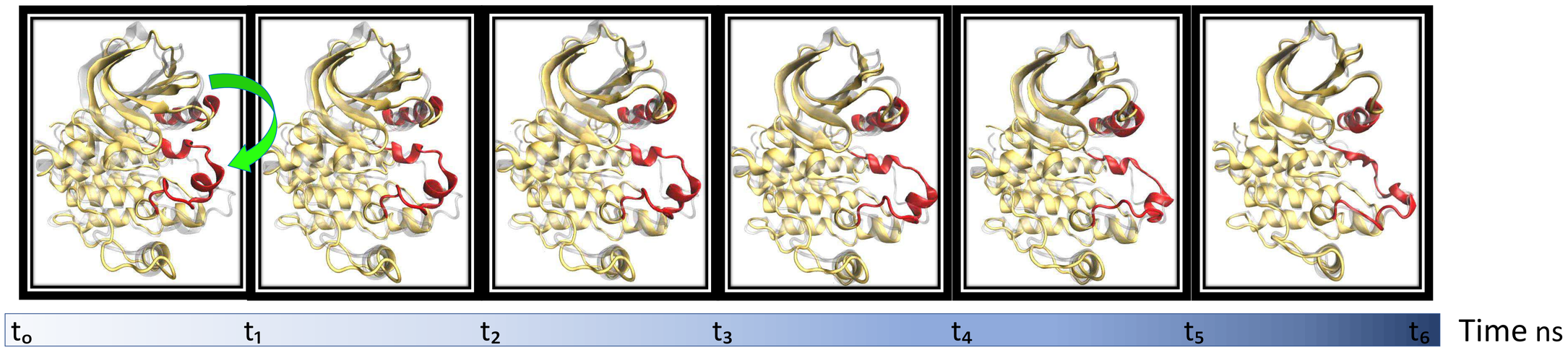
J.Alba [1*], V. D'Annibale[1], M. D'Abramo[1*]

1 Dep. of Chemistry, Sapienza University of Rome

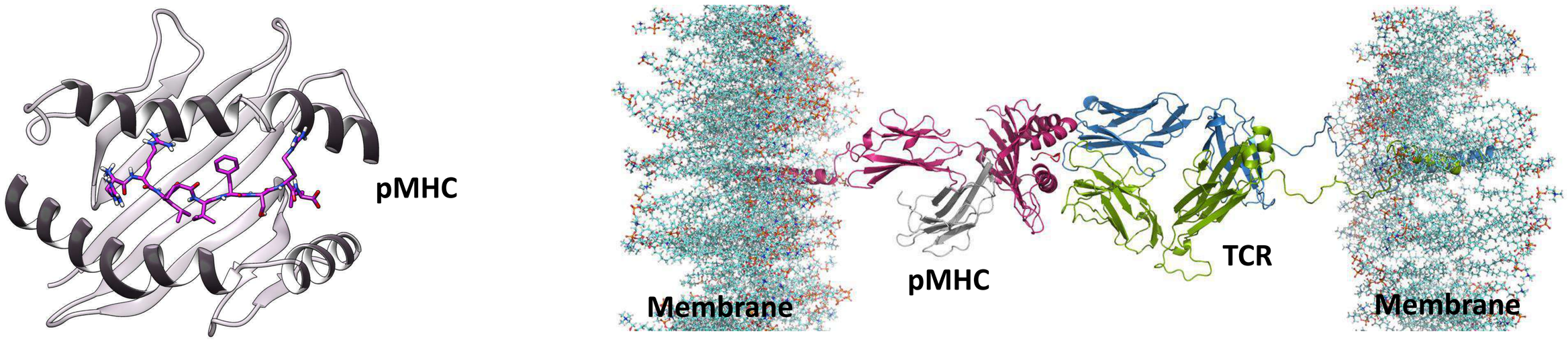
*email: josephine.alba@uniroma1.it, marco.dabramo@uniroma1.it

Molecular Dynamics Simulation

Integrating the Newton's second law, it is possible to follow the protein dynamics to characterize the conformational space sampled by such kind of systems. Such a method is useful to predict, among others, protein-protein and drug-protein interactions.



Using high performance computing, it is also possible to simulate a protein in its natural environment, i.e. in membranes.



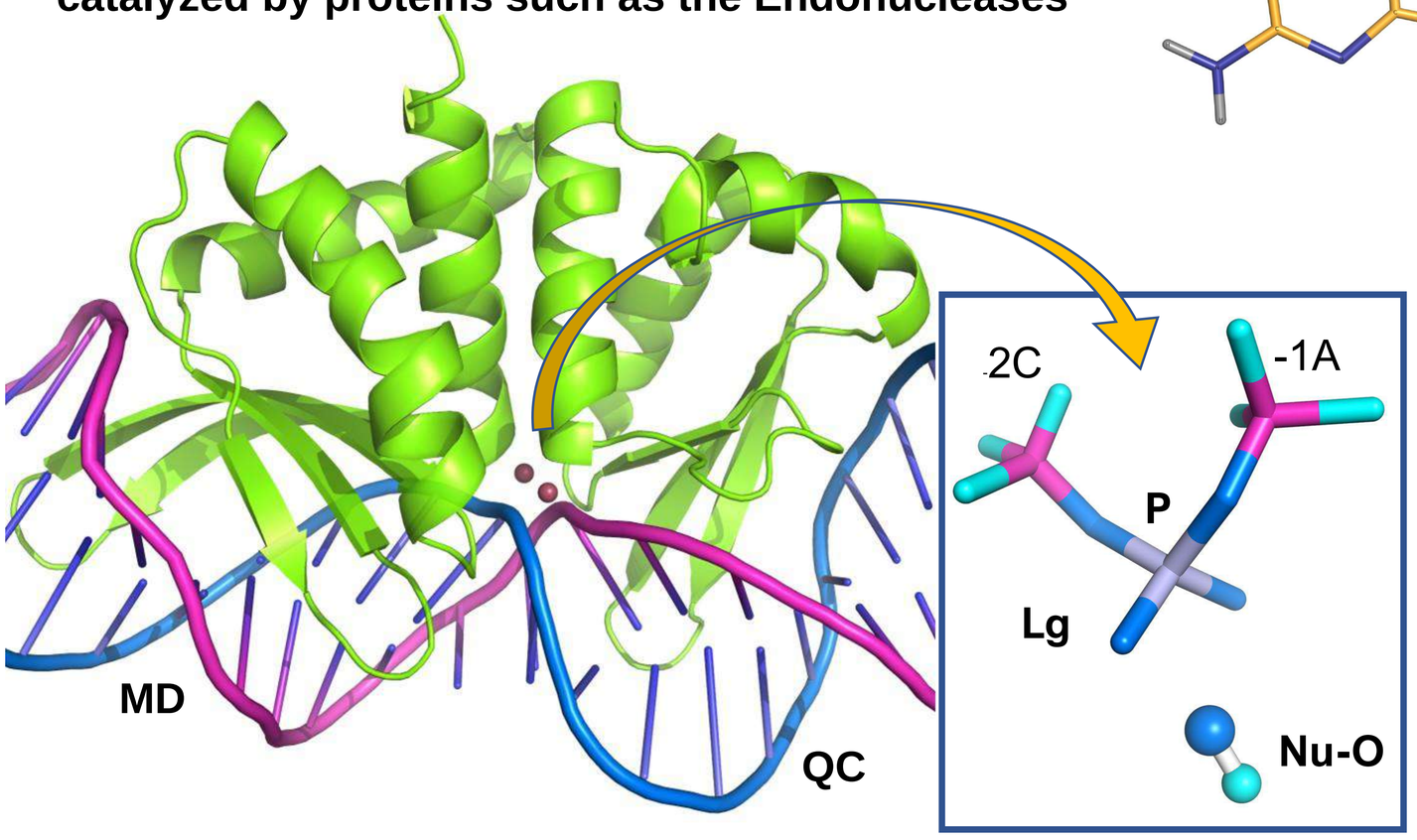
In a current resereach, we simulated the pMHC/TCR complex, a fundamental system in immunology.

Quantum Mechanics/Molecular Dynamics

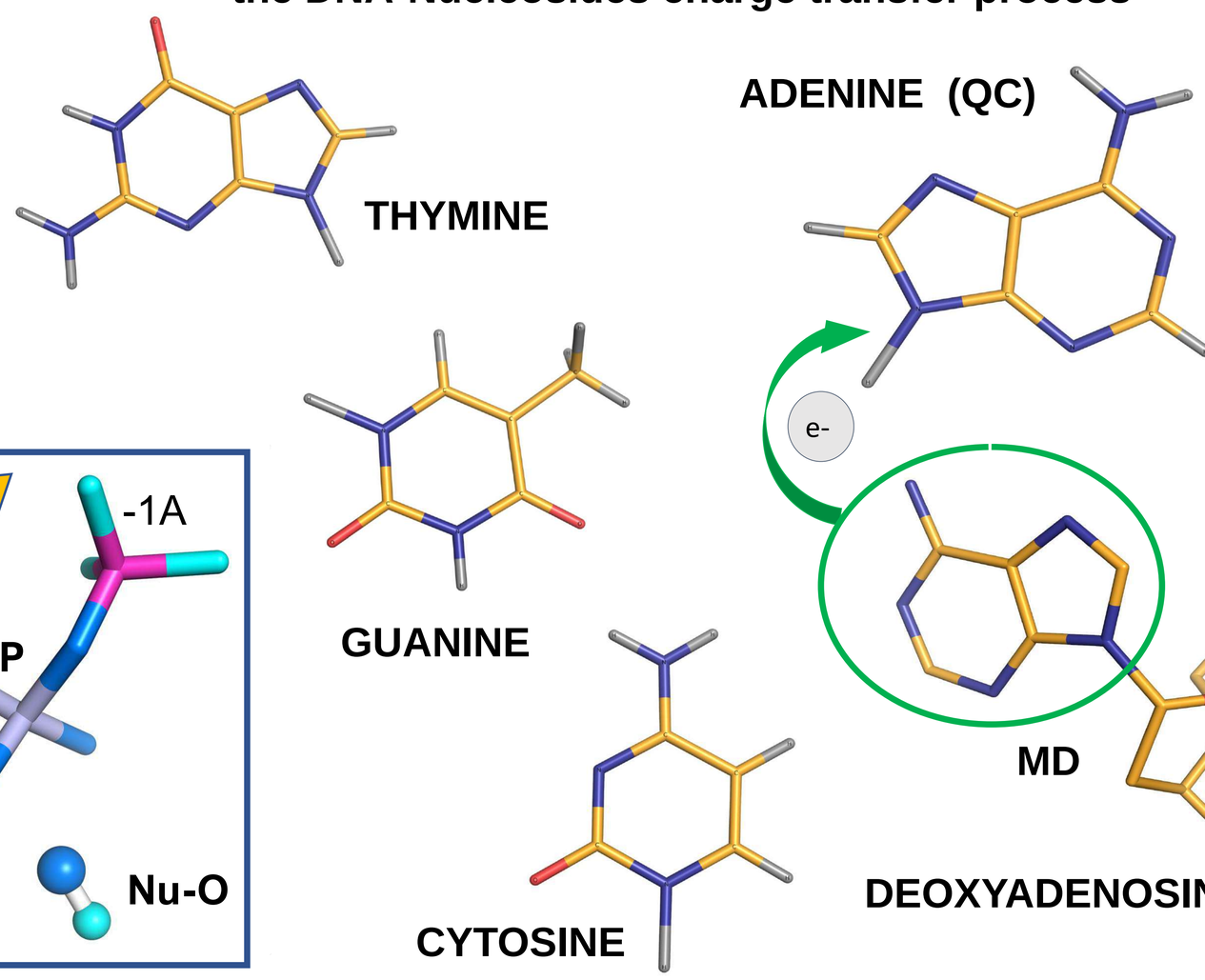
Combining quantum mechanical calculations and molecular dynamics simulations using advanced molecular theories, it is possible to model the perturbed electronic properties of systems in complex environments. Such an approach is able to provide the perturbed electronic-related observables, such as energies, electronic and magnetic dipole moments. By such an approach, we are studying:

the DNA cleavage

catalyzed by proteins such as the Endonucleases



the DNA-Nucleosides charge transfer process



References

[1] L. Zanetti-Polzi et al., (2018) Phys. Chem. Chem. Phys., DOI:10.1039/C8CP04190C.

[2] J. Alba, J, et al., (2017) Journal of Computer-Aided Molecular Design. DOI: https://doi.org/10.1007/s10822-017-0087-5

[3] V. Tedeschi J. Alba, et al., (2019) Cells, 8(6), 572; https://doi.org/10.3390/cells8060572

Rivelatori di posizione per applicazioni alla chirurgia Radioguidata con emettitori β-

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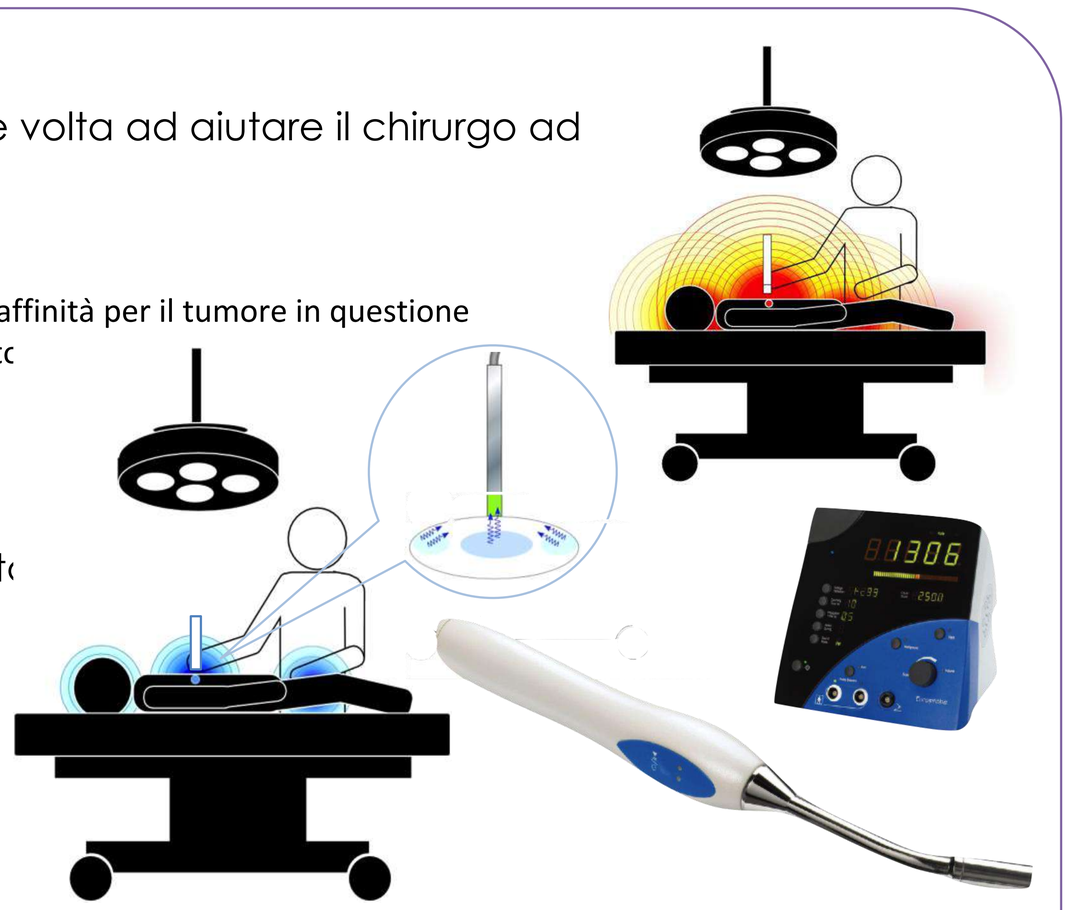
F. Collamati, V. Bocci, M. De Simoni, R. Faccini, M. Fischetti,
C. Mancini-Terracciano, R. Mirabelli, E. Solfaroli-Camillocci, S. Morganti
Dipartimento di Fisica - Email: riccardo.faccini@roma1.infn.it

CHIRURGIA RADIO GUIDATA

La chirurgia radioguidata (RGS) è una tecnica di medicina nucleare volta ad aiutare il chirurgo ad ottenere una più precisa e completa asportazione dei tumori:

➞ Ridotto rischio di recidive
➞ Riduzione dei sintomi

Al paziente viene iniettato prima dell'operazione un radiofarmaco che presenti particolare affinità per il tumore in questione
La radiazione emessa viene rivelata localmente dal chirurgo grazie ad un apposito strumento



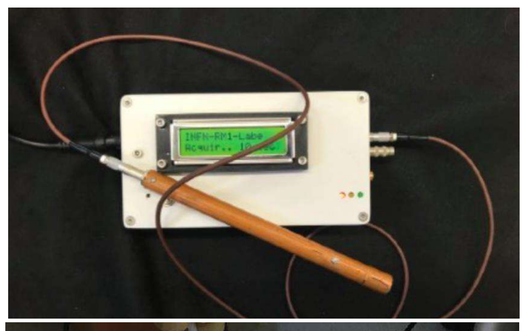
PROPOSTA INNOVATIVA

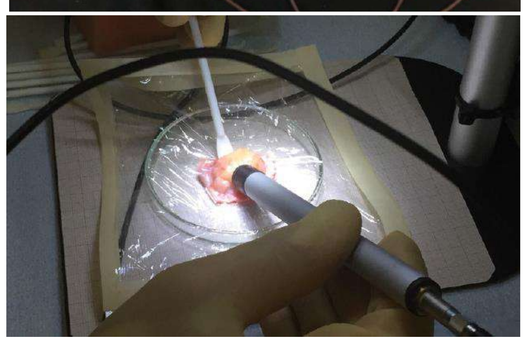
La RGS è oggi praticata usando isotopi che emettono fotoni **γ**
Circa 1/3 dei fotoni del ^{99}Tc attraversano più di 8 cm di tessuto
➞ Al rivelatore arriveranno anche fotoni emessi dagli organi sani lontani
➞Dose al personale
➞Rivelatore "ingombrante" per rivelare i fotoni

Tutti questi problemi sarebbero risolti usando isotopi emettitori **β-**
Elettroni di ~1MeV percorrono pochi mm nel tessuto umano
➞ minore contaminazione da fondo sano
➞ minore dose al personale
➞ Rivelatore compatto

STATO ATTUALE

La β- RGS è stata validata utilizzando radio farmaci contenendo ^{90}Y (E_e=2.2 MeV) e un rivelatore basato su scintillatore organico [1]





Nonostante la buona sensibilità dimostrata [2], questo tipo di rivelatore è sostanzialmente cieco agli elettroni sotto i 400 keV
➞ Ridotta efficienza a 90Y
➞ Impossibile applicazione a vari radio farmaci molto diffusi [3]

POSSIBILE SVILUPPO: RIVELATORE CMOS

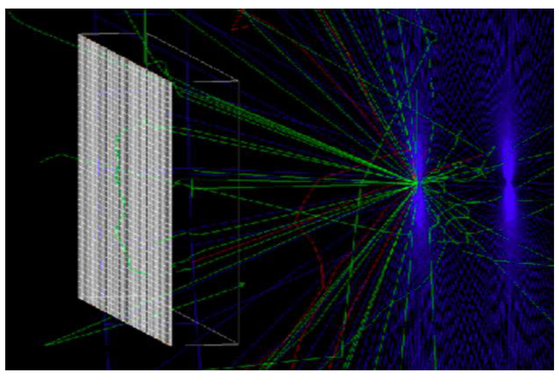
Un nuovo rivelatore è in fase di sviluppo, basato su un sensore CMOS commerciale [4]
Anche se originariamente pensato come fotocamera, risulta sensibile anche alle particelle beta di bassa energia, restando sostanzialmente trasparente ai **γ** > 100KeV

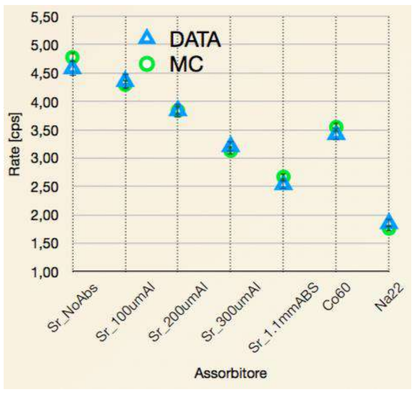
Modello	MT9V115 - OnSemi
Dimensione package	2.7x2.7 mm^2
Risoluzione	648x488=316'224 px
Dimensione pixel	1.75 um
Range dinamico	1024 ADC



SIMULAZIONE MONTECARLO

Una simulazione Monte Carlo completa è stata sviluppata in Geant4
➞ Tutti i 316k pixels
➞Processi fisici rilevanti
➞Varie sorgenti
➞Vari spessori
➞Simulata lettura CMOS





PROSPETTIVE MULTIDISCIPLINARI

1.Lo sviluppo di un rivelatore basato su sensore CMOS commerciale **estenderebbe il campo di applicazione della tecnica** ad una ampia classe di radiofarmaci con emissioni di elettroni con energie <500 keV, molto usati nella pratica clinica (18F, **β+**, E=500 keV, 68Ga, **β+**, E=1900 keV)
2. Per aumentare il numero di casi applicativi sono in corso di studio **nuovi radiofarmaci**. I primi test su cavie sono previsti per i prossimi mesi.
3.Dopo aver testato la tecnica su casi "ex-vivo", è in corso di perfezionamento una nuova sonda laparoscopica per estendere i test su pazienti ("**in-vivo**").

[1]E. Solfaroli Camillocci et al., *A novel radioguided surgery technique exploiting beta- decays* (2014) Scientific Reports, 4, art. no. 4401
[2]E. Solfaroli Camillocci et al., *First ex vivo validation of a radioguided surgery technique with β−radiation (*2016) Phys. Med. 32(9) 1139–1144
[3]C. Mancini Terracciano et al., *Feasibility of the **β**−Radio-Guided Surgery with a Variety of Radio-Nuclides of Interest to Nuclear Medicine* (2017) Physica Medica 43
[4]L. A. Solestizi et al., *Use of a CMOS image sensor for beta-emitting radionuclide measurements* (2018) JINST, 1

DIPARTIMENTO
DI BIOLOGIA AMBIENTALE

SAPIENZA
UNIVERSITÀ DI ROMA

Pollen studies in Archaeometry

Michelangeli F., Chassouant L., Fundurulić A., Paladugu R., Celant A., Di Rita F., Magri D.
Dipartimento di Biologia Ambientale, Edificio di Botanica (CU 022) piano 3°, laboratorio 307
Email: fabrizio.michelangeli@uniroma1.it

The Laboratory of Palaeobotany and Palynology, directed by Prof. Donatella Magri, participates in international projects in different aspects of Archaeometry. Spanning from Cultural Heritage to biological background, the lab is nevertheless unified by a common interest on pollen analysis. Through this multidisciplinary approach and in co-operation with geologists, sedimentologists, paleontologists, ecologists, archaeologists and genetists, our aim is to shed new light on vegetation history, in relation to dynamics of human communities and climate.

The analytical infrastructure consists of:

- Sterile palynological laboratory
- 4 transmitted light microscopes Zeiss
- 2 stereomicroscopes Zeiss
- 1 microscope Zeiss Axiolab 5 stand, Mat-TL/RL, DIC
- SEM Hitachi TM3000
- Hirox 3D Microscope

ERC panels:
SH6_2 Archaeology, archaeometry, landscape archaeology
PE10_6 Paleoclimatology, paleoecology
LS8_2 Population biology, population dynamics, population genetics, plant-animal interactions



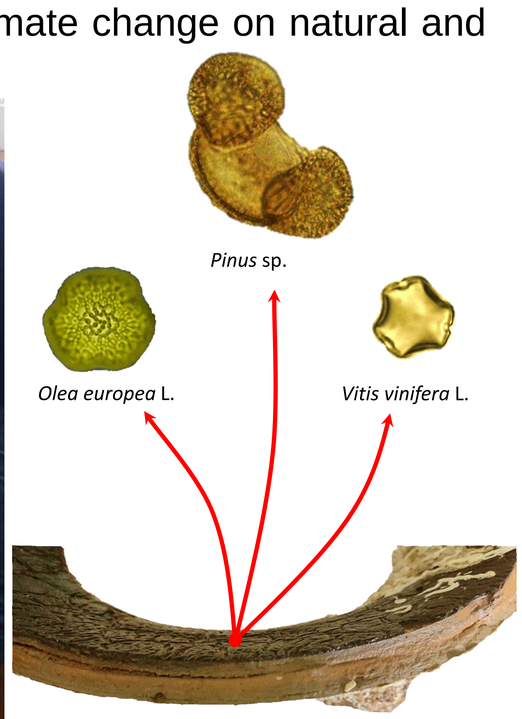


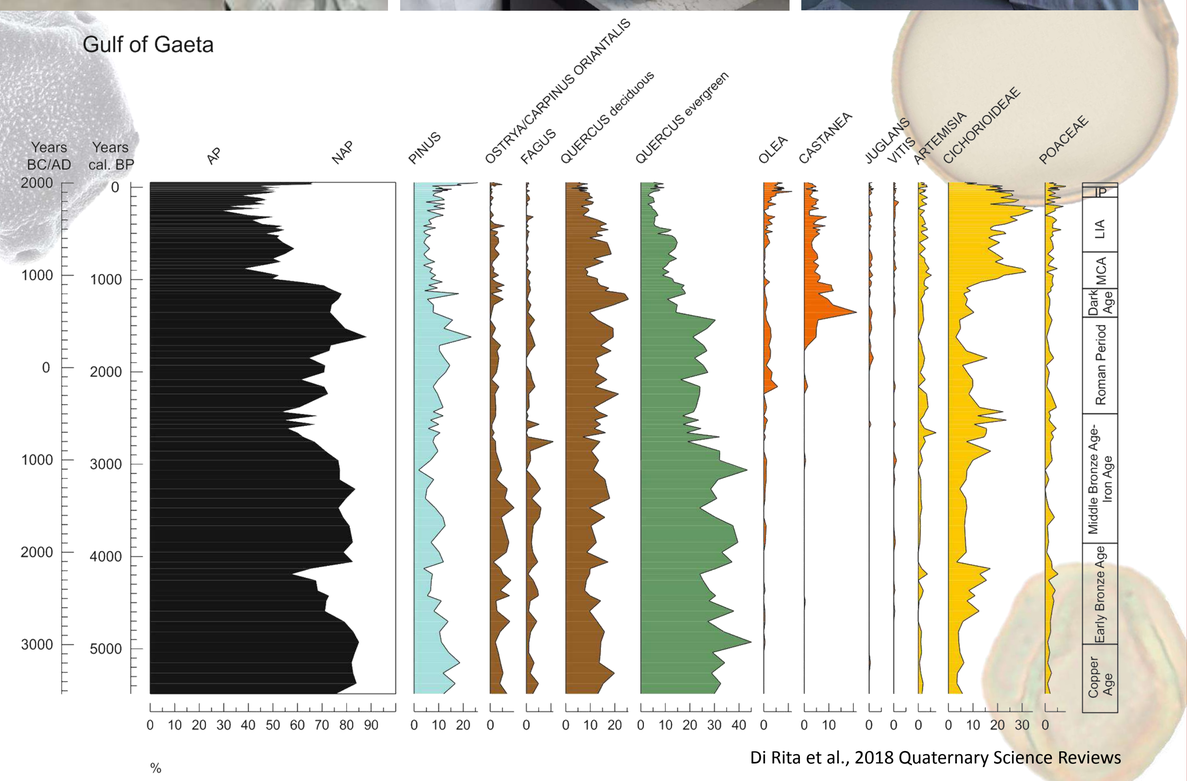


Gulf of Gaeta

Through pollen analysis, we reconstruct palaeoenvironmental conditions in relation to human activity at different time scales. This includes clearance of forest vegetation, pastoral activities, fire events, trade of plants, onset of cultivation and other practices of land use (e.g. salt-works). Pollen analysis provides also information on the effects of climate change on natural and anthropogenic landscapes.







Di Rita et al., 2018 Quaternary Science Reviews

Application of palynological investigations to burial sediments and archaeological resinous materials provides information about plant taxa used in food offerings, balms, ornamental and ritual habits, as well as on environmental conditions in the surrounding area. This information complements chemical analyses of organic residues and other contextual and analytical information, to gain a well-rounded picture of the funerary contexts and ritual cultures of ancient societies.

Palaeobotanical investigations may unravel the history of Cultural Heritage artefacts. One striking example would be deciphering of the content and ancient usage of *amphorae* under pollen identification. Indeed, *Vitis vinifera* L. or *Olea europaea* L. could target the historical presence of wine or olive oil respectively, their provenance and storage practices.





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- Wales N., Madrigal J.R., Cappellini E., Baez A.C., Samaniego Castruita J.A., Romero-Navarro J.A., Carøe C., Ávila-Arcos M.C., Peñaloza F., Moreno-Mayar J.V., Gasparyan B., Zardaryan D., Bagoyan T., Smith A., Pinhasi R., Bosi G., Fiorentino G., Grasso A.M., Celant A., Bar-Oz G., Tepper Y., Hall A., Scalabrin S., Miculan M., Morgante M., Di Gaspero G., Gilbert M.T.P. (2016) The limits and potential of paleogenomic techniques for reconstructing grapevine domestication. *Journal of Archaeological Science* 72, 57-70.

BIOCRYSTAL FACILITY

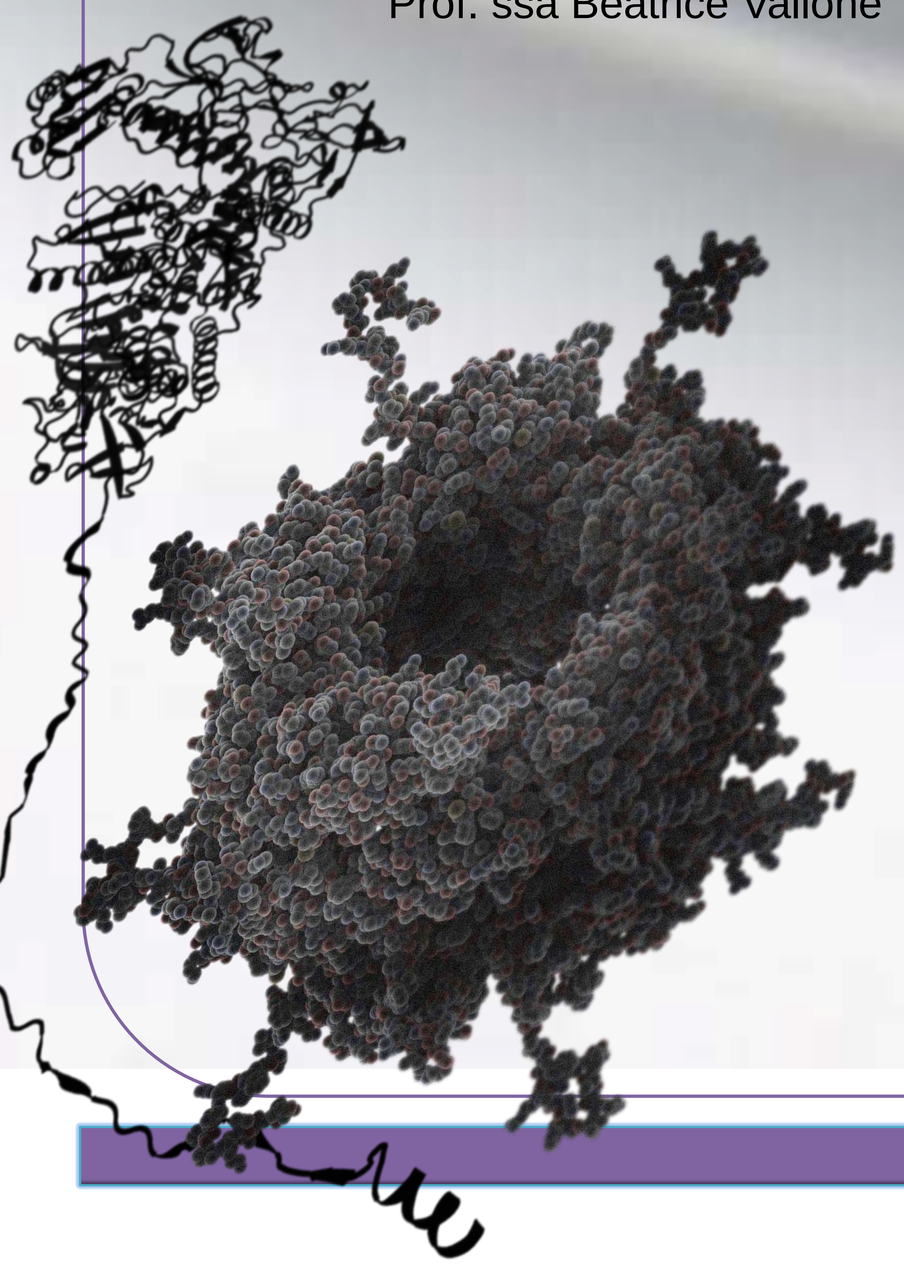
A. Di Matteo[a*], C. Savino[a], G. Colotti[a], V. Morea[a], G.Boumis[b], G. Giardina, A. Boffi[a,b], P. Baiocco, A. Fiorillo[b], L. Montemiglio[b], B. Vallone[a,b], A. Ilari[a].

[a]Istituto di Biologia e Patologia Molecolari, CNR-Roma; [b]Dipartimento di Scienze Biochimiche, "Sapienza" Università di Roma

Thanks to significant advances in the field of synchrotron light sources, expression of recombinant proteins and automation for protein crystal growth of, it is within the reach of molecular biologists. However, access to these technologies and to large international facilities is not fully exploited by the Italian scientific community.
It is therefore of essential to implement a connection between large international facilities and the Italian scientific community, in order to increase their use by life sciences researchers. These connecting structures shall provide support to users throughout the process of structure determination (choice of the construct, protein production, crystallization, data collection and analysis). In this context, it has been activated a BioCrystal, a biocrystallography facility that offers the access to production and interpretation of crystals of biological macromolecules.

The facility is based on practical and theoretical consultancy at critical steps of protein crystallography:

Staff
Dr. ssa Baiocco Paola
Prof. Alberto Boffi
Dott.ssa Giovanna Boumis
Dott. Gianni Colotti
Dott.ssa Adele Di Matteo
Dott.ssa Annarita Fiorillo
Dr. Giorgio Giardina
Dott. Andrea Ilari
Dott.ssa Linda Montemiglio
Dott.ssa Veronica Morea
Dott.ssa Carmelinda Savino
Prof. ssa Beatrice Vallone





• Setting the biomedical or biotechnological project in the context of structural biology: defining objectives and critical points.



•Consulting in the production and purification of proteins.



• Crystallization screening using robot, their analysis and optimization initially with our in-house equipment and then supporting the application to European initiatives.



• Collection of Diffraction data at synchrotron radiation

Contact:
www.biocrystalfacility.it
info@biocrystalfacility.it
Tel.: +39 06 49690276

Ambiente e Territorio

Imaging nell'infrarosso lontano per la sicurezza delle infrastrutture stradali e ferroviarie e per la diagnostica dermatologica

Leonetta Baldassarre[1], Paolo Mazzanti[2], Aldo Fiori[3], Francesco Pacillo[4], Alessandro Brunetti[5], Alfonso Tanga[1,6], Francesco Vitucci[6], Valeria Giliberti[7], Michele Ortolani[1,7]

[1]*Dipartimento di Fisica, Sapienza Univ. di Roma*
[2]*Dipartimento di Scienze della Terra, Sapienza Univ. di Roma*
[3]*Dipartimento di Ingegneria, Univ. Roma Tre*
[4]*Crisel s.r.l. soluzioni ad alto contenuto tecnologico*
[5]*Nhazca s.r.l. natural hazard control and assessment*
[6]*Crisel Instruments s.r.l. soluzioni per ricerca scientifica e industria*
[7]*Istituto Italiano di Tecnologia – Center for Life Nanoscience*

L'imaging nell'infrarosso termico è una tecnologia ben sviluppata e correntemente utilizzata nei sistemi di sicurezza e sorveglianza, nelle scienze ambientali ed agrarie, nell'analisi delle opere d'arte e nel controllo dei processi industriali. Tuttavia pochi utilizzatori conoscono il meccanismo fisico di emissione termica della radiazione, che dipende dalla funzione dielettrica e non solo dalla temperatura del corpo.

I recenti sviluppi dei sensori a stato solido nano-fabbricati permettono l'allargamento delle bande misurabili nell'infrarosso lontano, spesso detto "terahertz", dove l'imaging può essere effettuato anche con tecnologie elettroniche (radar). Le proprietà di riflessione e diffusione della radiazione nell'infrarosso lontano sono totalmente diverse da quelle della luce visibile.

Presentiamo due esempi di progetti regionali ancora in corso in cui, basandoci sulle leggi di fisica di base della termodinamica e della fisica dello stato solido, abbiamo allargato la banda di frequenze, ottenendo risultati innovativi nel campo biomedico e nel campo del monitoraggio delle infrastrutture ferroviarie.

Il metodo: imaging nel lontano infrarosso

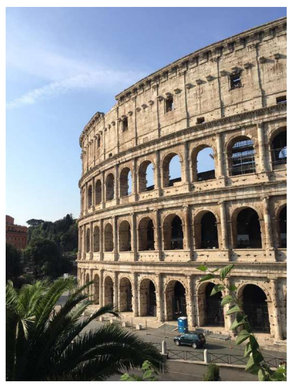
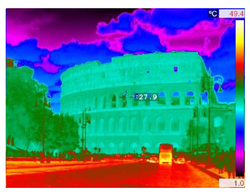
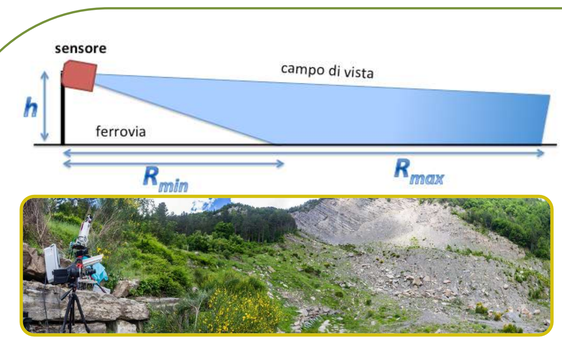




Immagine in falsi colori da telecamera commerciale in cui viene dichiarata una "temperatura"



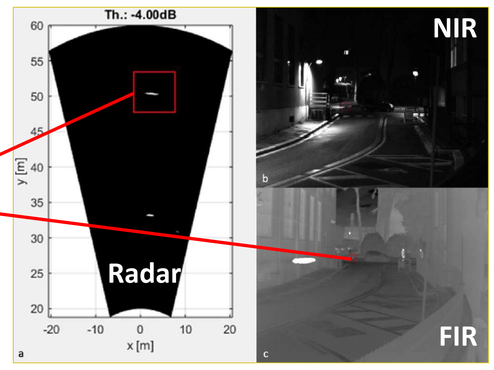
Il contrasto delle immagini con luce solare visibile sono basate su effetti di ombra e diffusione che non esistono nell'infrarosso lontano (far-infrared, FIR, lunghezze d'onda maggiori di 8micrometri). Il FIR penetra quindi nebbia, pioggia, polvere.
Il FIR può essere emesso dagli oggetti stessi, che diventano la sorgente (esempio: imaging termico di edifici).
Il FIR può essere anche prodotto da un generatore (Radar o Laser) ed essere riflesso in maniera speculare anche da superfici rugose ed opache (esempio: pelle umana, rocce)





Risultati:
Immagini radar e infrarosse di un *corner reflector* prese alla Sapienza e nel sito di una frana





Interdisciplinarità:
Ai test in laboratorio alla Sapienza hanno partecipato: *informatici, ingegneri elettronici, geologi, ingegneri idraulici, fisici, matematici*.

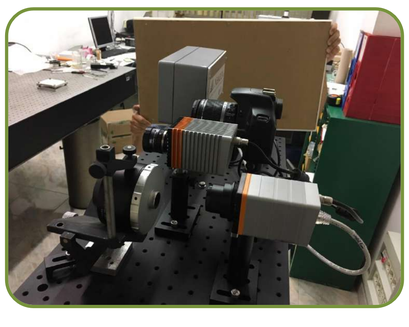
MARIIS Progetto cofinanziato dall'Unione Europea

Monitoraggio di infrastrutture ferroviarie e stradali critiche in qualunque condizione meteo

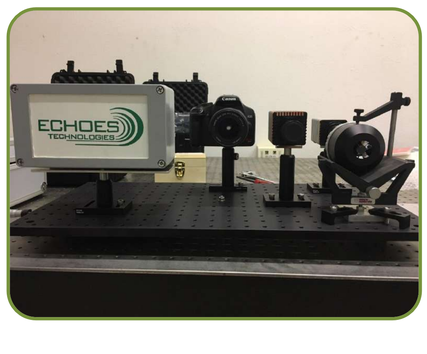
Dipartimento di Scienze della Terra
SAPIENZA UNIVERSITÀ DI ROMA

Dipartimento di Fisica
SAPIENZA UNIVERSITÀ DI ROMA

Strumentazione acquistata e disponibile su richiesta



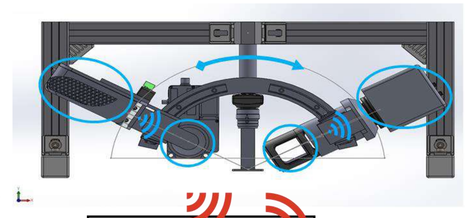
- Termocamera Xenics Gobi (medio infrarosso)
- InGaAs camera Xenics Bobcat (vicino infrarosso)
- RGB camera Canon (visibile)
- Radar Echoes a 24 GHz (MW)
- Terahertz camera i2s (THz)
- Sorgente Lytid a 0.6 THz

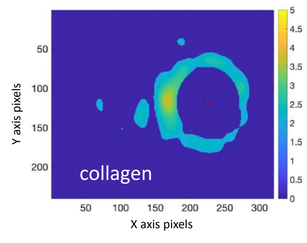


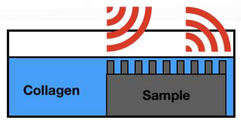
PROGETTO MICoTeD
Progetto cofinanziato dall'Unione Europea

Progettazione e Sviluppo di un nuovo Microscopio Terahertz in riflessione radente per la Diagnostica dermatologica di anomalie sotto pelle

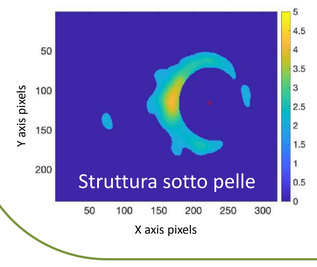
Risultati: dischi di Airy deformati da strutture sotto pelle.

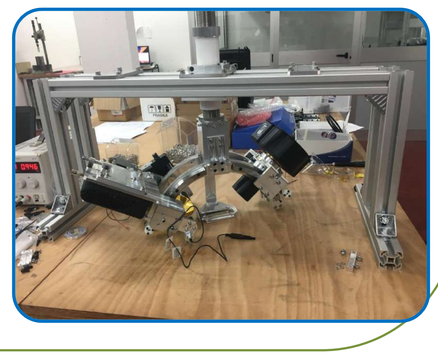






ν=0.6 THz
λ=0.5mm





Un approccio multi-disciplinare per combattere l'antibiotico-resistenza

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Introduzione: L'antibiotico-resistenza (ABR) è una delle maggiori sfide per la salute a livello globale. Riteniamo che questa coinvolga non solo la medicina e la microbiologia clinica, ma anche la biologia molecolare e la bioinformatica.
La complessità e l'estensione di tale problema richiedono l'implementazione di nuovi metodi di ricerca, con l'indicazione a trovare nuove forme di collaborazione per valutare l'efficacia delle pratiche di sorveglianza, fondamentali per contenere il problema dell'ABR, per identificarne i determinanti genetici, descriverne le dinamiche di trasmissione e di infezione, le caratteristiche epidemiologiche e l'impatto sulla scelta ed il consumo di antibiotici.
È stata quindi creata una rete di competenze per studiare l'ABR in generale ed in particolare le Enterobacteriaceae Resistenti ai Carbapenemi (CRE), un antibiotico di ultima scelta.

I **settori ERC** interessati da questa collaborazione sono **LS2_10** (Bioinformatica), **LS6_9** (Batteriologia) e **LS6_11** (Prevenzione e trattamento delle malattie infettive).
L'approccio di partenza è di tipo microbiologico e viene svolto nel laboratorio della Unità di Microbiologia e Virologia dell'AOU "Policlinico Umberto I" della Sapienza, dove attraverso tecniche come la spettrometria di massa mediante sistema MALDI-TOF e test di suscettibilità agli antibiotici vengono caratterizzati gli isolati CRE. L'analisi genomica è invece svolta presso il Dipartimento di Biologia Ambientale mediante MinION della Oxford Nanopore Technologies. Quest'ultima analisi è fondamentale per fornire un'immagine più ampia sull'origine e sulla diffusione dei geni di resistenza tra tali batteri.

Risultati: Questa collaborazione ha permesso di definire in modo accurato l'epidemiologia all'interno del "Policlinico Umberto I " di una specifica forma di resistenza ai carbapenemi.
La partecipazione congiunta della microbiologia, che si è occupata dell'isolamento delle specie batteriche resistenti, con la bioinformatica, dedita al sequenziamento completo dei batteri e dei loro plasmidi tramite MinION e la conseguente analisi delle sequenze genomiche, ha fornito indicazioni fondamentali sulla diffusione di tale resistenza a livello ospedaliero.

Conclusioni e prospettive future: Dal punto di vista di salute pubblica, la collaborazione e l'istituzione di questa rete di competenze ha permesso di accertare l'introduzione ha permesso di accertare l'introduzione di una nuova forma di CRE nell'ambito dei patogeni circolanti all'interno di un grande ospedale, ed di indentificare nuovi meccanismi di resistenza batterica anche nei confronti di molecole di ultima generazione.
L'applicazione della genomica alla microbiologia tradizionale offre quindi grandi possibilità per contrastare il fenomeno della ABR, soprattutto grazie alla possibilità di avere un accesso più rapido e dettagliato ai meccanismi molecolari che sottendono alla resistenza agli antibiotici.

Applying Rapid Whole-Genome Sequencing To Predict Phenotypic Antimicrobial Susceptibility Testing Results among Carbapenem-Resistant Klebsiella pneumoniae Clinical Isolates. (2018)
Tamma PD, Fan Y, Bergman Y, Pertea G, Kazmi AQ, Lewis S, Carroll KC, Schatz MC, Timp W, Simner PJ.

Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

Sviluppo di nuovi metodi analitici in ambito forense e clinico tramite LC-MS/MS

Camilla Montesano*, Flaminia Vincenti, Ilaria Serafini, Alessandro Ciccola, Roberta Curini
Dipartimento di Chimica, Edificio Cannizzazo, Laboratorio 062
Email: camilla.montesano@uniroma1.it

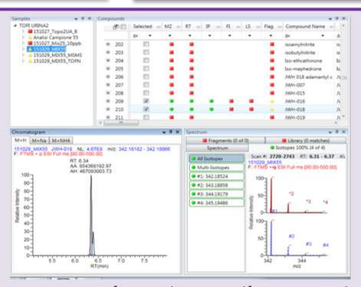
Il gruppo di ricerca guidato dalla Prof.ssa Curini, segue varie linee di ricerca nell'ambito della chimica analitica, con particolare riferimento allo sviluppo di metodologie innovative utilizzando come tecnica di riferimento la cromatografia liquida accoppiata alla spettrometria di massa tandem (LC-MS/MS). Il laboratorio è attualmente equipaggiato con tre strumenti a triplo quadrupolo e a breve verrà acquisita una nuova strumentazione dotata della tecnologia di mobilità ionica. Le principali linee di ricerca comprendono la tossicologia forense e lo studio di biomarcatori in ambito clinico. Di particolare interesse sono le metodologie per l'estrazione di sostanze d'abuso dalla matrice pilifera, lo sviluppo di metodi di screening per il riconoscimento di nuove sostanze psicoattive e lo studio del metabolismo in-vitro di nuove droghe. Il gruppo di ricerca si avvale della collaborazione con il Reparto Investigazioni Scientifiche (RIS-Roma).

SCREENING E IDENTIFICAZIONE DI NPS NEL PLASMA[1]



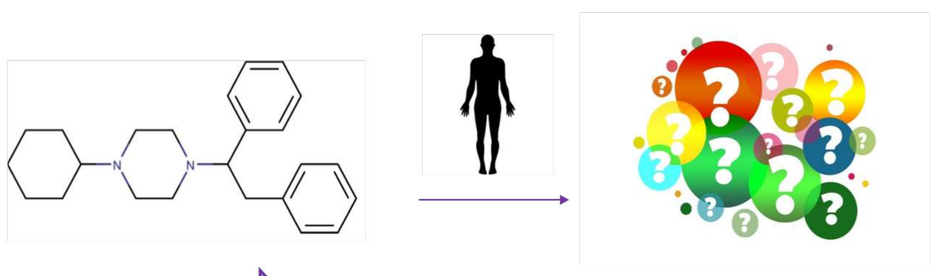
SCREENING POST-ANALYSIS

- Screening post-run e confronto in libreria con un database interno contenente oltre 300 NPS e metaboliti noti (Tracefinder Forensic).
- **Composizione Elementare** (formula molecolare)
  - ✓ **Massa Accurata**
  - ✓ **Tr** (se disponibile)
  - ✓ Massa esatta dei **Frammenti** (se disponibile)

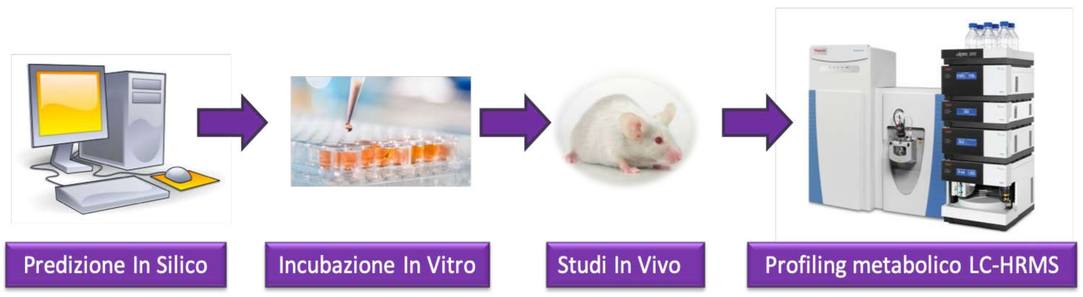


⇨ La libreria interna è dinamica e può essere aggiornata continuamente

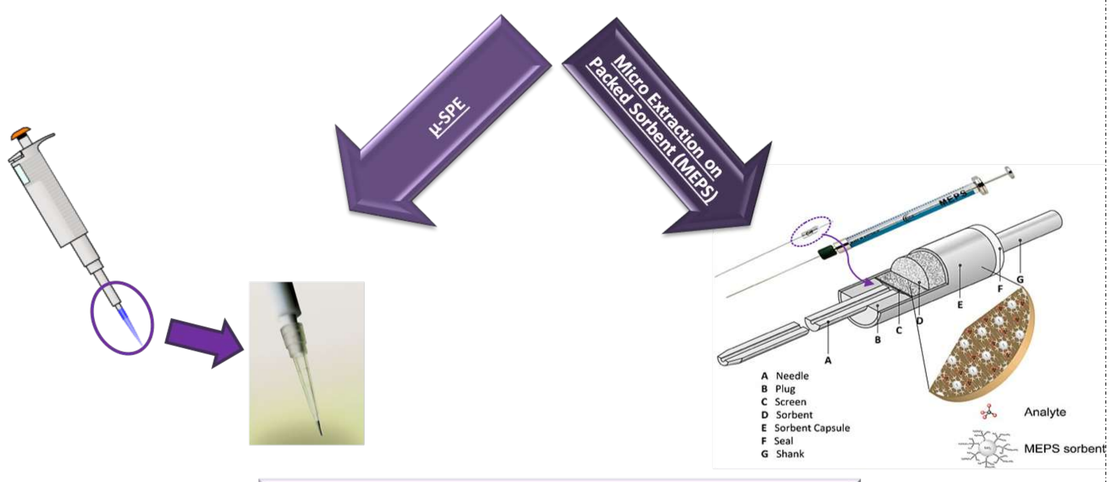
IDENTIFICAZIONE DEI METABOLITI DELLE NPS: MT-45[2]



⇨ Identification of Biomarkers of consumption



MINIATURIZZAZIONE DELLE TECNICHE ESTRATTIVE[3,4]

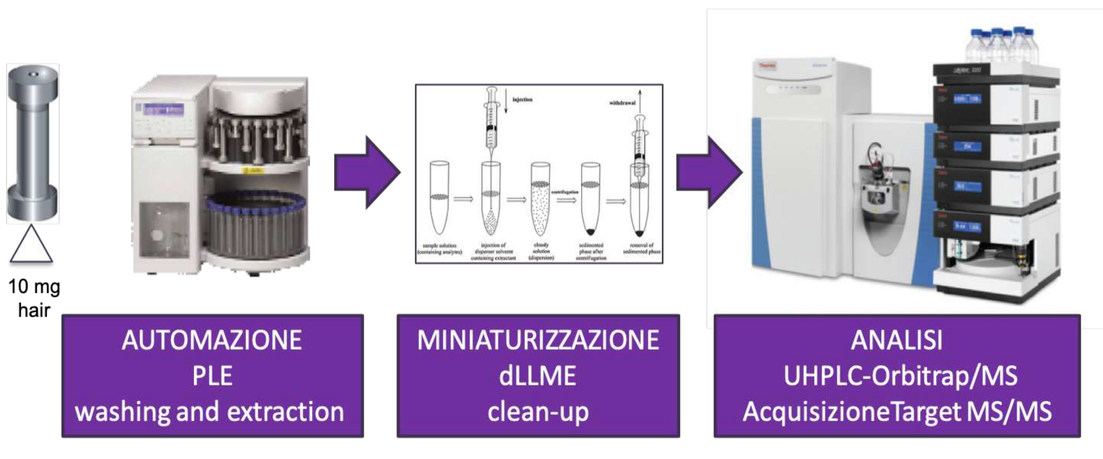


- ✓ Pochi mg di fasi stazionarie
- ✓ Riduzione del volume di campione necessario (10-100 µL)
- ✓ Riduzione del volume di solventi organici impiegati

➢ Applicazione all'estrazione di droghe d'abuso da matrici biologiche

▪ Sangue intero ▪ Plasma ▪ Urina ▪ Fluidi orali

ESTRAZIONE DI SOSTANZE D'ABUSO DALLA MATRICE PILIFERA[5]



- ✓ Estrazione simultanea di oltre 60 sostanze stupefacenti appartenenti a differenti classi chimiche e chimico-fisiche
- ✓ **Automazione:** la PLE consente il lavaggio del campione e l'estrazione degli analiti in meno di 20 minuti
- ✓ **Riduzione del volume di solventi organici necessari:** l'estrazione degli analiti avviene con circa 5 mL
- ✓ **Fattore di arrichhimento:** la dLLME consente un fattore di arricchimento di oltre 50 voltre
- ✓ **Rapidità:** l'analisi quali-quantitativa LC-MS viene completata in 13 minuti

Data la competenza del gruppo di ricerca nel trattare le matrici biologiche, e nell'analisi effettuata con tecnica HPLC-HRMS(/MS) le metodiche presentate possono essere estese ad altri tipi di analiti e quindi ad altri campi di applicazione come ad esempio il campo clinico o il settore biomedico.

[1] C. Montesano et al., Broad Screening and Identification of NPS in Plasma by UHPLC-HRMS and Post-run Library Matching, Anal Toxicol (2016) 40: 516-528
[2] C. Montesano et al., Identification of MT-45 Metabolites: In Silico Prediction, In Vitro Incubation with Rat Hepatocytes and In Vivo Confirmation, Anal Toxicol (2017) 1-10
[3] C. Montesano et al, Application of a rapid µ-SPE clean-up for multiclass quantitative analysis of sixteen new psychoactive substances in whole blood by LC–MS/MS Talanta (2017) 167:260-267
[4] C. Montesano et al. Determination of illicit drugs and metabolites in oral fluid by MEPS coupled with LC-MS/MS, Anal Bioanal Chem (2015) 407: 3647-3658
[5] F. Vincenti et al. Combination of Pressurized Liquid Extraction with dispersive Liquid-Liquid Micro Extraction for the determination of sixty drugs of abuse in hair, J. Chromatogr. A (2019) – *In press*

Agro Alimentare

Dipartimento di Chimica
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Metabolomica basata su spettroscopia NMR in AGRIFOOD

**Fabio Sciubba*, Giorgio Capuani, Maria Enrica Di Cocco,
Alberta Tomassini, Giorgia Conta, Ottavia Giampaoli, Alfredo Miccheli**
Dipartimento di Chimica, Edificio Cannizzaro, CU014, piano II stanza 247
Email: fabio.sciubba@uniroma1.it

Attività del gruppo di Ricerca nella tematica presentata

L'attività del gruppo di ricerca nel campo Agrifood è focalizzata alla caratterizzazione, miglioramento e valorizzazione di prodotti alimentari sia di origine vegetale che animale, come ad esempio il latte. L'attività si esplica principalmente mediante Spettroscopia di Risonanza Magnetica Nucleare (RMN) ad alta risoluzione per la definizione del profilo metabolico dell'alimento in termini di micronutrienti di basso peso molecolare, da mettere in relazione alle condizioni pedoclimatiche, geografiche, agronomiche, microbiologiche del terreno, come pure, nel caso di prodotti caseari, all'influenza della composizione della dieta dell'animale. La ricerca in campo AGRIFOOD prende in esame anche aspetti nutrizionali riguardanti la identificazione di biomarcatori di assunzione dell'alimento specifico e l'effetto delle molecole bioattive in essi contenute.
L'attività di ricerca si esplica attraverso collaborazioni con Aziende Agricole (Aureli Mario, Ortucchio , AQ), Aziende Agro-alimentari (Birra del Borgo, RI), (Valagro, Atessa, PE); (Medicina Veterinaria, UNIMI, Milano) Tale attività rientra nella categoria ERC delle Life Sciences, e nello specifico LS2_4 (Metabolomics) e LS9_6 (Food Sciences). Lo svolgimento di tale attività richiede competenze multidisciplinari nei settori della Chimica, della Botanica, nelle Biotecnologie Vegetali e Microbiche.

Strumentazioni e metodologie



Il gruppo di ricerca fa parte del NMR-based Metabolomics Laboratory of Sapienza, che è costituito dalla partecipazione multidisciplinare di 6 Dipartimenti dell'Università Sapienza di Roma (Dipartimento di Biologia e Biotecnologie "Charles Darwin", Dipartimento di Biologia Vegetale, Dipartimento di Chimica, Dipartimento di Chimica e Tecnologie del Farmaco, Dipartimento di Fisiologia e Farmacologia "Vittorio Erspamer" e Dipartimento di Medicina Sperimentale coordinati dal prof. Alfredo Miccheli). Il laboratorio dispone di strumentazione RMN ad alto campo, JEOL 600 ECZ (dotato di campionatore automatico e cryoprobe) e 400 Bruker Avance 3, e laboratori di preparazione di campioni biologici vegetali ed animali. Il gruppo di ricerca utilizza metodiche di analisi multivariata per poter classificare e discriminare le miscele in esame e identificare i biomarcatori caratteristici di funzione, assunzione ed effetto. L'analisi metabolomica mediante NMR permette di determinare quali-quantitativamente metaboliti di basso peso molecolare sia idrosolubili che liposolubili.

Esempi di attività pregressa e in corso

1) Valutazione dell'influenza delle condizioni pedoclimatiche sulla qualità del succo di carota

Succhi di carota processati nel medesimo impianto, ma ottenuti a partire da carote arancioni provenienti da regioni differenti

Alimenti derivati da fonti agricole

↓

Materia grezza



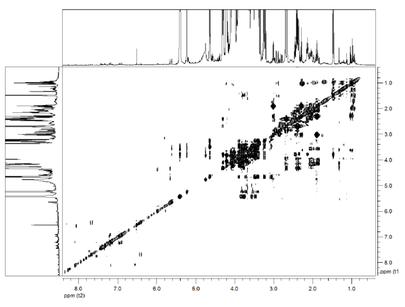
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Prodotto finito



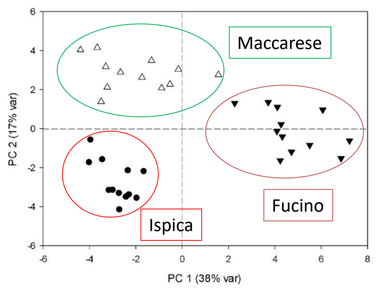


La ricerca in oggetto fa parte del progetto **VALFOOD** finanziato dal **Fondo europeo agricolo** per lo sviluppo rurale Reg. **CE 1698/2005: Progetto Regione Abruzzo: PSR 2007-201**3 Misura 1.2.4 responsabile prof A. Miccheli.

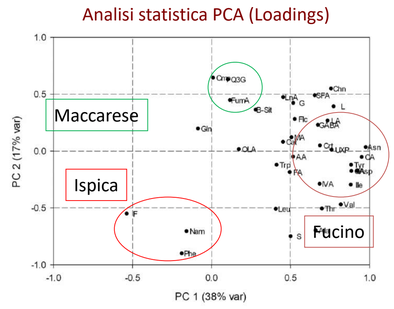


Spettro ^{1}H-^{1}H TOCSY Estratto Idroalcolico
di succo di carota arancione (definizione profilo metabolico)

Analisi statistica PCA (scores)



Analisi statistica PCA (Loadings)



Si osserva come i succhi "Ispica" e "Maccarese" siano più simili tra loro di quanto non lo siano rispetto a quelli "Fucino" (la loro separazione avviene sulla PC1) e dall'analisi dei loadings si osserva come i succhi "Fucino" siano maggiormente ricchi di amminoacidi rispetto agli altri.

2) Caratterizzazione dei micronutrienti durante lo sviluppo di carote viola per l'ottimizzazione della loro raccolta per un migliore rapporto qualità/impatto salutistico

Parametri convenzionali di maturazione delle carote:



Dimensioni

Colore

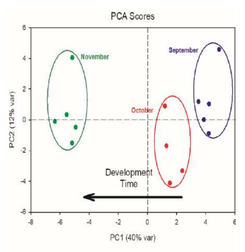
Croccantezza

Forma dell'apice

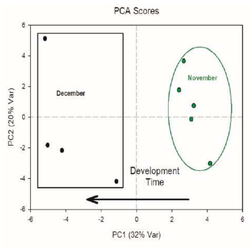
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Come mai carote simili posseggono un aroma più amaro?
(possono avere altri usi?)

Servono parametri più oggettivi



Variazione del profilo metabolico della carota viola durante la maturazione.



Variazione del profilo metabolico della carota viola durante la sovra-maturazione.

La ricerca in oggetto fa parte del progetto **INNOPAQ** finanziato dal **Fondo europeo** agricolo per lo sviluppo rurale **Reg. CE 1698/2005: Progetto Regione Abruzzo: PSR 2007-2013** Misura 1.2.4 responsabile prof A. Miccheli.

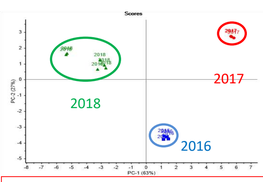
3) Analisi dell'influenza dell'annualità sul profilo metabolico di rapa rossa e identificazione di biomarcatori di assunzione



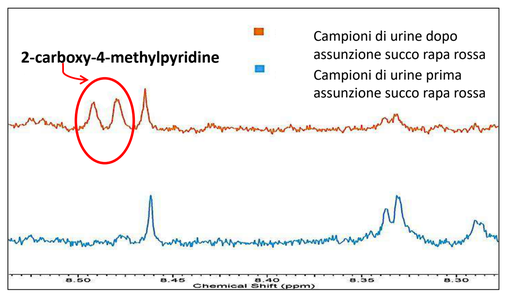
L'annualità influenza la composizione qualitativa di un alimento

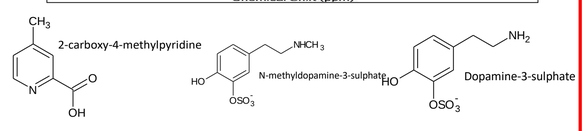
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Come valutarne l'effetto?
(possono essere usate per scopi differenti?)



Variazione del profilo metabolico della rapa rossa in funzione dell'anno di coltivazione. (analisi PCA)

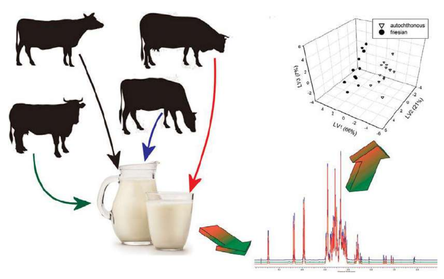




Biomarcatori di assunzione di rapa rossa individuati nelle urine

La ricerca in oggetto fa parte del progetto **G.A.P.INNO.** finanziato dal **Fondo europeo** agricolo per lo sviluppo rurale **Reg. CE 1698/2005: Progetto Regione Abruzzo: PSR 2007-2013** Misura 1.2.4, responsabile prof A. Miccheli

4) Studio della composizione del latte vaccino in funzione della specie e dell'alimentazione

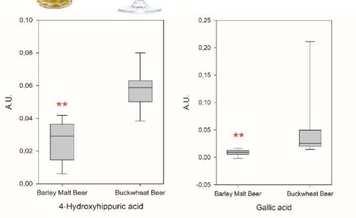


L'obiettivo del progetto è di confrontare e dimostrare, mediante ottimizzazione di metodiche analitiche tradizionali in laboratorio e messa a punto di strumentazioni innovative in situ, come il risultato di una alimentazione che utilizza mangimi innovativi prebiotici/probiotici renda il latte migliore sostituendo il processo di arricchimento successivo.

La ricerca in oggetto fa parte del progetto **STRALAQ (Strategie innovative per un latte di qualità)** finanziato dal **Ministero delle Politiche Agricole e Forestali (MIPAAF) 2019,** responsabile prof. S. Materazzi**.**

5) Studio della composizione di birra d'orzo e di grano saraceno ed identificazione di biomarcatori urinari di assunzione





Biomarcatori di assunzione di birra di grano saraceno individuati nelle urine

L'obiettivo dello studio è di valutare le variazioni del metaboloma urinario di atleti prima, alla fine e tre ore post esercizio, quando assume acqua, assume birra di grano saraceno o birra d'orzo (come controllo).

La ricerca in oggetto fa parte del progetto "**Impatto dell'ingestione di una birra a base di grano saraceno tartarico sullo stress ossidativo post esercizio in giocatori di rugby**" finanziato dal **Birra del Borgo 2019** responsabili prof N. Merendino - A. Miccheli**.**

Riferimenti recenti

Tomassini A., Sciubba F., Di Cocco M.E., Capuani G., Delfini M., Aureli W., Miccheli A. "^{1}H NMR-Based Metabolomics Reveals a Pedoclimatic Metabolic Imprinting in Ready-to-Drink Carrot Juices" *Journal of Agricultural and Food Chemistry,* 64(25), 5284-5291, 2016
Tomassini A., Curone G., Solè M., Capuani G., Sciubba F., Conta G., Miccheli A., Vigo D. "NMR-based metabolomics to evaluate the milk composition from Friesian and autochthonous cows of Northern Italy at different lactation times" Natural Product Research, 33(8), 1085-1091

Scienze della Vita

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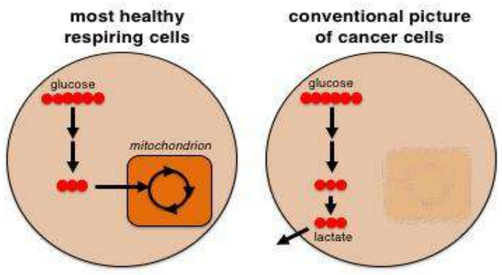
Numerical investigation of the Gatenby-Gawlinski model for tumour dynamics

Pierfrancesco Moschetta, Corrado Mascia and Chiara Simeoni
Email: moschetta@mat.uniroma1.it mascia@mat.uniroma1.it simeoni@unice.fr
Research fields: mathematical modeling, numerical analysis and scientific computing.

From a phenomenological point of view, the Gatenby-Gawlinski model of cancer invasion is inspired by the Warburg effect and relies on the acid-mediated invasion hypothesis. The main purpose consists in improving the understanding of its structural aspects, by means of a numerical approach based on finite volume approximations, and provide a space-averaged propagation speed estimate as a tool to investigate the phenomenon of traveling fronts. In particular, the multidimensional environment is explored with emphasis on some important qualitative aspects strongly linked to experimental observations.

Biomedical context and model presentation

The Warburg effect concerns the metabolism of cancer cells, essentially providing their glucose uptake rates: tumour cells tend to rely on glycolytic metabolism even in presence of huge oxygen amounts, while normal cells undergo glucose metabolism by employing oxidative phosphorylation pathways, which is the most effective process in terms of ATP production and requires oxygen as main resource. Tumour cells seems to forbear the conventional pathway and appeal to glycolysis, inducing lactic acid fermentation (generally released in hypoxia), thus leading to the so-called acid-mediated invasion hypothesis.



The model [*Gatenby and Gawlinski,*1996] is developed to reproduce cancer cells invasion within a healthy tissue: we deal with a reaction-diffusion system. The degenerate diffusion term within the second equation prevents tumour from spreading, unless the surrounding healthy tissue concentration is diminished from its carrying capacity. A generalized version of the model is proposed in [*McGillen et al*., 2014], including terms for acid-mediated tumour cells death and mutual competition between healthy and cancer cells.

$$\begin{cases} \dfrac{\partial u}{\partial t} = u(1-u) - duw \\ \dfrac{\partial v}{\partial t} = rv(1-v) + D\dfrac{\partial}{\partial x}\left[(1-u)\dfrac{\partial v}{\partial x}\right] \\ \dfrac{\partial w}{\partial t} = c(v-w) + \dfrac{\partial^2 w}{\partial x^2} \end{cases}$$

- $\mathbf{u(x,t)}$ healthy tissue density;
- $\mathbf{v(x,t)}$ tumour cells density;
- $\mathbf{w(x,t)}$ extracellular lactic acid concentration;
- $\mathbf{d}$ death rate for healthy cells;
- $\mathbf{r}$ growth rate for tumour cells;
- $\mathbf{c}$ growth and reabsorption rate for lactic acid;
- $\mathbf{D}$ diffusion constant for tumour cells;
- $\mathbf{[-1, 1]}$ experimental domain;
- the homogeneous Neumann problem is considered for the boundary data.

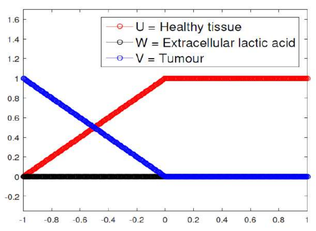
A numerical algorithm based on cell-centered finite volume approximations is employed for the spatial discretization: the interfacial quantities are approximated by building weighted averages involving the size of the adjacent finite volumes and the first order derivatives are discretized by means of an upwind formula. For the time discretization a semi-implicit approach is invoked: the reaction terms are treated explicitly, while the differential terms on the right-hand sides are approximated implicitly.

$$\begin{cases} u_j^{n+1} &= u_j^n + \Delta t[u_j^n(1-u_j^n) - du_j^n w_j^n] \\ v_j^{n+1} &= v_j^n + r\Delta t v_j^n(1-v_j^n) \\ &\quad + D\dfrac{\Delta t}{(\Delta x)^2}\Big[(1-u_j^{n+1})(v_{j+1}^{n+1} - 2v_j^{n+1} + v_{j-1}^{n+1}) \\ &\quad - \dfrac{1}{2}(v_{j+1}^{n+1} - v_j^{n+1})(u_{j+1}^{n+1} - u_j^{n+1}) - \dfrac{1}{2}(v_j^{n+1} - v_{j-1}^{n+1})(u_j^{n+1} - u_{j-1}^{n+1})\Big] \\ w_j^{n+1} &= w_j^n + c\Delta t(v_j^n - w_j^n) + \dfrac{\Delta t}{(\Delta x)^2}(w_{j-1}^{n+1} - 2w_j^{n+1} + w_{j+1}^{n+1}) \end{cases}$$

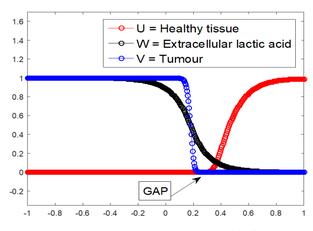
Simulations results

Parameters and initial profiles

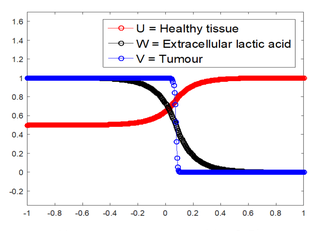
- $\mathbf{D = 4 \cdot 10^{-5}}$
- $\mathbf{r = 1}$
- $\mathbf{c = 70}$
- $\mathbf{d \in \{0.5, 12.5\}}$
- $\mathbf{T = 20}$ final time
- $\mathbf{\Delta x = 0.005}$ space-step
- $\mathbf{\Delta t = 0.01}$ time-step



Recognition of tumour invasions



Homogeneous case (d = 12.5)



Heterogeneous case (d = 0.5)

Propagating fronts are moving from left to right. The heterogeneous invasion (coexistence between tumour and healthy cells behind the wave front) takes place if $d < 1$; the homogeneous invasion (healthy tissue destruction behind the wave front) happens if $d >> 1$. In this last scenario, from the experimental point of view, is remarkable the formation of the tumour-host hypocellular interstitial Gap, namely a separation zone between cancer and healthy cells fronts.

LeVeque-Yee wave speed estimate

$$s^n = \frac{\Delta x}{[v]\Delta t}\sum_j (v_j^n - v_j^{n+1}), \quad \text{where} \quad [v] = v(+\infty) - v(-\infty)$$

Investigation case	Numerical	Analytical
Homogeneous i.e. $d = 12.5$	0.0124	$s \approx 2\sqrt{Dr} = 0.0126$
Heterogeneous i.e. $d = 0.5$	0.0058	$s \approx \sqrt{2Ddr} = 0.0063$

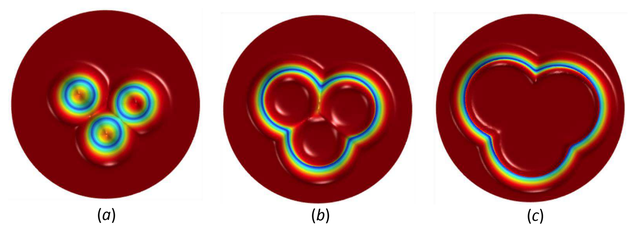
To get information about the propagating fronts speed, the LeVeque-Yee space-averaged approximation [*LeVeque and Yee,* 1990] is invoked: its strength lies in the absolute independence from the dynamics of the system solutions.

Multidimensional simulations

Use of Lagrange P2 finite elements for numerical functions. The COMSOL Multiphysics environment (www.comsol.it) is employed for simulations, while ParaView (www.paraview.org) is exploited for post-processing 3D graphical results.

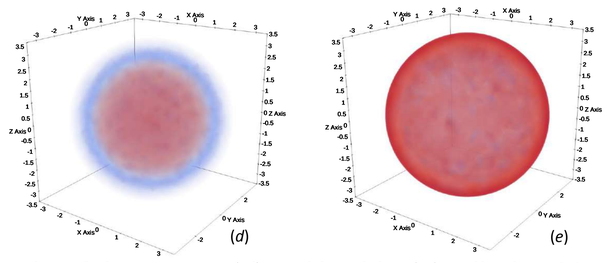
Gap detection for two-dimensional configurations

Three initial distinct cancerous peaks surrounded by the healthy tissue (*a*) are considered for the homogeneous invasion ($\mathrm{d} = 12.5$). By adopting a bird-eye viewpoint, it is possible to appreciate the Gap formation around the cancerous peaks: smaller blue rings, namely null zone densities, are detectable within the circular crowns located between the fronts. Through an intermediate evaluations (*b*), it is shown how these rings gradually increase their size and are opening, as the corresponding cancerous peaks are colliding and going into meltdown. Eventually, once the novel tumour core is well defined (*c*), the resultant Gap consists of a single contour cordoning off the cancerous crown from the surrounding marginal area, where the local healthy tissue is regressing.



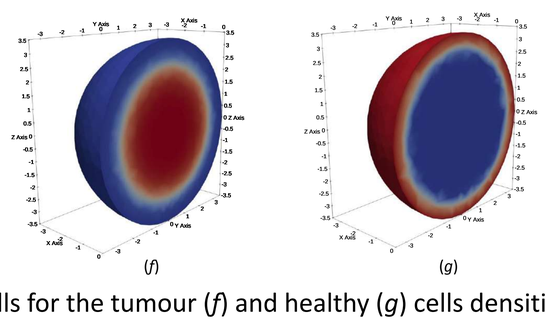
(*a*) (*b*) (*c*)

Gap detection for three-dimensional configurations



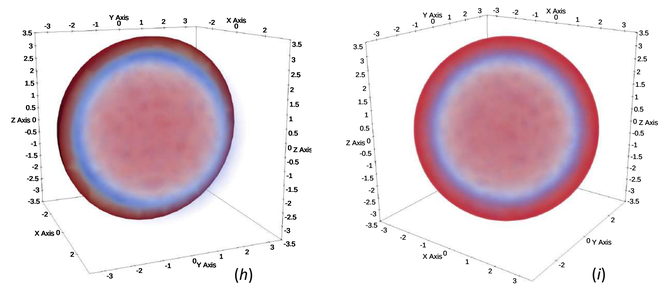
(*d*) (*e*)

Graphs of the tumour (*d*) and healthy (*e*) cells densities at the final time instant for the homogeneous invasion ($\mathrm{d} = 12.5$) by means of the transparency technique. The initial profile is a single cancerous peak surrounded by healthy tissue.



(*f*) (*g*)

Half balls for the tumour (*f*) and healthy (*g*) cells densities arising from domain sectioning and provided with numerical data throughout the external spherical surface. Through symmetry arguments, it is possible to infer that data distributions retain an analogous behaviour inside any inner layer.



(*h*) (*i*)

Graphical proof for assessing the presence of a separation zone between the tumour and healthy cells densities: simultaneous plot (*h*) of data merging from (*d*) and (*g*); simultaneous plot (*i*) of data from (*d*) and (*e*) allowing to notice the three-dimensional Gap, appearing as a null density solid shell.

References:

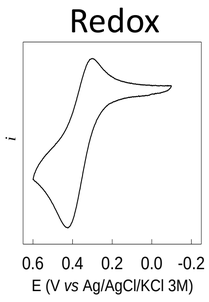
Gatenby, R. A., Gawlinski, E. T., 2002, A reaction-diffusion model of cancer invasion, *Appl. Math. Lett.,* **15**, 339-345.
LeVeque, R. J., Yee, H. C., 1990, A study of numerical methods for hyperbolic conservation laws with stiff source terms, *J. Comput. Phys.,* **86**, 187-210.
McGillen, J. B., Gaffney, E. A., Martin, N. K., Maini, P. K., 2014, A general reaction-diffusion model of acidity in cancer invasion, *J. Math. Biol.,* **68**, 1199-1224.
Moschetta, P., Simeoni, C., online first 2019, Numerical investigation of the Gatenby-Gawlinski model for acid-mediated tumour invasion, *Rend. Mat. Appl.,* 31 pp.

Photochemical behavior of 2-(hydroxyimino)aldehydes

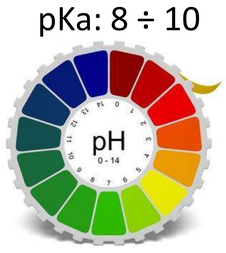
Dario Filippini[a], Laura Mancini[a], Francesca D'Acunzo[b], Patrizia Gentili[a,b]
[a]*Dipartimento di Chimica, Sapienza Università di Roma;* [b]*Istituto per i Sistemi Biologici*, CNR
E –mail: filippini.1648506@studenti.uniroma1.it

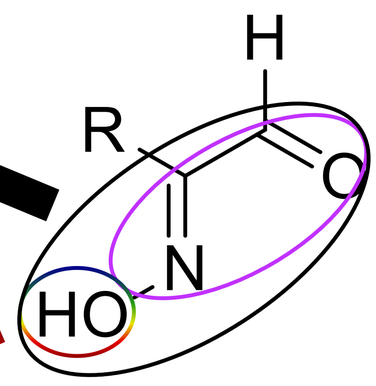
HIA general properties

Redox



pKa: 8 ÷ 10



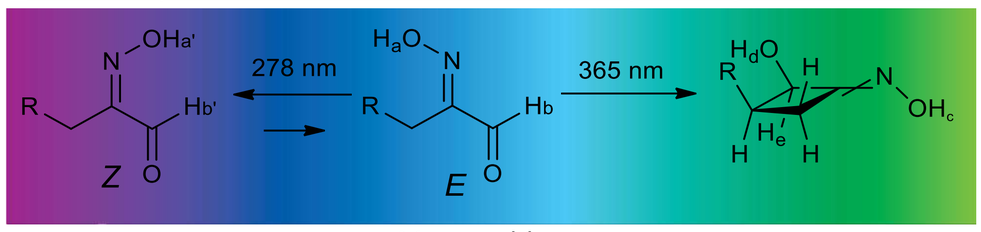


UV Light



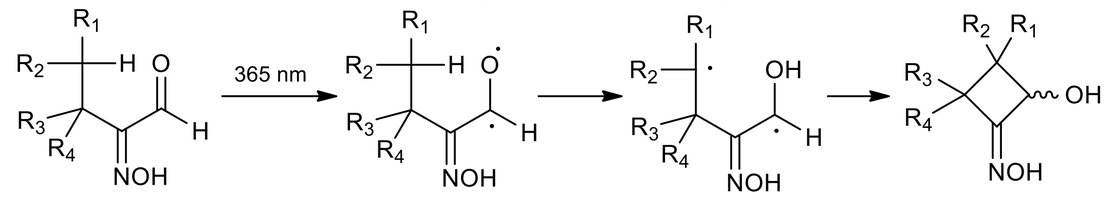
Gentili, P. et al. *Chem. Eur. J.* **2018**, *24*, 7683 – 7694

HIA photochemical properties



Less stable isomer | More stable isomer | CBO

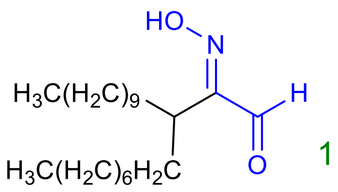
CBO formation through a Norrish-Yang mechanism



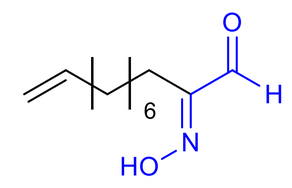
1: R_1 = H; R_2 = $CH_3(CH_2)_6$-; R_3 = $CH_3(CH_2)_9$-; R_4 = H
2: R_1 = CH_2=$CH(CH_2)_5$-; R_3 = R_4 = H
3: R_1 = $CH_3(CH_2)_7$-triazole-; R_2 = R_3 = R_4 = H
4: R_1 = $mPEG_{350}$-triazole-; R_2 = R_3 = R_4 = H

Gentili, P. et al. *Chem. Eur. J.* **2018**, *24*, 7683 – 7694

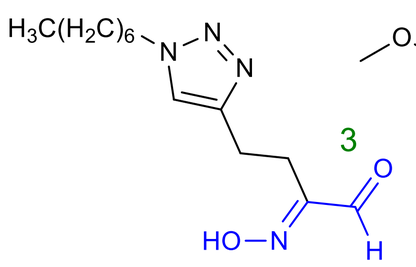
Synthesized HIAs

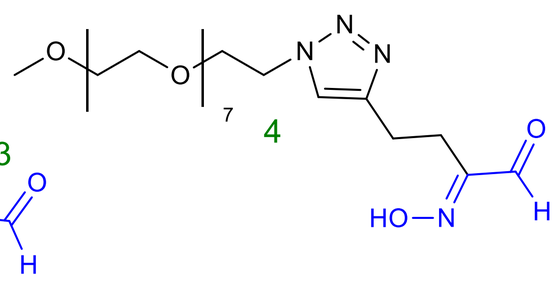


aliphatic HIA



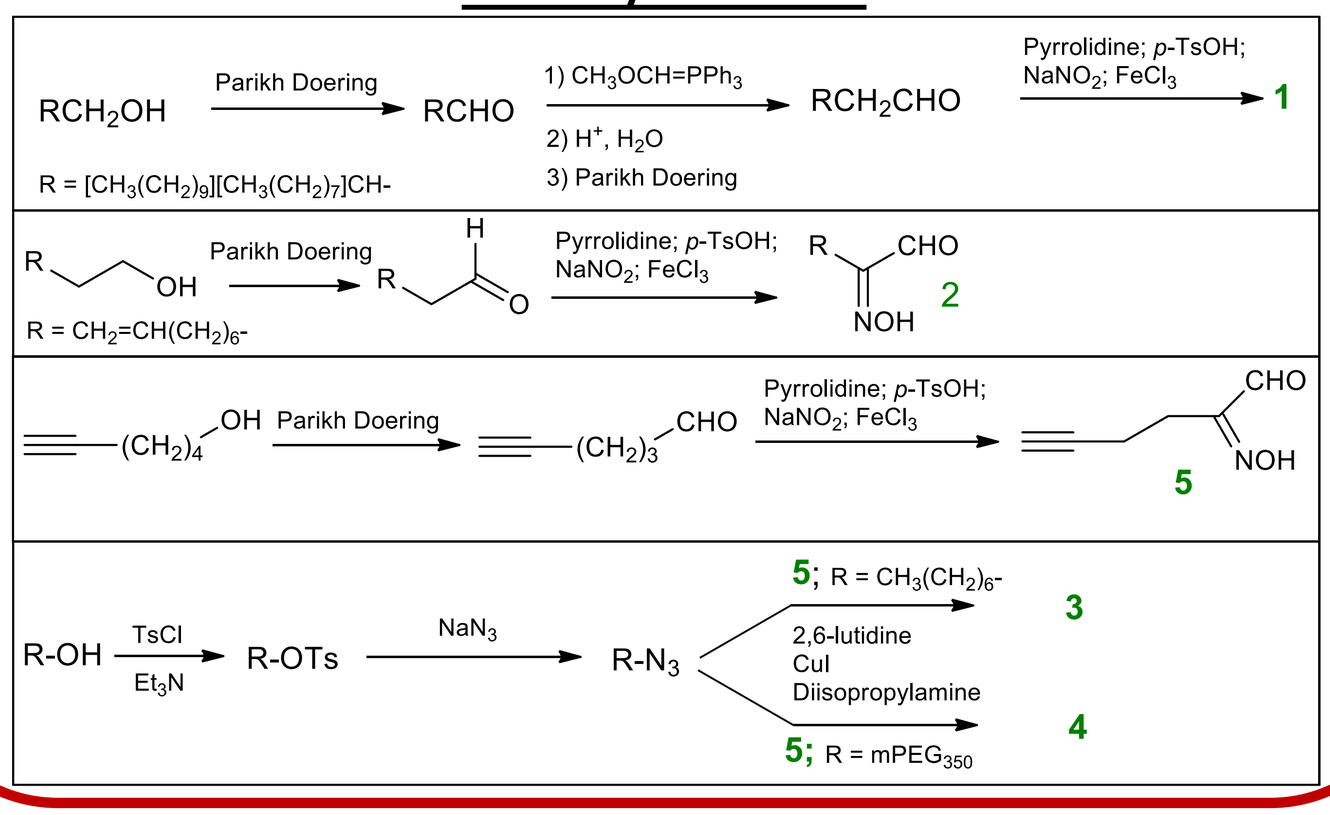
HIA with a remote double bond



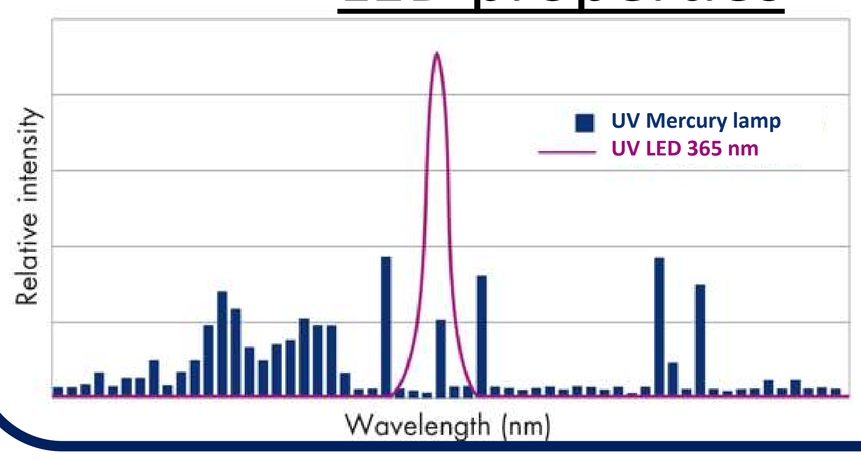


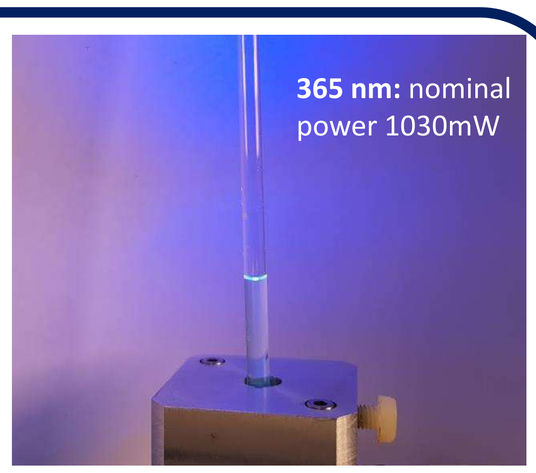
HIA linked via click chemistry to a hydrophobic (3) and hydrophylic group (4)

HIA synthesis



LED properties





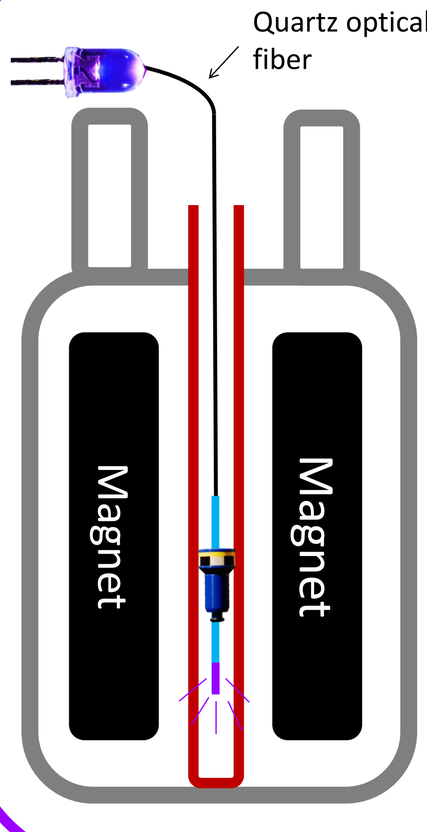
LED assembly by Mr. **Carlo Sperilli**

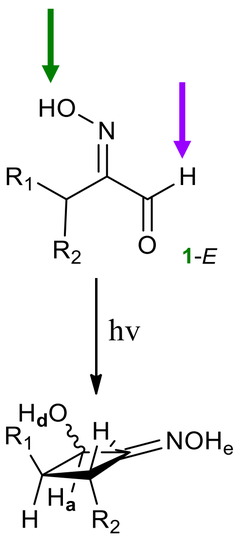
Fiber properties

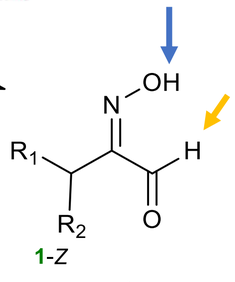
Composition:
Fused silica core 600 µm
Fluorine doped fused cladding 660 µm
Silicone elastomer cladding 760 µm
Optical properties:
Operating wavelength: 200 to 1100 nm
NA: 0.22
Length:
2 m



Light and NMR









Gschwind, R.M. et al Angew. *Chem. Int.* Ed. **2018**, *57*, 7493 –7497

New multi-stimuli responsive methacrylates bearing the 2-(hydroxyimino)aldehyde group and their behavior in aqueous solution

Francesca D'Acunzo,*[a] Giancarlo Masci,[b] Anita Scipioni,[c] Patrizia Gentili,[d] Polyssena Renzi, Davide Arena

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[b] *stanza 363; giancarlo.masci@uniroma1.it;* [c] *stanza 371; anita.scipioni@uniroma1.it;* [d] *stanza 187, patrizia.gentili@uniroma1.it*

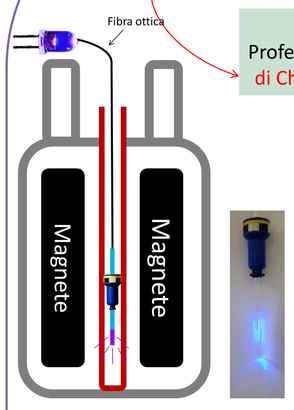
Sintesi di 2-(idrossiimmino)aldeidi (HIA) mediante organocatalisi e click chemistry

Sintesi RAFT di polimeri multi stimolo-sensibili

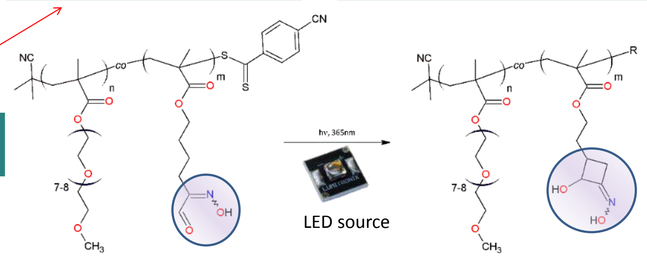
Patrizia Gentili
Professore Associato Dipartimento di Chimica Università La Sapienza

Francesca D'Acunzo
Ricercatore Istituto per i Sistemi Biologici CNR

Giancarlo Masci
Professore Associato Dipartimento di Chimica Università La Sapienza

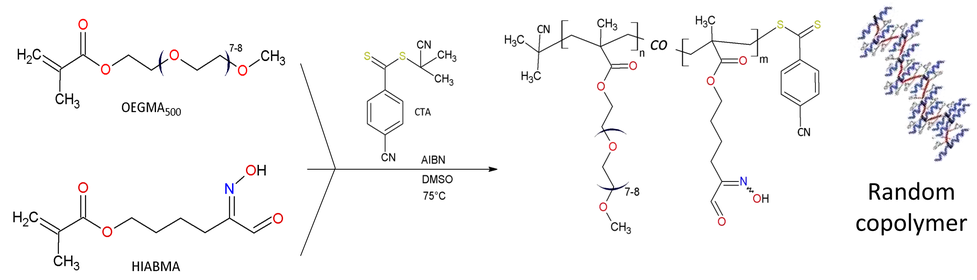


Fotochimica delle HIA
Foto-NMR

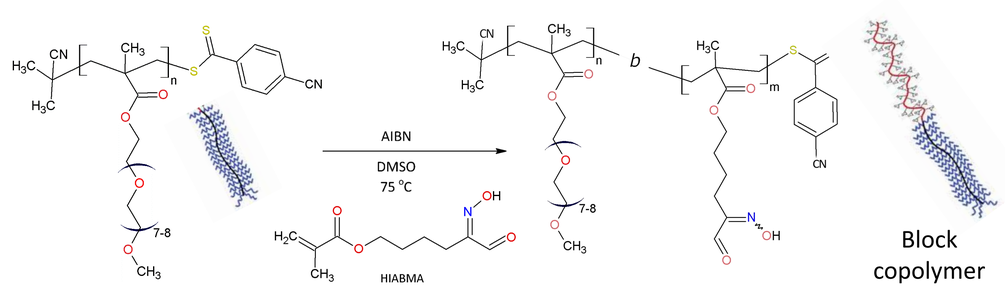


Synthesis

The HIA-functionalized monomer **HIABMA** (4-[(hydroxyimino)aldehyde]butyl methacrylate) was polymerized in RAFT conditions. Random copolymers of HIABMA and oligo(ethylene glycol) methyl ether methacrylate (**OEGMA$_{500}$**) in different proportions were obtained (HIABMA/ OEGMA$_{500}$ from 7:3 to 3:7). Monomers conversion >95%.[1, 2]

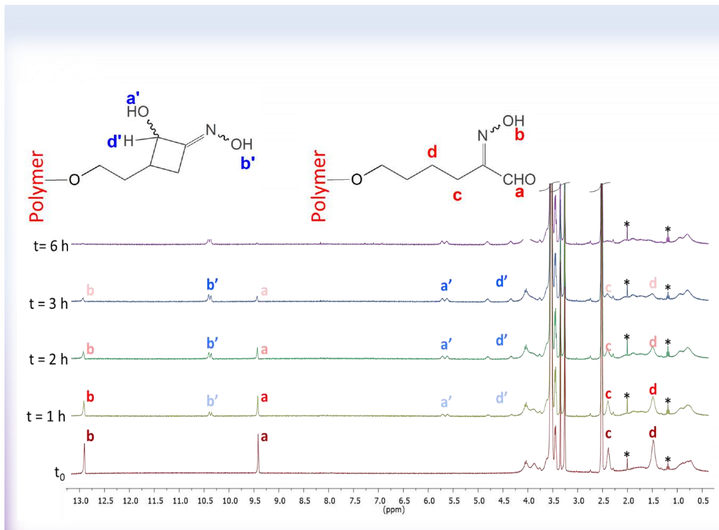


Through a living-chain extension approach, the elongation of polyOEGMA$_{500}$ with HIABMA afforded a 1:1 block copolymer

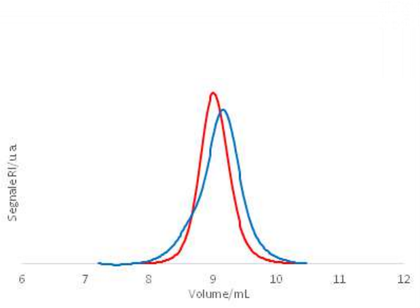


	Polymer	HIABMA/OEGMA$_{500}$	M_n/kDa	Đ
1	*poly*-OEGMA$_{500}$	-	13.5	1.10
2	*poly*-(HIABMA-*b*-OEGMA$_{500}$)	1:1	24.0	1.14
3	*poly*-(HIABMA-*r*-OEGMA$_{500}$)	1:1	12.8	1.20
4		3:7	14.1	1.23
5		7:3	13.8	1.08
6	*poly*-HIABMA	-	12.5	1.10

Number-Average Molecular Weight (Mn) and Disperion Đ by GPC, relative to linear PEO standards. Mn values are underestimated by a factor of approximately 2 due to the brush-like structure of OEGMA$_{500}$ polymers.

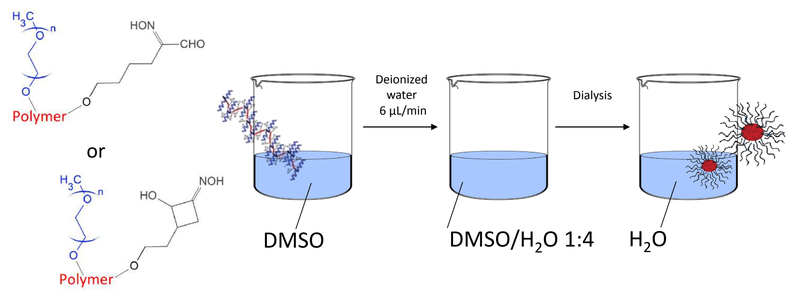


Photoisomerization



GPC curve before and after photoisometization

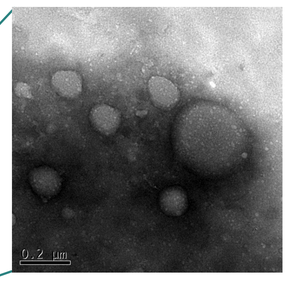
Formation of polymeric micelles



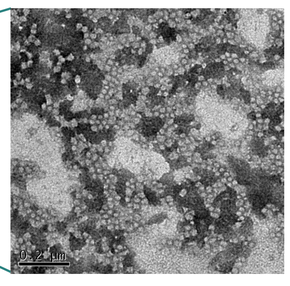
Polymer (HIABMA/OEGMA$_{500}$)	DMSO/Water 1:4	Water
Random (3:7)	No aggregation	Dh (nm) 332 poly 0.261 kpcs 19.1
Random (1:1)	Dh (nm) 303 poly 0.278 kpcs 31.5	
Random (7:3)	Dh (nm) 65 poly 0.049 kpcs 149	
Block (1:1)	Dh (nm) 39 poly 0.109 kpcs 17.5	Dh (nm) 57 poly 0.094 kpcs 29.6

Photoisomerized copolymers lose aggregation capability

Dynamic Light Scattering measurements of nanoparticles

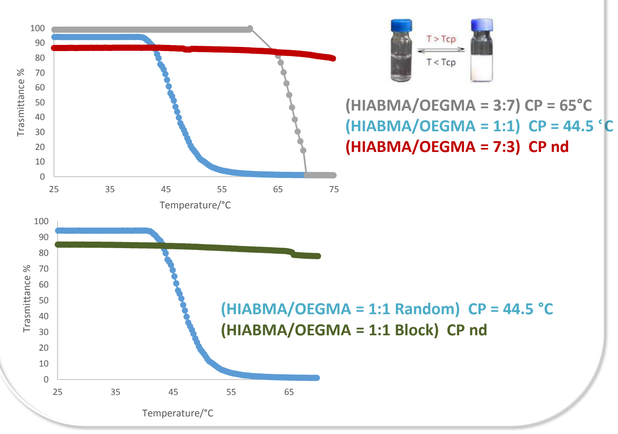


TEM images of nanoparticles with negative staining (PTA)



Thermoresponsivity

Cloud Point (CP)
Temperature at 90% Transmittance (λ= 700 nm)



Summary

HIA-functionalized copolymers are light- and thermo-responsive

Response to stimuli is dependent on composition and architecture

Potential applications

Laser nanoprinting

Drug delivery

And more….

Acknowledgements

Dr. Carlo Sperilli – Sapienza University, Chemistry Department — LED –fiber optics assembly

Dr. Stefano Casciardi - INAIL Research, Rome, Italy — TEM imaging

Riferimenti recenti

[1] M. Nardi, F. D'Acunzo, M. Clemente, G. Proietti, P. Gentili, *Polym. Chem.* **2017**, *8*, 4233.

[2] P. Gentili, M. Nardi, I. Antignano, P. Cambise, M. D'Abramo, F. D'Acunzo, A. Pinna, E. Ussia, *Chem. Eur. J.* **2018**, *24*, 7683.

[3] F. D'Acunzo, S. De Santis, G. Masci, M. Nardi, P. Renzi, A. P. Sobolev, *Macr. Chem. Phys.* **2019**, *220*, 1900200.

Dipartimento di
Biologia Ambientale
SAPIENZA
UNIVERSITÀ DI ROMA

Fungal biodiversity as a bioresource for sustainable applications

Veronica Spinelli*, Andrea Ceci, Anna Maria Persiani
Dipartimento di Biologia Ambientale, Edificio Botanica, CU022, piano 2 stanza 212
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FUNGAL BIODIVERSITY LAB OF SAPIENZA • FBL •

Attività

- Isolamento e caratterizzazione ceppi fungini da matrici ambientali
- Conservazione e mantenimento dei ceppi della micoteca
- Studi delle potenzialità dei funghi nel biorimedio
- I funghi: biorisorse per la *plant growth promotion*

Nel nostro laboratorio

Microscopia
Tecniche colturali
Test di *plant growth promotion*
Phenotype Microarray
Conservazione ceppi fungini
Test di *bioremediation*

- Gestione della *Fungal culture collection* del laboratorio costituita da oltre 600 ceppi fungini, conservati in forma liofilizzata o in liquido, isolati da diverse aree geografiche e matrici ambientali tra cui suoli naturali e contaminati, lettiera ed acque.
- Isolamento e caratterizzazione di ceppi fungini, identificazione mediante approccio polifasico (morfologico e molecolare), studi di caratteri fisiologici, metabolici, fenotipici e genomici.
- Valutazione delle potenzialità di ceppi fungini nella *bioremediation* e nella *plant growth promotion* di specie di interesse agrario e medicinale.

Settori ERC:

LS8_2 - Biodiversity, conservation biology, conservation genetics
LS8_10 - Microbial ecology and evolution
LS9_4 - Applied plant sciences
LS9_7 Environmental biotechnology
LS1_2 Biochemistry and metabolism

Le nostre collaborazioni multidisciplinari

Prof. Alfredo Miccheli - Dipartimento di Chimica, Sapienza
Metabolomica mediante spettroscopia NMR

Dr. Flavia Pinzari– CREA Centro di ricerca Agricoltura e Ambiente
Biotecnologie per le applicazioni agrarie

Prof. Silvia Canepari - Dipartimento di Chimica, Sapienza
Chimica analitica

Dr. Domenico Davolos – Inail
Genomica e tecniche molecolari

Prof. Marco Petrangeli Papini- Dipartimento di Chimica, Sapienza
Chimica industriale e risanamento siti contaminati

Prof. Gabriella Pasqua- Dipartimento di Biologia Ambientale, Sapienza
Biotecnologie Cellulari Vegetali

Funghi per la *bioremediation* dell' HCH

- Isolamento di 52 taxa da campioni di suolo e matrici ambientali provenienti rispettivamente da aree naturali e da reattori in situ per il trattamento delle acque contaminate da isomeri di HCH di un sito (Repubblica Ceca).
- 12 ceppi fungini testati sono risultati tolleranti ad elevate concentrazioni di isomeri di HCH, di questi ceppi sono stati individuati i metaboliti secondari prodotti della biotrasformazione degli isomeri di HCH.
- Di due dei 12 ceppi, *Trichoderma harzianum e Penicillium simplicissimum,* è stata rilevata l'attività di enzimi antiossidanti in risposta allo stress ossidativo.

Funghi e arsenico: tolleranza e bioaccumulo

- 4 ceppi fungini, *Absidia spinosa, Purpureocillium lilacinum, Metarhizium marquandii and Cephalotrichum nanum*, isolati da siti naturali con elevate concentrazioni di background di As, sono stati testati per differenti concentrazioni di arsenito di sodio in diverse condizioni nutrizionali.
- Tutti i ceppi sono risultati tolleranti anche alle più elevate concentrazioni di arsenito e in grado di accumulare nelle biomasse, in misura differente, il metalloide.

Funghi per la *bioremediation* del DDT

- Tra i 38 taxa isolati da suoli agricoli contaminati (Polonia), 24 specie sono risultate tolleranti ad elevate concentrazioni di DDT e dei suoi isomeri.
- 2 ceppi fungini tra i 24, testati per lo stress ossidativo e per il profilo fenotipico, *Rhizopus arrhizus* e T*richoderma hamatum*, hanno mostrato alcune differenze significative nei profili fenotipici in presenza degli xenobiotici e l'attivazione di meccanismi di risposta allo stress ossidativo.

Biorisorse fungine per la solubilizzazione del fosforo

- 30 ceppi fungini testati in Pikovskaya medium hanno solubilizzato il tricalcio fosfato mediante differenti meccanismi, rilasciandolo nel terreno di coltura.
- 9 dei 30 ceppi sono stati testati anche in coltura liquida e la solubilizzazione e l'accumulo di P nelle biomasse sono stati valutati mediante ICP/MS.
- *Aspergillus niger, Penicillium griseofulvum* e *Rhizopus stolonifer* var. *stolonifer* sono risultate le specie più efficaci
- In alcune specie è stata osservata mediante SEM la produzione di minerali di precipitazione secondaria.

Progetti in corso

- Sustainable cultivation of the medicinal plant *Hypericum perforatum* (L.): soil saprotrophic fungi for growth-promoting and resistance induction
- Fungi and arsenic: tolerance and bioaccumulation by soil saprotrophic strains

Riferimenti recenti

Ceci, A., Pinzari, F., Russo, F., Persiani, A.M., and Gadd, G.M. (2019). Applied Microbiology and Biotechnology *103*, 53–68.
Russo, F., Ceci, A., Pinzari, F., Siciliano, A., Guida, M., Malusà, E., Tartanus, M., Miszczak, A., Maggi, O., and Persiani, A.M. (2019). Applied and Environmental Microbiology.
Russo, F., Ceci, A., Maggi, O., Siciliano, A., Guida, M., Petrangeli Papini, M., Černík, M., and Persiani, A.M. (2019). Environmental Science and Pollution Research *26*, 24445–24461.
Ceci, A., Pinzari, F., Russo, F., Maggi, O., and Persiani, A.M. (2018). Ambio *47*, 30–40.

Dipartimento di Fisica
SAPIENZA Università di Roma

Applicazioni di tecniche di Fisica delle Particelle alla Terapia con Particelle

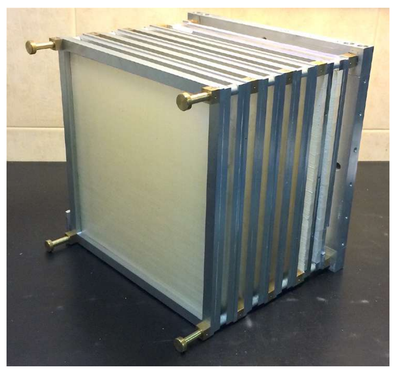
Marta Fischetti, Micol De Simoni, Riccardo Faccini, Carlo Mancini Terracciano, Michela Marafini, Riccardo Mirabelli, Alessio Sarti, Angelo Schiavi, Adalberto Sciubba, Elena Solfaroli Camillocci, Marco Toppi, Giacomo Traini, Vincenzo Patera

Dipartimento di Fisica, Edificio Marconi, piano 2
Email: riccardo.faccini@roma1.infn.it

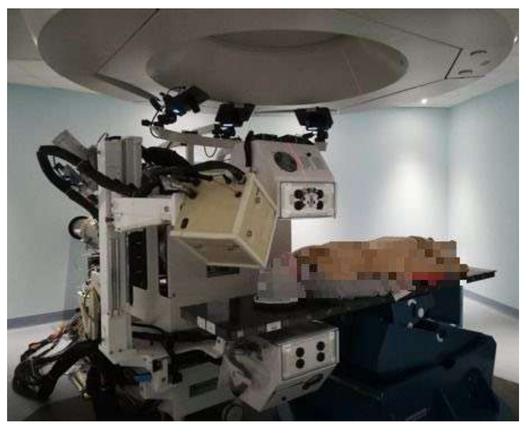
Dipartimento SBAI, Edificio RM009, piano terra
Email: vincenzo.patera@roma1.infn.it

La collaborazione ARPG è attiva dal 2011 per trasferire le competenze acquisite nel campo della fisica delle particelle delle alte energie ad applicazioni in diversi campi. Un contributo particolarmente significativo riguarda le applicazioni alla Terapia con Particelle.

Il **Dose profiler** (DP), sviluppato all'interno del progetto INSIDE (INnovative Solutions for In-beam DosimEtry in hadron therapy), è stato progettato e costruito per misurare il profilo di emissione delle particelle cariche secondarie (principalmente protoni) prodotte durante un trattamento con ioni Carbonio tra l'interazione del fascio principale e i tessuti del paziente.

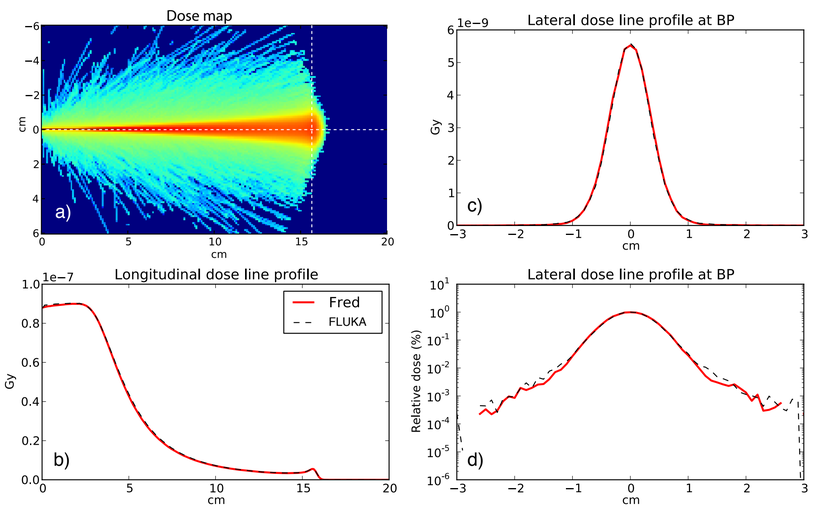


Il DP è costituito da 8 piani (mostrati in figura) di fibre scintillanti plastiche usate per il tracciamento delle particelle. Quando i protoni attraversano il rivelatore viene generato un segnale luminoso letto da SiPM che comunicano, tramite FPGA, con il software di acquisizione dati che si occupa di distribuire il segnale di trigger di lettura e inviare i dati ad un server per il data processing. Il DP è in grado di fornire informazioni sull'effettiva profondità a cui si fermano le particelle durante l'irraggiamento di un paziente e in questo modo ottimizzare il rilascio di dose, minimizzando il rilascio ai tessuti sani. Il sistema INSIDE è installato al CNAO (Centro Nazionale di Adroterapia Oncologica) di Pavia dal 2017 ed ha monitorato il primo paziente nel mese di agosto 2019, nell'ambito di un trial clinico che si propone di monitorare 40 pazienti con trattamenti nelle regioni Testa-Collo ed Encefalo, valutando la qualità del trattamento lungo tutta la durata della terapia (tipicamente 4 settimane per trattamenti con ioni carbonio). Grazie alle misure del trial sarà possibile valutare la stabilità dello strumento e la significatività della misura.



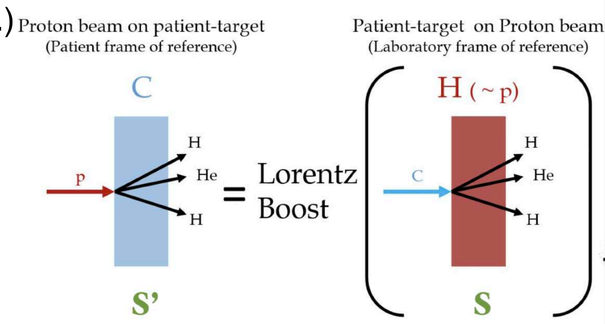
L'attività di ricerca portata avanti comprende: lo sviluppo del rivelatore, la relativa simulazione MC, la progettazione e realizzazione del DAQ e del relativo trigger.

FRED (Fast paRticle thErapy Dose evaluator) è un codice fast-MC sviluppato per realizzare piani di trattamento e verifica della dose nella terapia con particelle. Attualmente i piani di trattamento utilizzati sono analitici e solo in casi particolarmente difficili vengono usati dei Monte Carlo (MC) il cui limite principale è l'elevato tempo computazionale richiesto. Con FRED è possibile descrivere le interazioni di fasci di protoni a energie terapeutiche con la materia con l'accuratezza di un full-MC con il vantaggio di ridurre il tempo di simulazione di un fattore 1000. Gli eccellenti risultati ottenuti con fasci di protoni hanno aperto la strada al suo utilizzo per diverse applicazioni mediche in cui il fattore tempo è cruciale. In particolare permette una riottimizzazione del piano di trattamento in pochi minuti eseguendo il codice su schede GPU, invece che in molte ore con hardware CPU. Il prossimo obbiettivo da raggiungere è ottenere gli stessi risultati con fasci di ioni pesanti in cui bisogna tener conto anche della frammentazione del proiettile e con fasci di elettroni.
L'attività di ricerca portata avanti comprende: lo sviluppo e l'implementazione di modelli fisici(multiple scattering, nucleare, RBE ecc) nel codice e il test del MC confrontandolo con altri full-MC e con dati sperimentali.

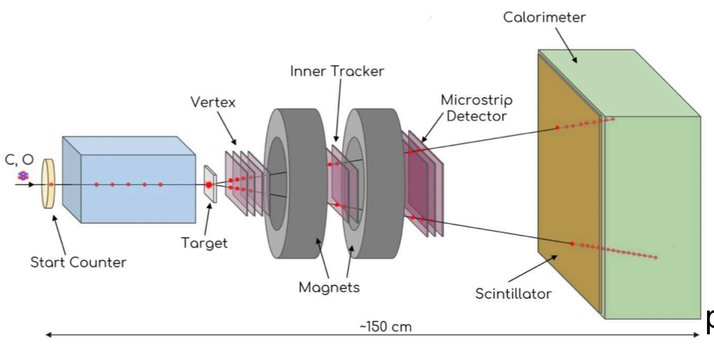


Nell'immagine un esempio della distribuzione di un fascio di protoni simulato in un bersaglio d'acqua (a), e il confronto tra il profilo di dose longitudinale lungo la direzione del fascio e laterale al picco di Bragg in Fred e nel full-MC FLUKA

La collaborazione internazionale **FOOT** ha come obiettivo principale quello di misurare le sezioni d'urto dei processi di frammentazione di interesse nella terapia con particelle e per la radioprotezione nello spazio. Per lo studio dei frammenti prodotti in protonterpia verrà seguito un approccio (cinematica inversa) in cui per studiare la frammentazione indotta dai protoni si 'sparano' gli elementi costituenti del paziente (C, O, ..) su un bersaglio 'arricchito' in protoni per poi applicare un boost di Lorentz per calcolare le sezioni d'urto di interesse, ovviando al range estremamente ridotto (μm) dei frammenti prodotti direttamente in 'PT'.

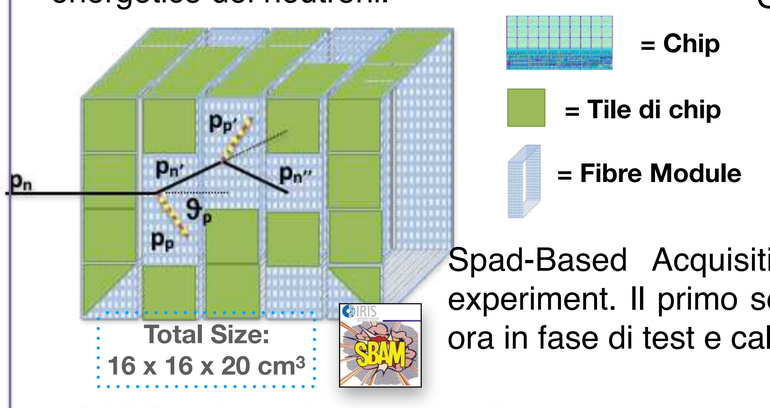


Per ricostruire completamente il quadrimpulso dei proiettili e delle particelle prodotte è necessario un apparato sperimentale ridondante (mostrato in figura) che comprende rivelatori a scintillazione (misura di tempi di volo e contatori di particelle), rivelatori traccianti (monitor di fascio e rivelatori al silicio in campo magnetico per la misura dell'impulso), calorimetri (misura di energia).

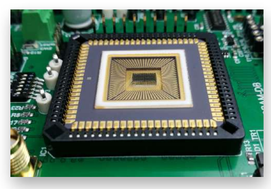


L'attività di ricerca portata avanti comprende: lo sviluppo dei rivelatori a scintillazione, dei tracciatori e del calorimetro, la relativa simulazione MC, l'implementazione del DAQ e del relativo trigger. Una delle principali sfide tecnologiche poste dall'esperimento è l'effettuare tali misure all'interno delle sale sperimentali di trattamento di centri quali il CNAO (Pavia), HIT (Heidelberg), GSI (Darmstadt). L'impiego di simulazioni MC (FLUKA) e algoritmi di ricostruzione (c++, ROOT, Kalman filtering, Runge-Kutta,..) si rivelano fondamentali nell'ottimizzare il layout dell'esperimento.

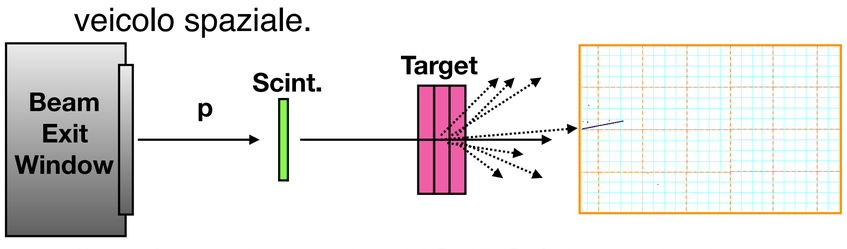
MONDO - Monitor for Neutron Dose in hadrOntherapy - è un progetto dedicato alla caratterizzazione dei neutroni secondari prodotti dalle interazioni dei fasci adroterapici con il paziente. I neutroni infatti possono rilasciare una dose significativa e altamente dannosa anche lontano dalla regione tumorale irraggiata. Il rivelatore di MONDO sfrutta il doppio scattering elastico del neutroni su una matrice di fibre plastiche sottili per ricostruire la direzione e lo spettro energetico dei neutroni.



Oltre alla matrice tracciante per MONDO si sta sviluppando, in collaborazione con la Fondazione Bruno Kessler di Trento, un sensore per il readout delle fibre scintillanti SBAM: Spad-Based Acquisition readout for the Mondo experiment. Il primo sensore è stato realizzato ed è ora in fase di test e calibrazione.



SPARE - SPAce Radiation shiElding - è un progetto (finanziato dal premiale 2016 del MIUR) dedicato all'ottimizzazione delle esplorazioni spaziali.
I rischi per la salute causati dall'esposizione alle radiazioni cosmiche sono riconosciuti come il principale ostacolo alla colonizzazione sicura dei sistemi solari. La schermatura è l'unica contromisura pratica disponibile e nuovi materiali altamente idrogenati sono in fase di sviluppo per la schermatura del veicolo spaziale.



Il rivelatore innovativo MONDO è in grado di tracciare sia i neutroni che le particelle cariche.

SPARE condurrà delle campagne di misura di materiali attivi e passivi utilizzando protoni e neutroni ad alta energia presso gli impianti di accelerazione di Trento e Legnaro.

G. Traini et al, **Review and performance of the Dose Profiler, a particle therapy treatments online monitor** (2019), Physica Medica, 65, pp. 84-93. DOI: 10.1016/j.ejmp.2019.07.010
E. Gioscio et al, **Development of a novel neutron tracker for the characterisation of secondary neutrons emitted in Particle Therapy (2019), Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment,** art. no. 162862, DOI: 10.1016/j.nima.2019.162862, in Press
Morrocchi M. et al, **Development and characterization of a ΔE-TOF detector prototype for the FOOT experiment (2019) Nuclear Instruments and Methods in Physics Research,** SectionA: Accelerators, Spectrometers, Detectors and Associated Equipment, 916, pp. 116-124. DOI: 10.1016/j.nima.2018.09.086

Dipartimento di Matematica
SAPIENZA UNIVERSITÀ DI ROMA

Seminario MoMA
Modelli Matematici nelle Applicazioni

Organizzatrici: Giada Basile e Adriana Garroni
Dipartimento di Matematica «G. Castelnuovo"
http://www1.mat.uniroma1.it/ricerca/seminari/moma/

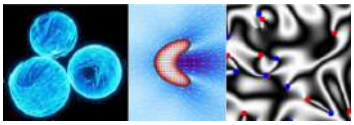
Seminario mensile attivo dal 2011 dallo stile abbastanza divulgativo e interdisciplinare. Ha ospitato relatori di rilievo in molti settori della scienza dalla fisica alla geologia, dalla bioinformatica alla scienza dei materiali, dalle scienze sociali alla finanza.
Filo conduttore: Il rigore scientifico nella ricerca in cui la matematica può dare contributo e permette un salto di qualità.
Obbiettivo: La comunicazione scientifica e la ricerca di possibili interazioni interdisciplinari.

ALCUNI ESEMPI

MATERIA ATTIVA

L. Di Leonardo (2017), Sapienza
The Physics and Engineering of Active Matter

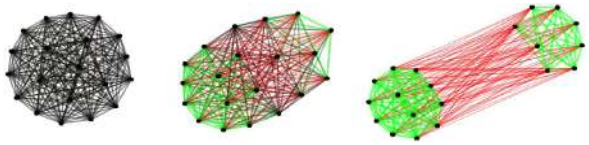




L. Giomi (2017), Leiden NL
Active fludis: from liquid crystals to living systems

DATA SCIENCE

S. Strogatz (2012), Cornell University
Social networks that balance themselves
Consider a fully-connected social network of people, companies, or countries, modeled as an undirected complete graph with real numbers on its edges. Positive edges link friends; negative edges link enemies....



SISTEMI COMPLESSI

I. Giardina (2012), Sapienza
Birds, spins and entropy:
a theoretical physics approach to collective animal behaviour



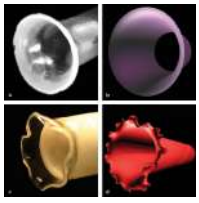
MATERIALI

G. Parisi (2018), Sapienza-Accademia dei Lincei
The physics of glasses form the viewpoint of theoretical physicists

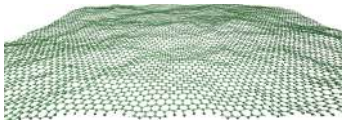


Glassy materials are characterized by being solid (for all practical purpose) at low tempera-ture in absence of a sharp transition from the liquid phase to the solid state. They are ubiquitous in nature: among them, we find window glasses, wax, honey, mozzarella cheese...

E. Sharon (2018), Ebrew University
The Geometry and Mechanics of Growing Elastic Sheets

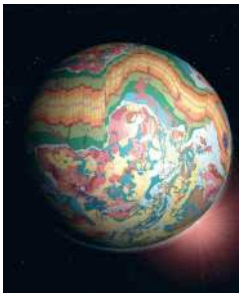


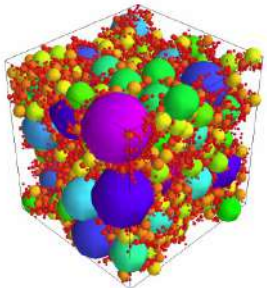
A. Fasolino (2015), Radboud NL
The wonderful structure of graphene



GEOLOGIA-GEOTECNICA

C. Doglioni (2011), Sapienza-INGV
Tectonic asymmetry of the Earth: any relation with tides?

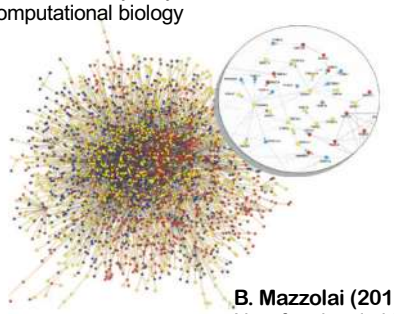




G. Viggiani (2013), Cambridge-Tor Vergata
Grain crushing in polydisperse granular media:
from experimental evidence to modeling

BIOLOGIA-MEDICINA

A. Tramontano (2016), Sapienza
The ultimate mystery is ourselves: the fascinating challenge of computational biology





B. Mazzolai (2017), IIT
New frontiers in biology based robotics

Altri relatori (matematici esclusi): M. Arroyo (Barcelona-tech), S. Barbarossa (Sapienza), A. Barra (Univ. Salento), M. Battaglia (Sapienza), M.G Betti (Sapienza), D. Bigoni (Trento), M. Bizzari (Sapienza), A. Carcaterra (Sapienza), A. Cavagna (CNR), E. Clement (Paris), G. Contini (CNR), M. Crespi (Sapienza), M. Cuffaro (Sapienza), A. D'Avella (Messina), **A. De Simone** (SISSA-Sant'Anna Pisa), **G. Jona Lasinio** (Sapienza), **V. Loreto** (SONY Lab-Sapienza), M. Mattoni (Cagliari), L. Marrucci (Napoli), M. Mattoni (Cagliari), E. Messina (Sapienza), F. Pellaccini (Sapienza), **M. Porfiri** (NYU, New York), A. Puglisi (CNR), **D. Quéré** (Paris), S. Sabatini (Sapienza), V. Vitelli (Leiden), **C. Zannoni** (Bologna), **S. Zapperi** (Milano).

Algoritmi Machine Learning e Deep Learning ultraveloce su FPGA

DIPARTIMENTO DI FISICA
SAPIENZA
UNIVERSITÀ DI ROMA

S. Giagu*, F. Riti, L. Sabetta, S. Francescato
**Dipartimento di Fisica, Edificio G.Marconi, CU013, piano 3° , stanza 318*
Email: stefano.giagu@uniroma1.it



1 - Problema fisico

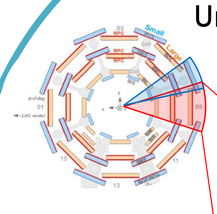
Per gli esperimenti di fisica delle alte energie è essenziale filtrare in tempo reale gli eventi interessanti.

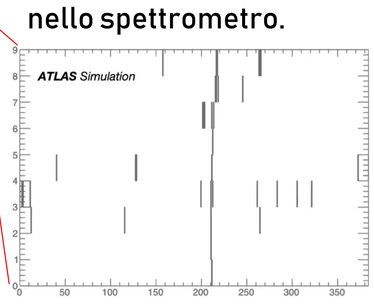
- Eventi ogni 25 ns
- ~100 Milioni di canali di acquisizione
- ~100 Miliardi di particelle al secondo

Un flusso di dati che si otterrebbe se tutte le persone del mondo intrattenessero 20 conversazioni ciascuno allo stesso tempo.

2 - Input e Output

Un tipico evento a un muone appare così nello spettrometro.



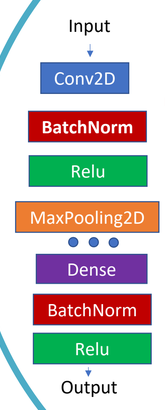


Gli eventi interessanti sono quelli ad alta energia.

Gli ingredienti necessari sono questi:

$(p_T^{lead},\ \eta^{lead},\ p_T^{sublead},\ \eta^{sublead},\ N^{muons})$

3 - Rete Neurale Convoluzionale Ternaria (t-CNN)



Per il riconoscimento immagini le CNN raggiungono prestazioni incredibili.

Assegnando un valore ternario ai pesi che descrivono la rete, è possibile ottenere un'occupazione delle risorse computazionali 16 volte inferiore ed al tempo stesso un ottimizzazione delle prestazioni.

4 – Field Programmable Gate Array (FPGA)



Composto da semplici blocchi logici che possono essere programmati e connessi tramite connessioni programmabili.

Questo tipo di dispositivo si adatta perfettamente al problema:

- Veloce
- Flessibile

5 - Strumentazione

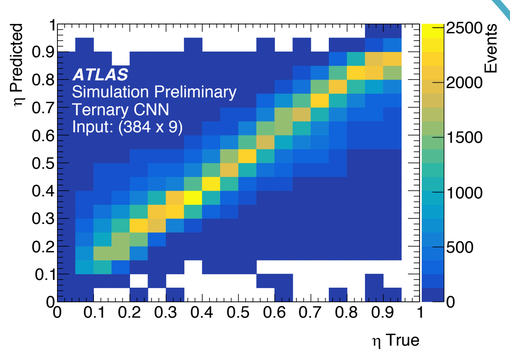
Creazione della rete con framework TensorFlow e Keras.

Allenamento della rete su GPU.

Creazione librerie C/C++ per la t-CNN.

Sintesi ed implementazione della t-CNN su FPGA con Xilinx Vivado HLS.

6 - Prestazioni



Miglioramento del 20% in efficienza rispetto all'algoritmo attualmente utilizzato.

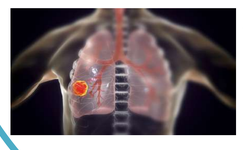
Sintetizzato con latenza max ~1 µs

7 - Potenzialità applicative

L' intelligenza artificiale ad altissima velocità può essere utilizzata in ogni problema che richiede risposte in tempo reale:

- Guida autonoma di automobili





- Costruzione ed analisi di immagini per applicazioni mediche

Progetto con applicazioni multidisciplinari:
Settori ERC PE2 e PE6

Dipartimento di Biologia
e Biotecnologie
Charles Darwin

SAPIENZA
UNIVERSITÀ DI ROMA

Analisi della comunità microbica presente nel moonmilk delle tombe etrusche di Tarquinia

Cirigliano A.[1], Mura F.[2], Negri R.[1] and Rinaldi T.[1*]

[1] Dipartimento di Biologia e Biotecnologie Edificio Fisiologia CU026 piano rialzato stanza 18*
Email: teresa.rinaldi@uniroma1.it
[2] CNIS – Centro di ricerca per le nanotecnologie applicate all'ingegneria della Sapienza

Le tombe etrusche di Tarquinia, datate tra il VI e III sec A.C., sono scavate in una roccia calcarenitica chiamata macco. In questi ambienti ipogei gli etruschi dipinsero affreschi che solo in parte sono rimasti preservati. Durante il restauro della Tomba degli Scudi, con la supervisione della Soprintendenza Archeologia, Belle Arti e Paesaggio, abbiamo indagato la natura di una patina bianca che ricopriva gli affreschi con tecniche di microscopia elettronica, microbiologia classica e metagenomica.

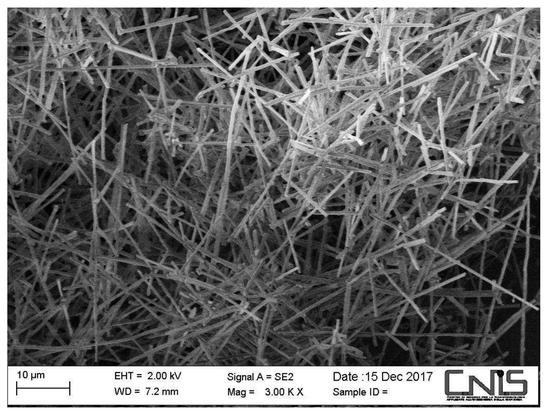


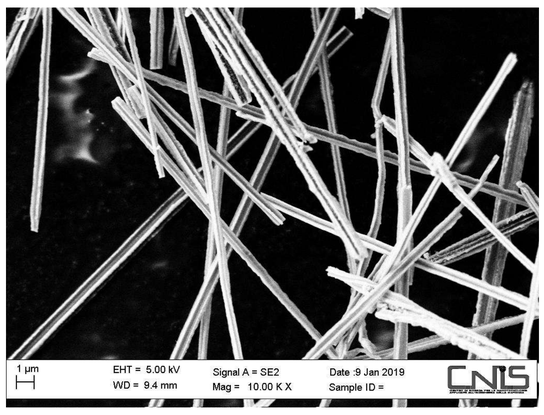
Test iniziali prima dell'intervento di restauro. La zona dell'affresco in cui la patina bianca è stata asportata rivela colori ben conservati. (Foto della restauratrice Maria Cristina Tomassetti).

Esempio di restauro di un affresco nella Tomba degli Scudi in cui è stato asportato il carbonato di calcio che ricopriva le pareti. (Foto della restauratrice Maria Cristina Tomassetti).



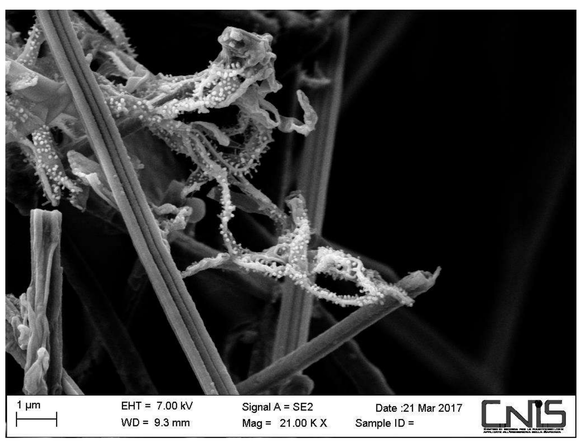
Un'indagine piu' approfondita ha stabilito che la patina bianca nella Tomba degli Scudi è una deposizione di carbonato di calcio costituita da cristalli nanostrutturati, conosciuta con il nome moonmilk, abbondante nelle grotte carsiche ma mai descritta in tombe ipogee.

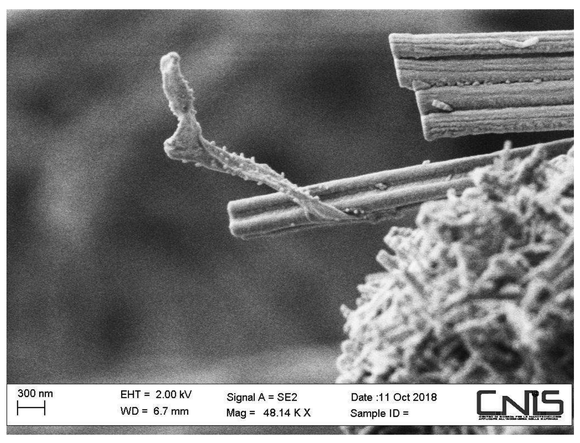




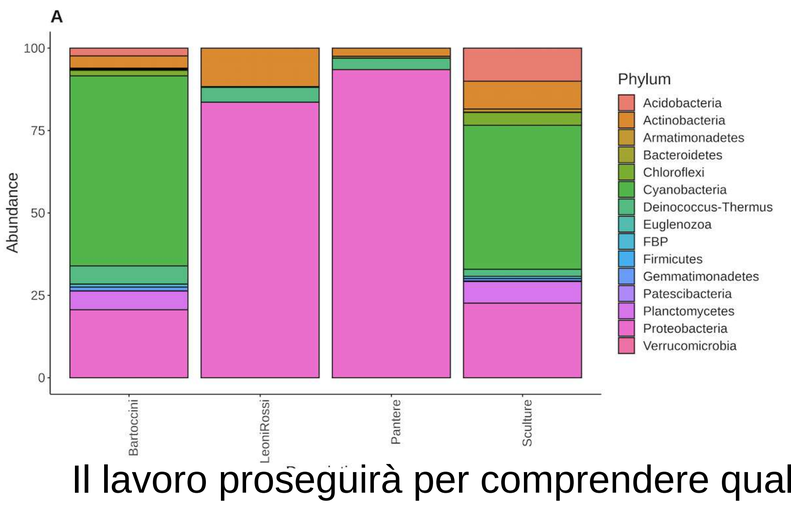
Un'analisi della patina con il microscopio elettronico a scansione ha rivelato una struttura di carbonato di calcio di grandezza nanometrica.

E' ormai dimostrato che un contributo fondamentale nella formazione di questa deposizione è dato da una comunità microbica complessa, ma non è ancora noto il meccanismo che porta alla formazione di queste strutture di carbonato di calcio.





Un'analisi con il microscopio elettronico a scansione ha rivelato una stretta connessione tra batteri (attinomiceti) ed il moonmilk.



Per comprendere quali tipi di batteri siano implicati nella produzione del moonmilk, abbiamo confrontato la comunità microbica presente nel moonmilk in quattro tombe della necropoli di Tarquinia (Tomba Bartoccini, Tomba dei Leoni rossi, Tomba delle Pantere e Tomba delle Sculture) ed abbiamo identificato i Phyla presenti in questi ambienti ipogei dove esiste un perfetto equilibrio metabolico che concorre alla formazione del moonmilk.

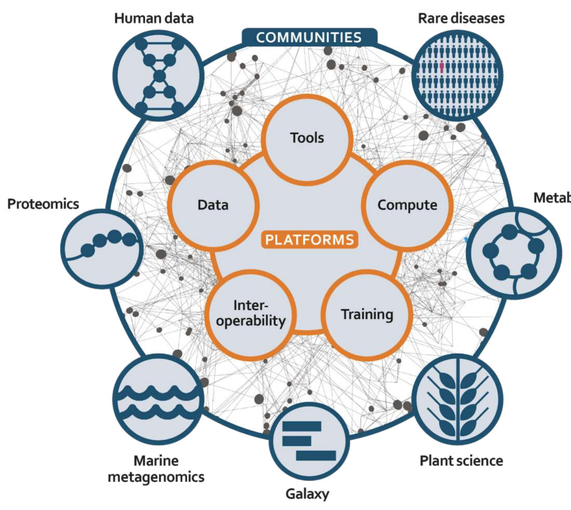
Il lavoro proseguirà per comprendere quale sia la relazione tra il macco e queste comunità microbiche e quale sia il processo che innesca la produzione del moonmilk.
Questa ricerca si è basata su una collaborazione interdisciplinare tra restauratori, archeologi, biologi e chimici. I risultati hanno permesso ai restauratori di adattare gli interventi di restauro e di mantenimento degli affreschi. Dal punto di vista biologico abbiamo selezionato dal moonmilk, con metodi microbiologici, una serie di batteri che depongono carbonato di calcio e batteri che lo sciolgono, con lo scopo di utilizzarli per applicazioni biotecnologiche in interventi di biorestauro e bioconsolodamento.

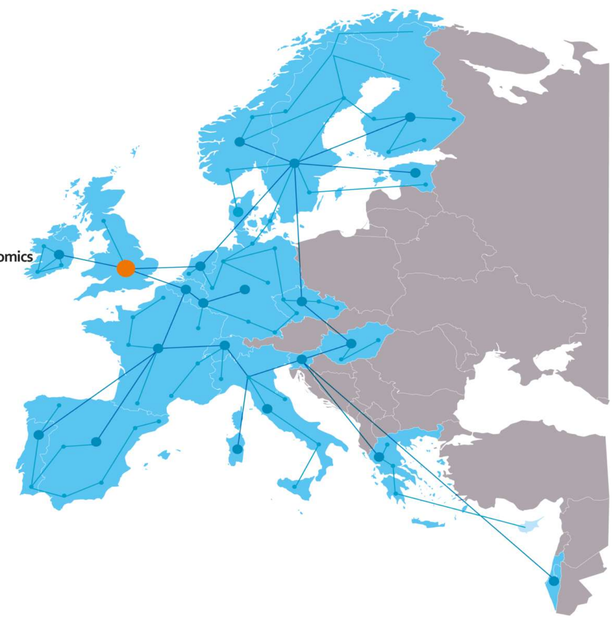
Referenze
Tomassetti, M. C., Cirigliano, A., Arrighi, C., Negri, R., Mura, F., Maneschi, M. L., Gentili M.D., Stirpe M., Mazzoni C., Rinaldi, T. (**2017**). A role for microbial selection in frescoes' deterioration in Tomba degli Scudi in Tarquinia, Italy. Scientific Reports, 7: 6027.
Cirigliano, M. C. Tomassetti, M. Di Pietro, F. Mura, M. L. Maneschi, M. D. Gentili, B. Cardazzo, C. Arrighi, C. Mazzoni, R. Negri and T. Rinaldi. (**2018**). Calcite moonmilk of microbial origin in the etruscan Tomba degli Scudi in Tarquinia, Italy. Scientific Reports, 8:15839.
Cirigliano A., Cecchini A., Tomassetti M.C., Cavalieri D., Quagliariello A., Mura F., Negri R. and Rinaldi T. (**2019**). Analysis of the microbial community in nanomeric-scale crystals of calcium carbonate in the Etruscan tombs of Tarquinia. In preparation.

ELIXIR-IIB: a growing support to national and international research in life sciences

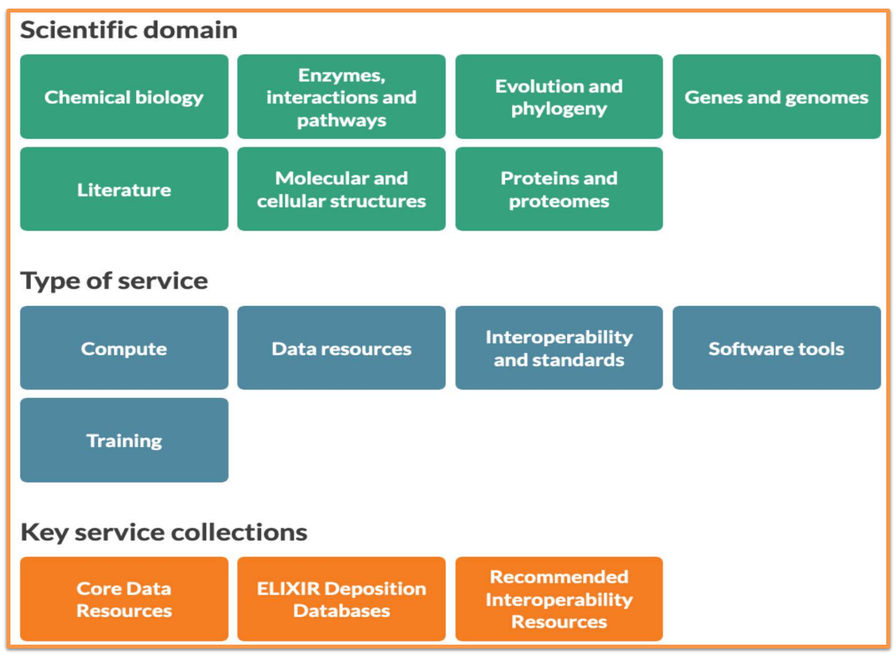
Allegra Via[1,2], Loredana Le Pera[1,2,3], Veronica Morea[1,2], David Sasah Staid[4,2], Stefano Pascarella[4,2]
[1]IBPM-CNR; [2]ELIXIR Italy; [3]IBIOM-CNR; [4]Dipartimento di Scienze Biochimiche «A. Rossi Fanelli»
Email: stefano.pascarella@uniroma1.it; allegra.via@cnr.it

ELIXIR is a European Research Infrastructure that supports and brings together resources (databases, software tools, training materials, cloud storage and supercomputers) from across Europe, to sustain research in life sciences. The goal is to make it easier for scientists from academia, research institutions and industry to find and share data, exchange expertise and agree on best practices. The scientific and technical activities in ELIXIR are run by five Platforms and a number of Communities. The five Platforms (**Data**, **Tools**, **Compute**, **Interoperability** and **Training**) comprise experts who define strategies and provide services such as tool development, data management, etc. Communities comprise experts who work in specific scientific areas (e.g. structural bioinformatics, rare diseases, marine metagenomics). ELIXIR adopts a "Hub and Nodes" organisation model. The national Nodes are the >20 participating member states. Each Node is, in turn, a network of organizations.



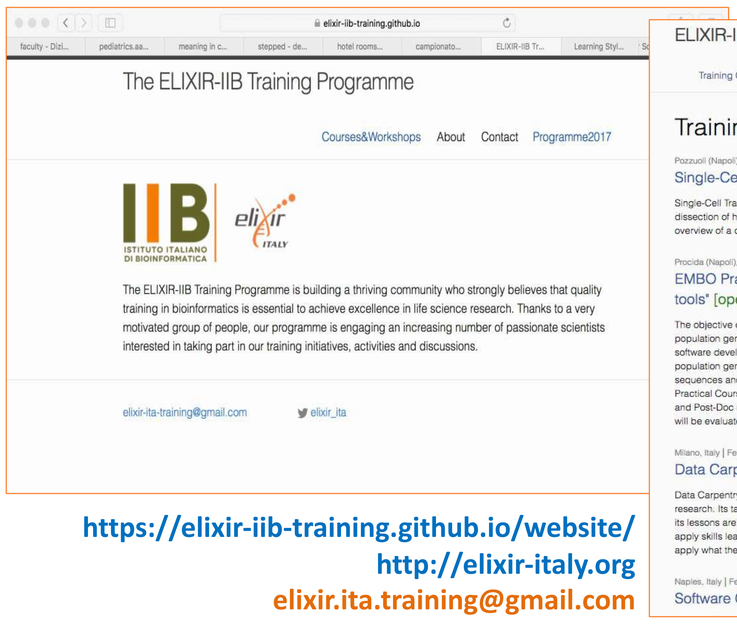


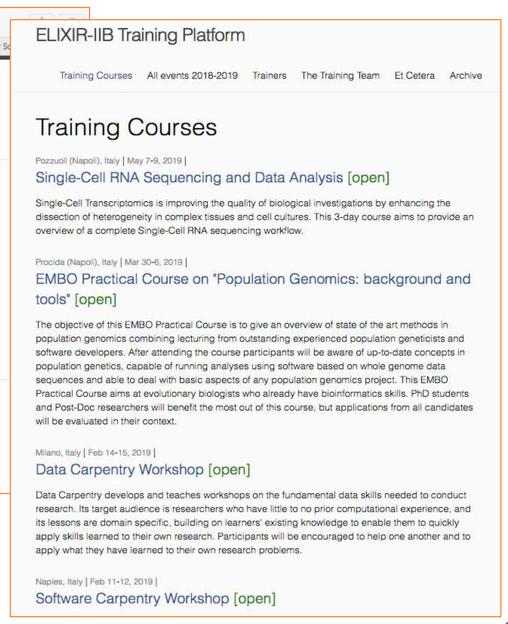
The Italian Node of ELIXIR has been formally established as a Joint Research Unit named ELIXIR - Infrastruttura Italiana di Bioinformatica (ELIXIR-IIB). It is in charge of the coordination and delivery of existing bioinformatics services at a national level. ELIXIR-IIB is led by the National Research Council (CNR) of Italy. It currently involves 23 partners, including universities and research institutions/facilities of national relevance, including "Sapienza" University of Rome and INFN. The organization of ELIXIR-IIB mirrors ELIXIR at the European level. It includes five operational Platforms (Data, Tools, Compute, Interoperability and Training) and several thematic communities.



The ELIXIR-IIB Training Platform is coordinated by the Bioinformatics group at IBPM-CNR, in Rome. This Platform has set-up a training community spanning all ELIXIR members states, which comprises instructors and learners who actively embrace the idea that quality education is essential to perform high quality research in the life sciences. The Platform supports researchers and professionals in the acquisition of specialised bioinformatics, computational and data management skills; it aims to strengthen national training programmes, grow bioinformatics capacity and competence, and empower users to utilise ELIXIR's services and tools; it closely collaborates with other ELIXIR Nodes in Europe by developing and promoting a large variety of national and international training and training-related events, projects and initiatives. These include:

- Development of targeted training programmes for researchers, developers, infrastructure operators, trainers
- Bioinformatics courses
- Training courses in computational and data management
- 'Train the Trainer' workshops
- Training material development
- E-Learning courses
- Dissemination of best practices for software development
- Workshops for the Rare Disease community
- Bring Your Own Data events
- Quality and Impact program





https://elixir-iib-training.github.io/website/
http://elixir-italy.org
elixir.ita.training@gmail.com
@elixir_it

Riferimenti recenti

1) Gurwitz KT et al. A framework to assess the quality and impact of bioinformatics training across ELIXIR. PLoS Computational Biology. *Under revision*.
2) Via A et al. (2017). A new pan-European Train-the-Trainer Programme for bioinformatics: Pilot results on feasibility, utility and sustainability of learning. Briefings in Bioinformatics.
3) Morgan SL et al. (2017) The ELIXIR-EXCELERATE Train-the-Trainer pilot programme: empower researchers to deliver high-quality training. F1000Research.

Dipartimento di Fisica
SAPIENZA Università di Roma

ArielRad: the ARIEL Radiometric Model

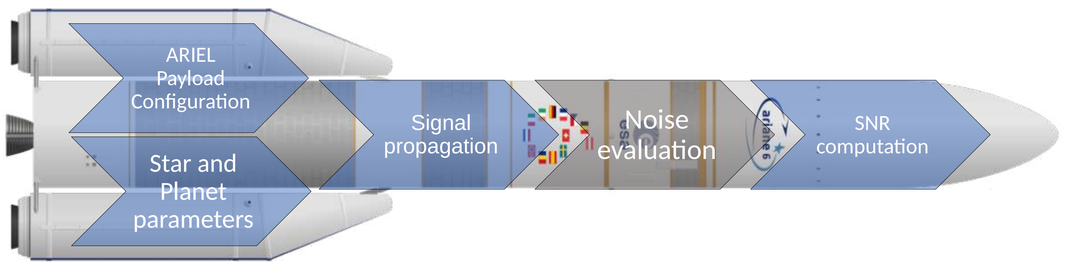
Lorenzo Mugnai*, Billy Edwards, Andreas Papageorgiou, Enzo Pascale, Subhajit Sarkar
Dipartimento di Fisica, Edificio Marconi, CU013, piano terzo, stanza 301
Email: lorenzo.mugnai@uniroma1.it

ArielRad simulator software

The ArielRad simulator is a python software. The package has a complete documentation, compliant to the python standards. It is completely customizable in the simulation, thanks to two xml configuration files and a user defined target list in MS Excel format.



Starting from these input files, the code propagates the star signal through the payload, evaluates the noise and, simulating the expected planet signal, estimates the SNR on the detection of atmospheric features in transmission and emission.



Implemented Noise Model

ArielRad implements a physically motivated noise model, able to reproduce stationary systematics

$$\frac{Var(s)}{S^2} = \left[\frac{\sigma_R^2}{R^2}\left(1+\frac{N_{pix} I_D}{k\eta_s QE\, N_0}\right)^2 + \frac{\sigma_t^2}{\Delta t^2} + \frac{\sigma_{\eta_s}^2}{\eta_s^2} + \frac{\sigma_{QE}^2}{QE^2}\right]\times\frac{\Delta t}{T} + \quad \text{(gain terms)}$$

$$+\frac{1}{k\eta_s QE\, N_0}\times\frac{1}{\epsilon T} + \quad \text{(photon noise term)}$$

$$+\frac{N_{pix} I_D + N_{pix}\sigma_{rd}^2/(\epsilon\Delta t)}{(k\eta_s QE\, N_0)^2}\times\frac{1}{\epsilon T} + \quad \text{(dark current and read noise)}$$

$$+p_0^2 \quad \text{(Payload noise floor)}$$

20% margin are included on CBE parameters estimates and the photon noise term is artificially increased to account for astrophysical and data processing. Also the detector ramp fitting is simulated, using the MULTIACCUM equation from Rauscher (2007):

$$\sigma_{total}^2 = \frac{12(n-1)}{n(n+1)}\,\sigma_{read}^2 + \frac{6(n^2+1)}{5n(n+1)}(n+1)t_g f$$

From the noise, ArielRad estimates the observable contrast ratio, and its variance

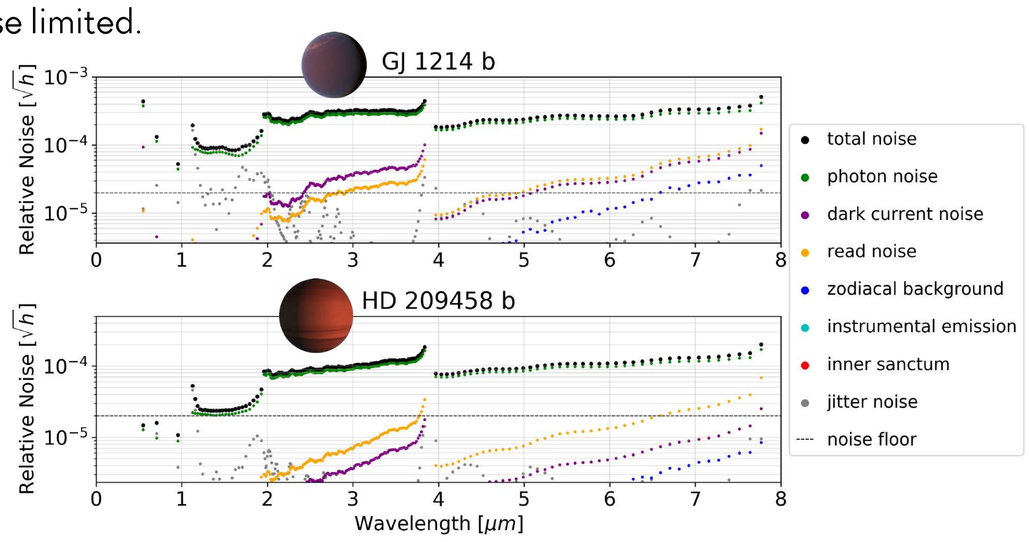
$$CR = \frac{S_{OOT}(\lambda) - S_{IT}(\lambda)}{S_{OOT}(\lambda)},\ VAR(CR,\lambda) = \frac{VAR(S_{OOT}) + VAR(S_{IT})}{E[S(\lambda)]^2} + \sigma_{floor}^2$$

and then the SNR, simulating the transit or eclipse detection

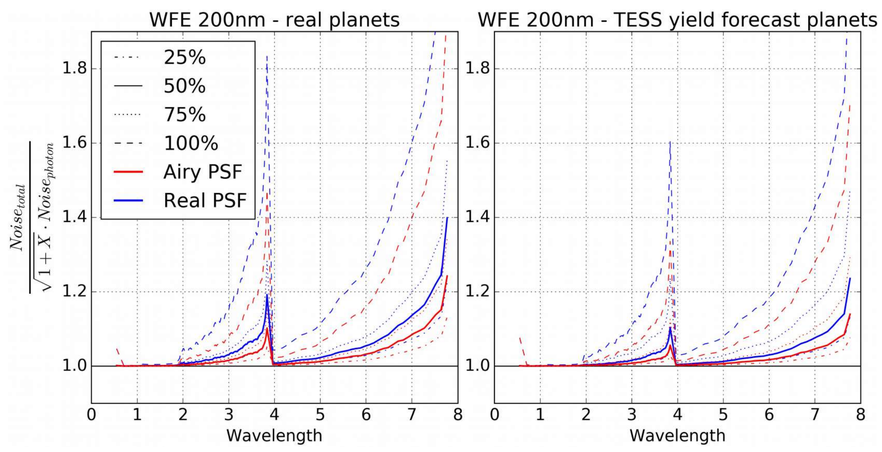
$$SNR = \frac{S_{planet}(\lambda)/E[S(\lambda)]}{\sqrt{VAR(CR,\lambda)}}$$

Case studies

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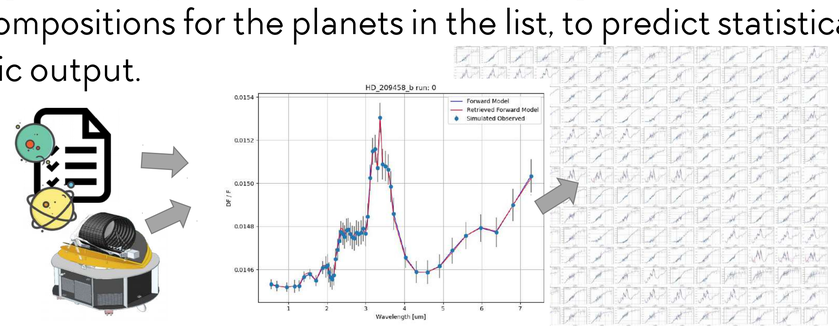


ArielRad is being also used to demonstrate that an observing programme with 1000 exoplanetary targets can be completed within the boundary of the mission lifetime, reaching SNR>7 in the IR spectral channels. The list currently includes a combination of exoplanets already discovered and a yield forecast for the TESS space mission (see Edwards et al. 2019).



Future applications

ArielRad has been combined to other software as the retrieval code TauREx. Combining the two we build a new simulator that , given the payload configuration, scrolls the target list and for each planet produces an *ARIEL* realistic simulated observation and performs a spectral retrieval.
Allowing the analysis of hundreds of planets at once, this simulator will be used to investigate multiple scientific cases, exploring different atmosphere compositions for the planets in the list, to predict statistically *ARIEL* scientific output.



Edwards, B., Mugnai, L., Tinetti, G., Pascale, E. & Sarkar, S. [2019] *AJ* **157**, 242, *"An Updated Study of Potential Targets for Ariel"*

Dipartimento di Fisica
SAPIENZA Università di Roma

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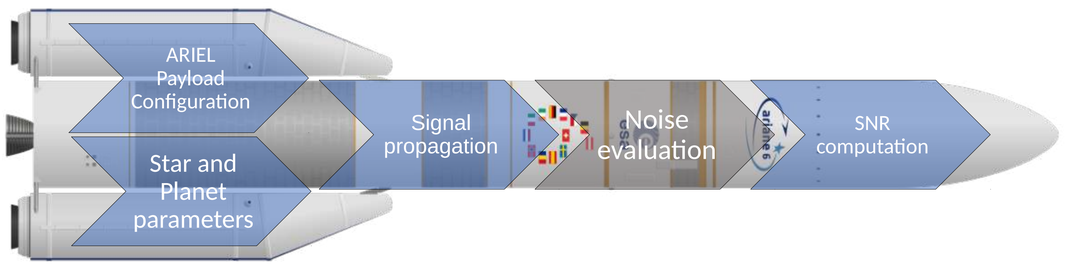
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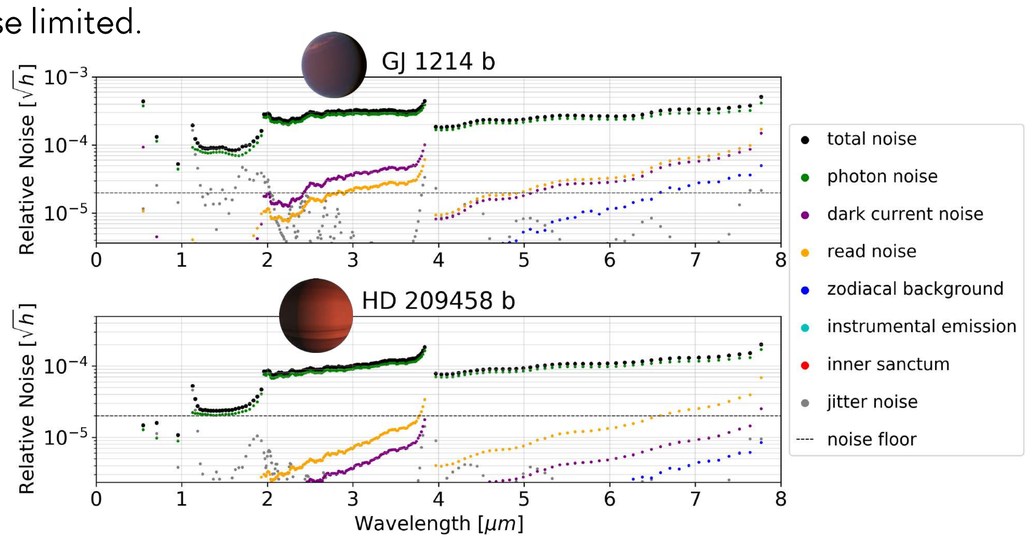
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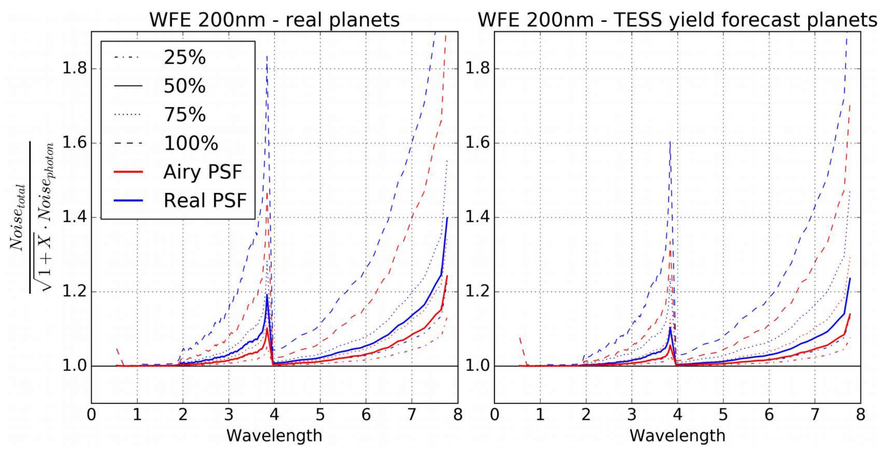
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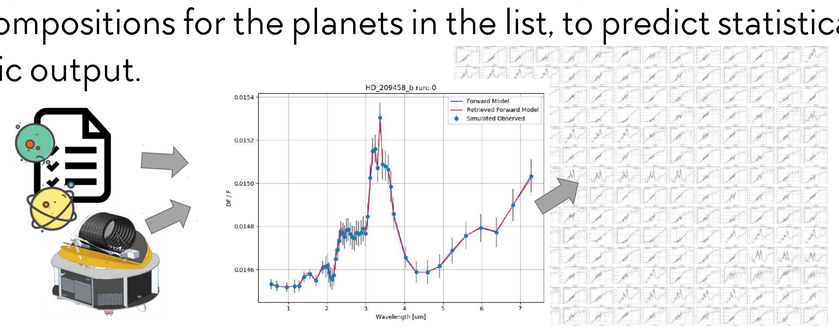


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Dipartimento di
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The Mediterranean Region risks aridification – Hints from the oldest lake of Europe

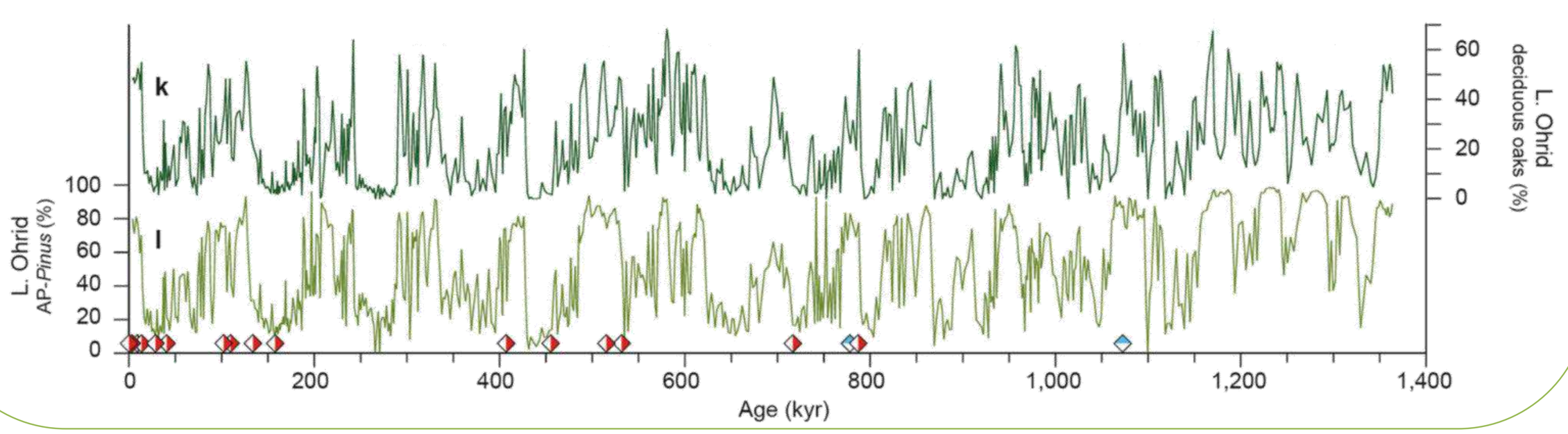
Alessia Masi, Laura Sadori
Dipartimento di Biologia Ambientale, Edificio Botanica, CU022, piano III, stanza 311
Email: alessia.masi@uniroma1.it, laura.sadori@uniroma1.it

Mediterranean Region is becoming more and more arid. The study of the past environmental changes is essential in order to assess the possible future scenarios. The SCOPSCO (Scientific COllaboration on Past Speciation Conditions in lake Ohrid) International Scientific Team provide the paleo-environmental study on Europe's oldest lake, Lake Ohrid which is located on the boundary between Albania and Northern Macedonia (Wagner et al. 2019). The lake is well-known for its exceptional biodiversity, it hosts over 300 endemic animal and plant species.



The objective of the research was to study the climate of the last 1,36 million years using geochemical and pollen analyses. The coring campaign has reached a depth of 568 metres below 245 metres of water. It took the researchers five years to analyse the lakebed cores describing the alternance of glacial and interglacial periods.
One of the most important results is provided by the fossil pollen, studied by an international group of palynologists, the SCOPSCO Pollen Group. During warmer periods, with higher CO2 content in the atmosphere, seasonal contrast increased with very arid summers and wet autumns with strong precipitations. Moreover, the study also revealed important relations between the Mediterranean climatic system and the African monsoon system. The comparison between the climatic data and models developed in the article indicates the intensification of storms generated in the Western Mediterranean, especially in the autumn. The increase in cyclogenesis is related, according to the research, to the anomalous heating up of the sea surface during the summer.
Similar effects could be caused by recent anthropic climatic warming. Indeed, in this context, research conducted on Lake Ohrid could help to solve a number of uncertainties that linger in the report of the UN Inter-governmental Panel on Climate Change (IPCC) and improve its future projections.

nature
International journal of science



Wagner B. Vogel H., Francke A., Friedrich T., Donders T., Lacey J., Leng M., Regattieri E., Sadori L., Masi A. et al., 2019. Mediterranean winter rainfall in phase with African monsoon during past 1.36 million years. Nature 573, 256-260.

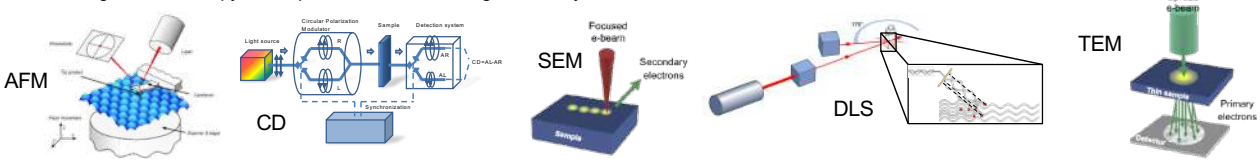
Il poster tratta un argomento specifico di una linea di ricerca sviluppata di recente

Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

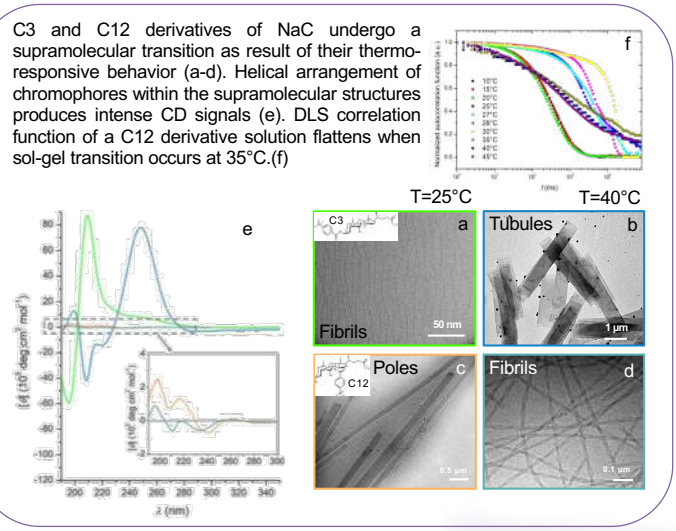
Natural amphiphiles: supramolecular and supracolloidal building blocks for nanotechnology applications

Jacopo Cautela*, Emilia Severoni*, Luciano Galantini
Dipartimento di Chimica, Edificio Cannizzaro, CU 014, piano 2°, stanza 261
Email: Jacopo.cautela@uniroma1.it, Emilia.severoni@uniroma1.it, Luciano.galantini@uniroma1.it

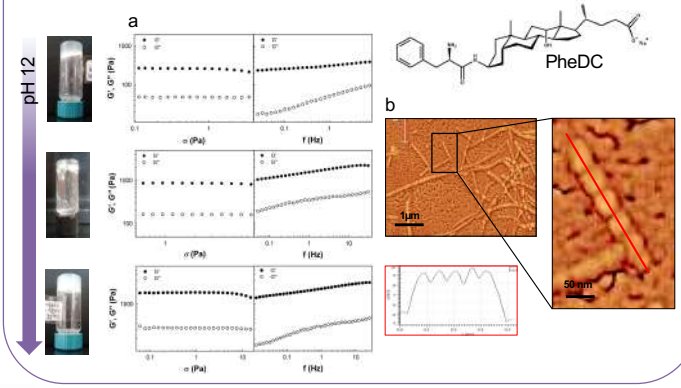
Bile salts, a class of natural surfactants, and their synthetic derivatives are characterized by the ability in water to aggregate in supramolecular structures with peculiar morphological and physico-chemical properties. A depeer comprehension of their self-assembly behavior expands the landscape of potential applications in nanotechnology, from the stabilization of carbon nanotubes suspensions or the encapsulation of drugs, to the preparation of supracolloidal frameworks and chiral inorganic structures. Scattering and Microscopy techniques are used to investigate such systems.



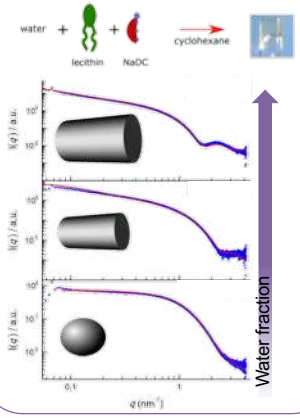
C3 and C12 derivatives of NaC undergo a supramolecular transition as result of their thermo-responsive behavior (a-d). Helical arrangement of chromophores within the supramolecular structures produces intense CD signals (e). DLS correlation function of a C12 derivative solution flattens when sol-gel transition occurs at 35°C.(f)

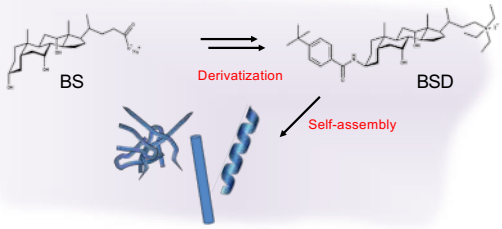


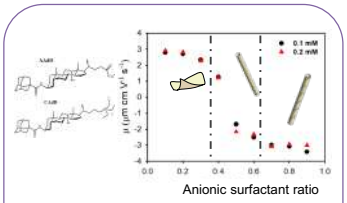
Specific phenylalanine derivatization on C3 of NaDC can vary the self-assembly properties of phenylalanine, giving rise to more efficient gelling systems than the precursor. Dynamic rheology measurements show improved mechanical properties of the gels upon lowering the pH from 12 to 10 (a). AFM micrographs show the presence of helical ribbons (b).



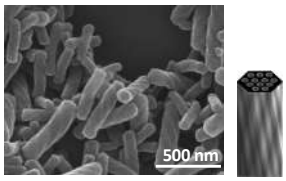
In oil, the interplay between lecithin and NaDC gives rise to a micellar sphere-to-rod transition in presence of small amounts of water. The elongation process, monitored through SAXS, culminates in the formation of a gel of wormlike micelles.





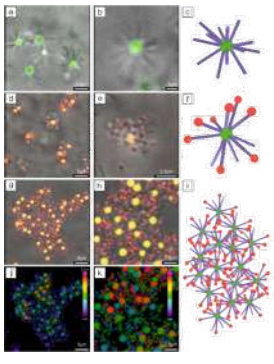


Bile salt derivative based catanionic mixtures assemble in tubules and lamellae depending on the mixture composition. They present exceptional stability close to the equimolar ratio and morphology and charge tunability.



Bile salts as co-directing agent in mixture with CTAB enable the production of chiral mesoporous silica nanoparticles. They can be used as a chiral environment to allow specific metallic nanoparticles patterns.

A controlled supracolloidal assembly is induced exploiting specific interactions between BSD supramolecular tubules and fluorescent microgels, obtaining supracolloidal hierarchical frameworks. The association is imaged through confocal laser scanning microscopy (a-k).



Cautela J., Severoni E., Redondo-Gómez C., di Gregorio M. C., Del Giudice A., Sennato S., Angelini R., D'Abramo M., Schillén K., Galantini L., *Colloid Surfaces B*, 2019, **110556**
Cautela J., Giustini M.,Pavel N. V., Palazzo G., Galantini L., *Colloid Surfaces A*, 2017, **532**, 411-419
Travaglini L., di Gregorio M. C., Severoni E., D'Annibale A., Sennato S., Tardani F., Giustini M., Gubitosi M., Del Giudice A., Galantini L., *J. Colloid Interf. Sci.*, 2019, **554**, 453-462
di Gregorio M. C., Severoni E., Travaglini L., Gubitosi M., Sennato S., Mura F., Redondo – Gómez C., Jover A., Pavel N. V., Galantini L., *Phys. Chem. Chem. Phys., 2018,* ***20****, 18957 -18968*
Cautela J., Lattanzi V., Månsson L. K., Galantini L., Crassous J., *Small*, 2018, 1803215

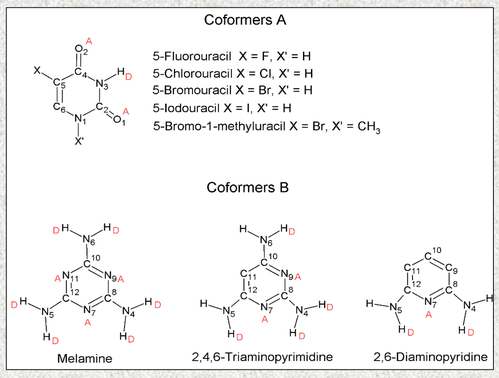
Scienze della Vita Exploring the role of neutral/ionized TPI hydrogen bonds and halogen bonds for multifacial recognition in 5-halouracils/aminoazine cocrystals

Gustavo Portalone[1] and Kari Rissanen[2]

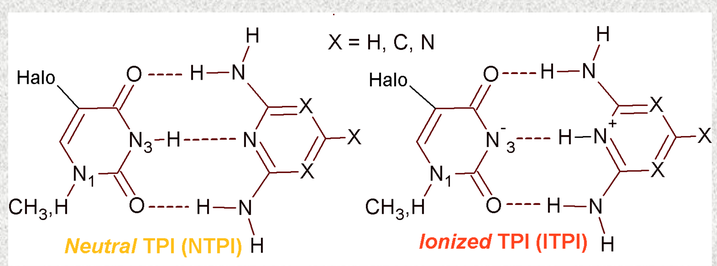
[1]*Department of Chemistry, Ed. "S. Cannizzaro", ground floor, room 43, gustavo.portalone@uniroma1.it*

[2]*Department of Chemistry, University of Jyväskylä, 40014 Jyväskylä, Finland*

A systematic analysis using single crystal X-ray diffraction was performed to explore the role exerted by potential proton-transfer reactions in the supramolecular structures of A-B cocrystals formed by 5-haloderivatives of uracil (A) coupled with 2-aminoadenine simulants (aminoazines, B). Twelve new heterodimers were synthesized in different stoichiometry and cocrystallized by solvent co-grinding followed by solution crystallization. In the A-B cocrystals, uracil or 1-methyluracil with halide modification at the 5 position (F, Cl, Br, I) were coupled with amino-aromatic *N*-heterocycles (melamine, Mel, 2,4,6-triaminopyrimidine, Tap, 2,6-diaminopyridine, Dap) as multivalent site for pyrimidine nucleobase recognition (Scheme 1). The XRD analysis showed that, next to the expected *neutral* three-point hydrogen bonds (NTPI), *ionized* three-point hydrogen bonds (ITPI), depending on the acid/base properties of the components, were used for *WC* multifacial recognition (Scheme 2). Noteworthy, *the formation of the charged TPI, favored by A → B proton transfer, takes always place between the more acidic site of the 5-halonucleobases (N3 atom) and the more basic site (N_{ring} atom) of 2,4,6-triaminopyrimidine or 2,6-diaminopyridine*, and melamine recognition unit results to be insufficiently basic to accept a proton.

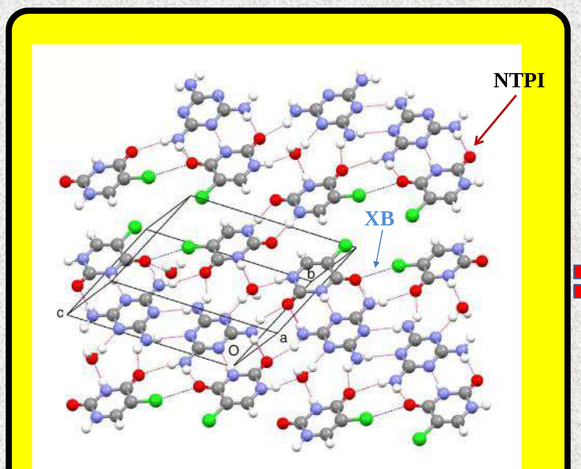


Scheme 1

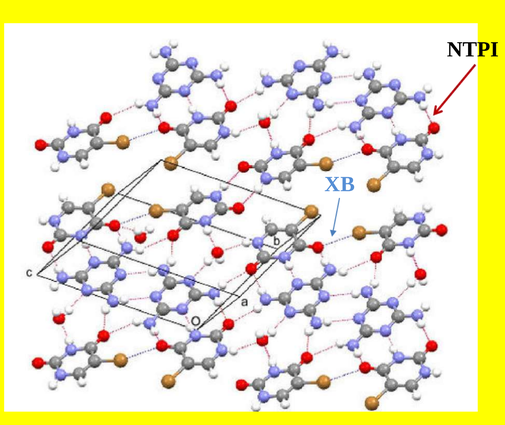


Scheme 2

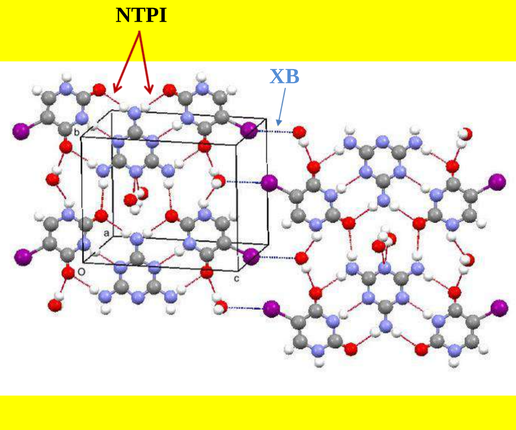
Here, neutral WC-pairs are observed for ΔpKa < ~ -3 (Mel as coformer B), and ionized acid-base WC-pairs are observed for ΔpKa > ~ -1 (Dap as coformer B). In the domain of ΔpKa between ~ -3 and ~ -1, i. e. when Tap is coformer B, proton transfer may (BruraTap, IuraTap and BrmuraTap) or may not occur (CluraTap). The general ability of pyrimidine nucleobases to provide electron donating groups to *halogen bonding* has been confirmed in seven cocrystals containing the 5-chloro, 5-bromo or 5-iododerivatives coupled with melamine or 2,4,6-triaminopyrimidine.



CluraMel Monofacial recognition

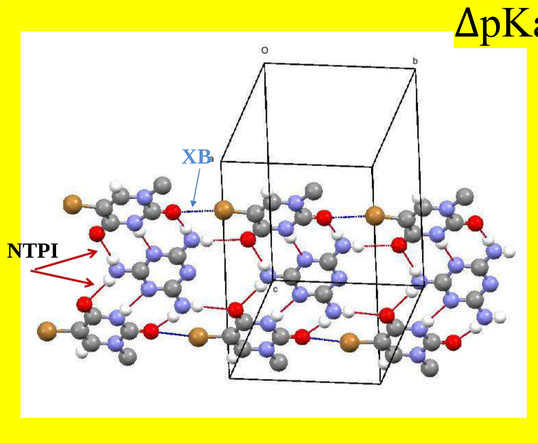


BruraMel Monofacial recognition

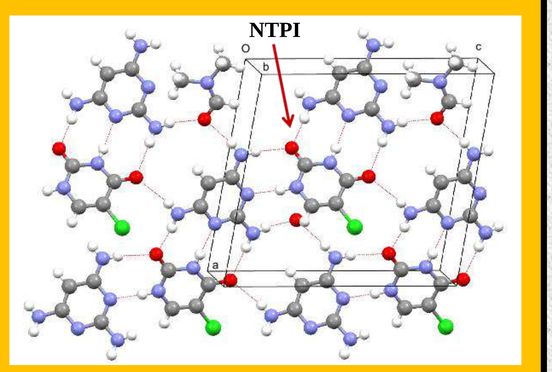


IuraMel Bifacial recognition

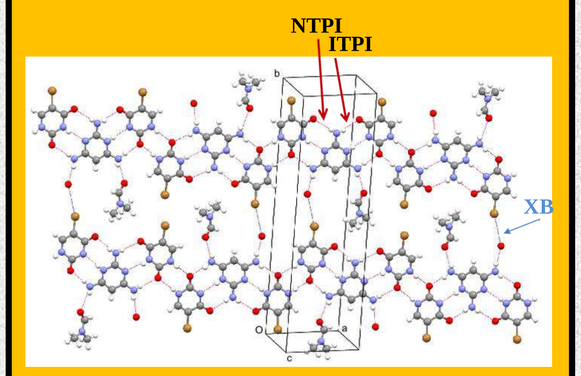
ΔpKa < ~ -3



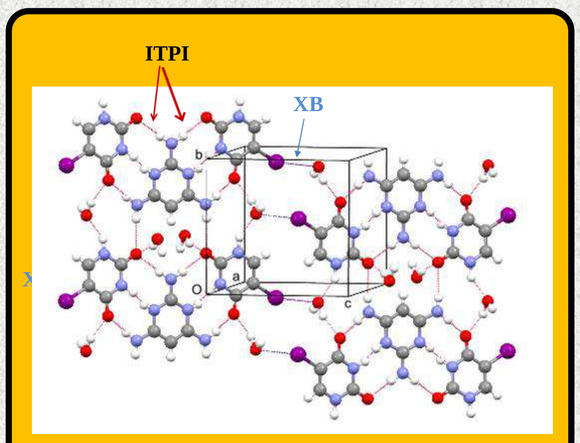
BrMuraMel Bifacial recognition



CluraTap Monofacial recognition

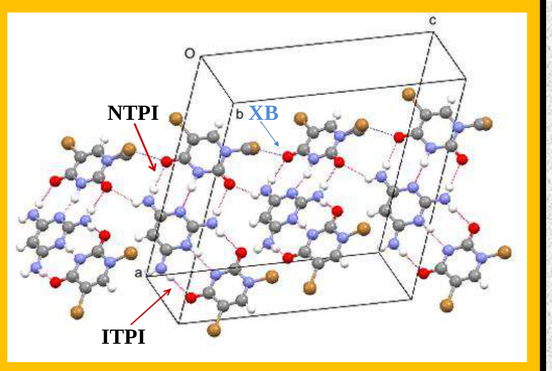


BruraTap Bifacial recognition

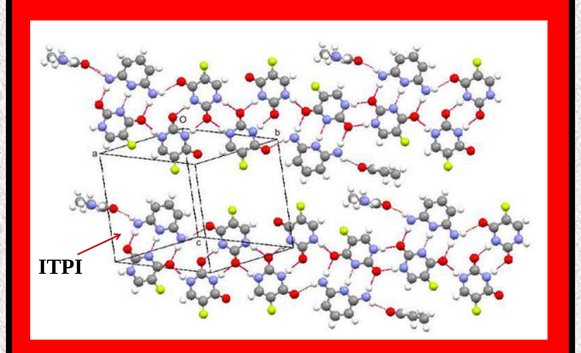


IuraTap Bifacial recognition

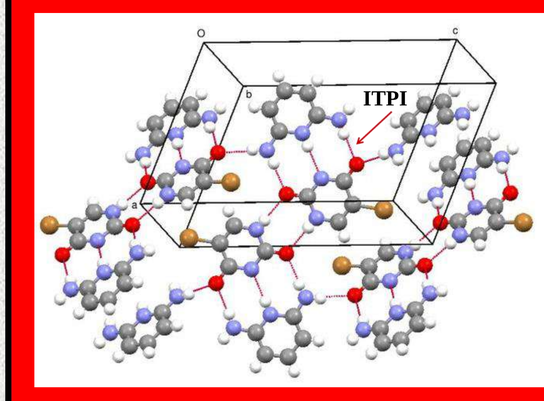
ΔpKa between ~ -3 and ~ -1



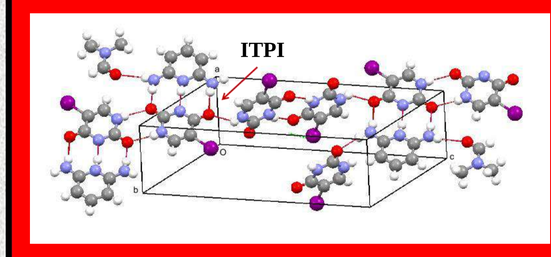
BrMuraTap Bifacial recognition



FuraDap Monofacial recognition

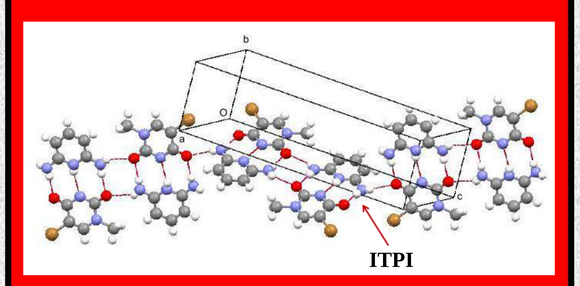


BruraDap Monofacial recognition

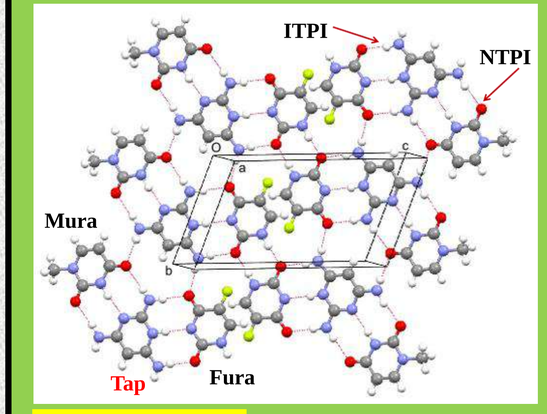


IuraDap Monofacial recognition

ΔpKa > ~ -1



BrMuraDap Monofacial recognition



FuraTapMura Bifacial recognition



Considerations of the relative acidities of coformers A and of the relative basicities of coformers B allowed us to design and characterize by single-crystal X-ray diffraction the *first ternary pyrimidine nucleobase-containing cocrystal based on the JANUS-WEDGE concept*: the nucleobase-*Janus*-nucleobase (1:1:1) triad showing a 2,4,6-triamino pyrimidine (Tap) molecule wedged *via* neutral and ionized TPI between the 1-methyluracil/5-fluorouracil pair in reverse *WC* fashion.

Ref: G. Portalone, K. Rissanen:"Multifacial Recognition in Binary and Ternary Cocrystals from 5-Halouracil and Aminoazine Derivatives". Cryst. Grow Des., 18, 5904-5918 (2018). G. Portalone:"Site Selectivity of Halogen…Oxygen Bonding in 5- and 6-Haloderivatives of Uracil". Crystals, 9, 467 (2019).

Ambiente e Territorio

Dipartimento di Scienze della Terra
SAPIENZA UNIVERSITÀ DI ROMA
Dipartimento di Chimica
SAPIENZA UNIVERSITÀ DI ROMA

Integrated Approach to Support the Remediation of Contaminated Sites

Carlo Esposito*, Marco Petrangeli Papini, Paolo Ciampi
Department of Earth Science, Mineralogy building, CU 005, 2nd floor, room 320
Email: carlo.esposito@uniroma1.it

1. Introduction

The research is inscribed within the framework of activities held by a multidisciplinary group of researchers (GEO/05, ING-IND/25, GEO/11, ICAR/03) that work together to bring innovative solutions for remediation strategies. Integrated data management processes have important implications on the efficiency of the selection, planning, and control of remediation operations.

2. Methodology

The experimental work carried out in sites that exhibit different geological and contamination contexts highlighted the contribution of the multitemporal and multidisciplinary geodatabase that was created for the integrated management, representation and analysis of different data. The creation of a 3D hydrogeophysical model represents an effective "near real time" decision support system able to manage and release data during the different remediation phases (Binley et al., 2015). The construction of a multi-source conceptual model along with LIF (Laser Induced Fluorescence), ERT (Electrical Resistivity Tomography), and multilevel piezometers, capture the information related to the hydrogeochemical sphere in all its dimensions.

3. Results

The hydrogeophysical model reaches a high-resolution characterization of underground geological heterogeneities (Fig. 1-2) and contaminated areas (Fig. 3).

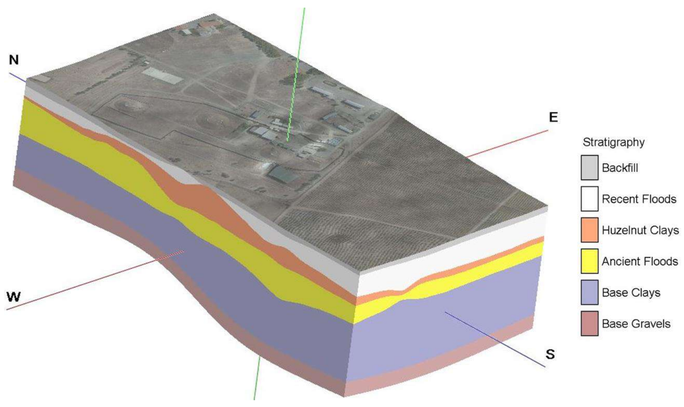


FIGURE 1. Geological model of the Decimomannu military base. The three-dimensional lithostratigraphic model uses a vertical exaggeration factor to mark the lithological steps

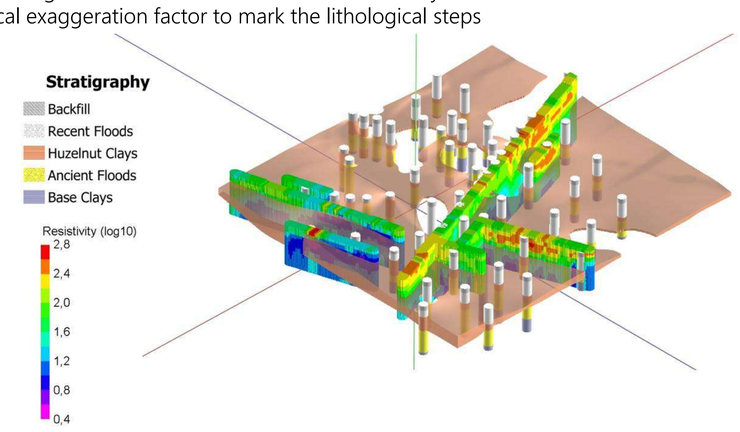


FIGURE 2. 3D model illustrating the results of the ERT investigations, the layer of hazelnut clays and stratigraphic logs at Decimomannu. Data show a good correlation between the low resistivity layers and the clay levels ascribable to the hazelnut clays, characterized by a greater relative electrical conductivity

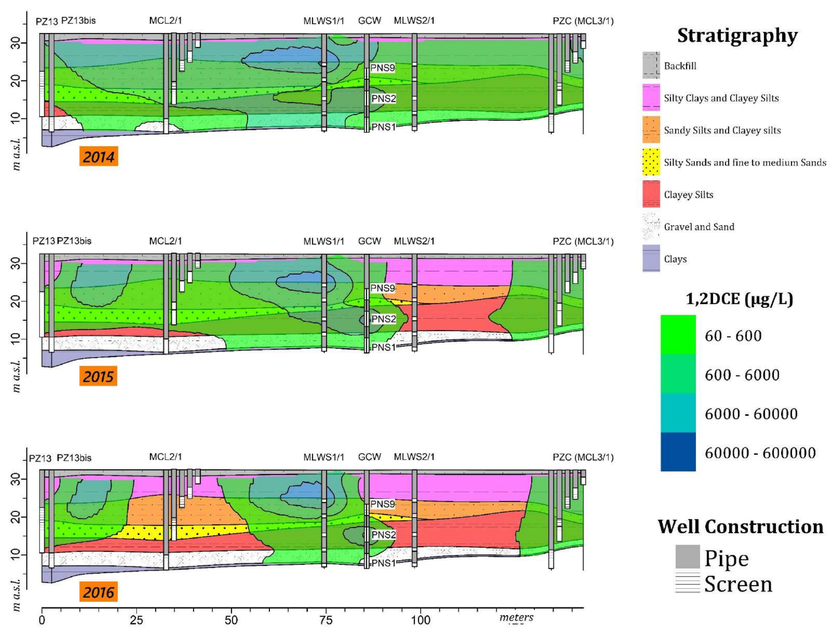


FIGURE 3. Hydrogeochemical sections relating to concentrations of 1,2-Dichloroethene (1,2-DCE) detected in multilevel piezometers at an industrial site operating in north Italy. The high-resolution characterization, in geological and chemical terms, displays the association of a significant mass of contaminants with lenses of fine materials (slow-release sources of contaminants) (Ciampi et al., 2019)

The continuous convergence of different types of geomodelling ensures the interchangeability of information in the multidisciplinary nature of the elements involved. The information exchange, the overlapping of knowledge, and the high-resolution characterization of environmental variability capture the hydrogeological uniqueness, the geophysical peculiarity and the contamination dynamics (Fig. 4).

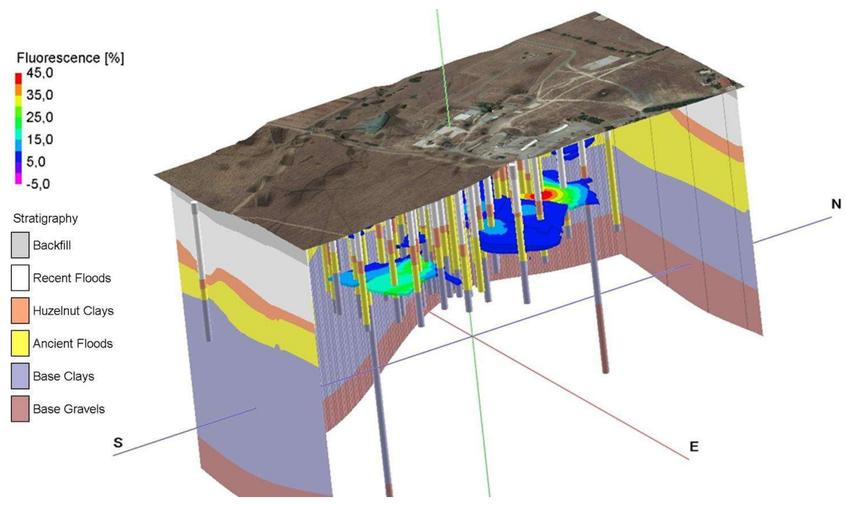


FIGURE 4. Multi-source model of Decimomannu base, showing stratigraphic logs and 3D geological fence diagrams. Fluorescence peaks obtained using the LIF technique on 32 investigation points determined the presence of the residual fraction of spilled fuel (secondary contamination source)

A pilot test is the last step of the evaluation process and is designed to monitor (Fig. 5), calibrate, adjust, and optimize the operating conditions at the field scale (Fig. 6). The results obtained during the experimentation support a definitive design choice that provides, for the full-scale intervention, the application of strategy able to determine the remediation of the entire identified contamination source (Fig. 7).

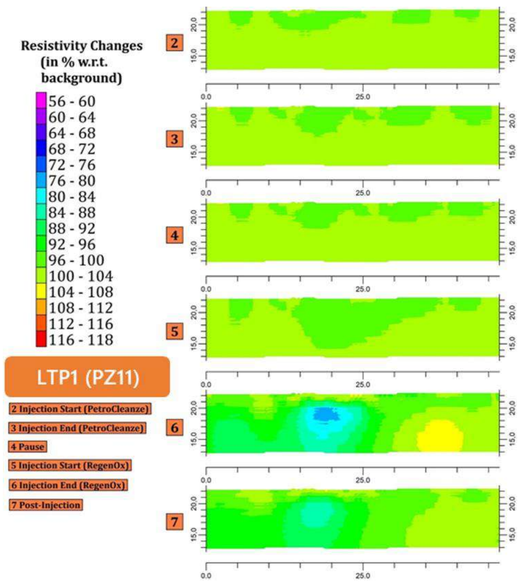


FIGURE 5. ERT profiles realized during the activities of reagent injection at the pilot scale (Decimomannu). The sections reveal a good diffusion of the second reagent in the aquifer (tested by the blue band)

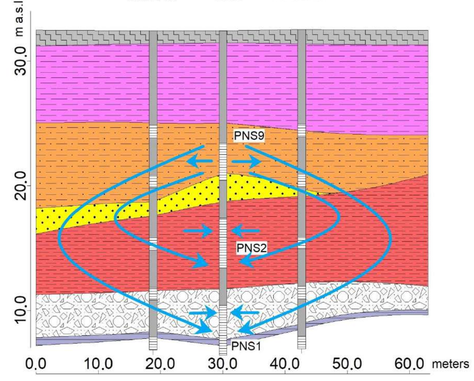


FIGURE 6. Configuration of the Groundwater Circulation Well (GCW) implemented in the specific lithostratigraphic situation at an industrial site operating in north Italy. The recirculation system evidenced the mobilization of contaminants adsorbed and/or trapped as a residual phase on low permeability horizons (Ciampi et al., 2019).

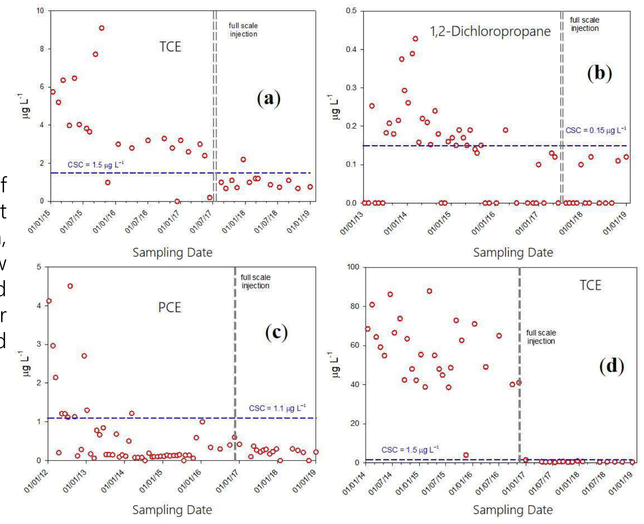


FIGURE 7. Concentration trends of chlorinated solvents measured in different intervention areas at Bologna railway station, after the reagent injection. The graphs show a reduction in chlorinated solvents detected after full scale intervention in the aquifer below the threshold limits (CSC) established by Italian legislation

4. Conclusions

The hydrogeophysical model and the thematic database act as integrated and continuously updated tools, able to optimize the investigations during the characterization phase, support the choice of the strategies in planning phase, managing and calibrating in progress the intervention modalities according to innovative approaches during the remediation phase.

Binley, A.; Hubbard, S.S.; Huisman, J.A.; Revil, A.; Robinson, D.A.; Singha, K; Slater, L.D. The emergence of hydrogeophysics for improved understanding of subsurface processes over multiple scales. Water Resour. Res. 2015, 51, 3837 - 3866, doi:10.1002/2015WR017016;
Ciampi, P.; Esposito, C.; Petrangeli Papini, M. Hydrogeochemical Model Supporting the Remediation Strategy of a Highly Contaminated Industrial Site. Water. 2019, 11, 1371. https://doi.org/10.3390/w11071371;

LA MICROZONAZIONE SISMICA DEL TERRITORIO QUALE STRUMENTO INTERDICIPLINARE DI MITIGAZIONE DEL RISCHIO GEOLOGICO INDOTTO DA TERREMOTI: LA RECENTE ESPERIENZA MATURATA IN APPENNINO CENTRALE

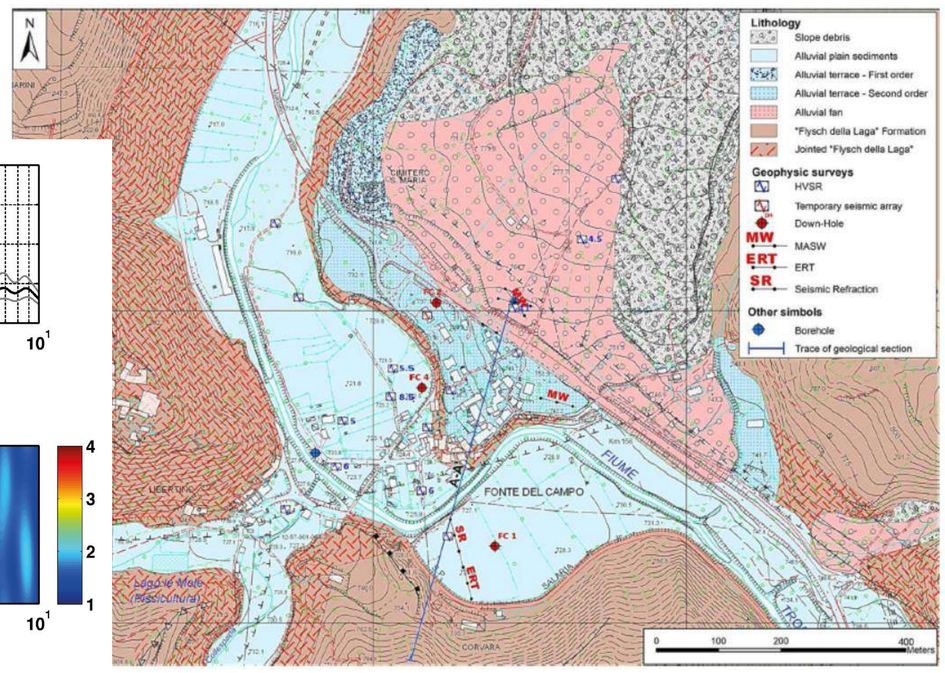
Martino S.*[1], Bozzano F.[1], Della Seta M.[1], Cercato M.[2], Esposito C.[1], Hailemikael S.[3], Martini G.[3], Paciello A.[3], Peloso A.[3], Scarascia Mugnozza G.[1], Troiani F.[1]

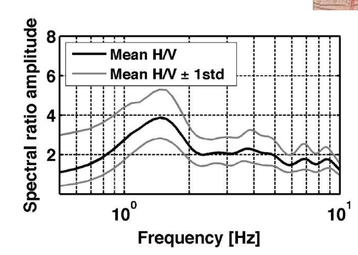
**Dipartimento di Scienze della Terra (DST-Sapienza), Edificio Mineralogia, CU005, piano 3 stanza 336*

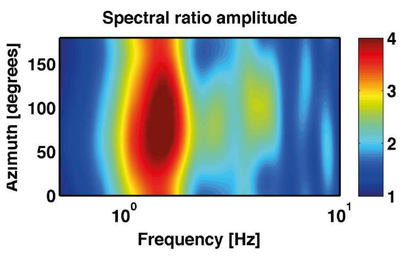
Email: salvatore.martino@uniroma1.it, [1] DST (Sapienza), [2] DICEA (Sapienza), [3] ENEA (Frascati e Casaccia, Roma)

L'Italia è tra i pochi paesi al mondo ad essere dotato di linee guida (redatte dalla Protezione Civile Nazionale) per la gestione tecnica della zonazione del territorio in prospettiva sismica, i così detti **studi di Microzonazione Sismica** (MS), atti a mitigare il rischio connesso all'accadimento di terremoti ed al loro potenziale distruttivo o di danneggiamento nei confronti di strutture ed infrastrutture antropiche.

Carta geologico-tecnica (Accumoli - RI) frutto di rilievi geologici e geomorfologici





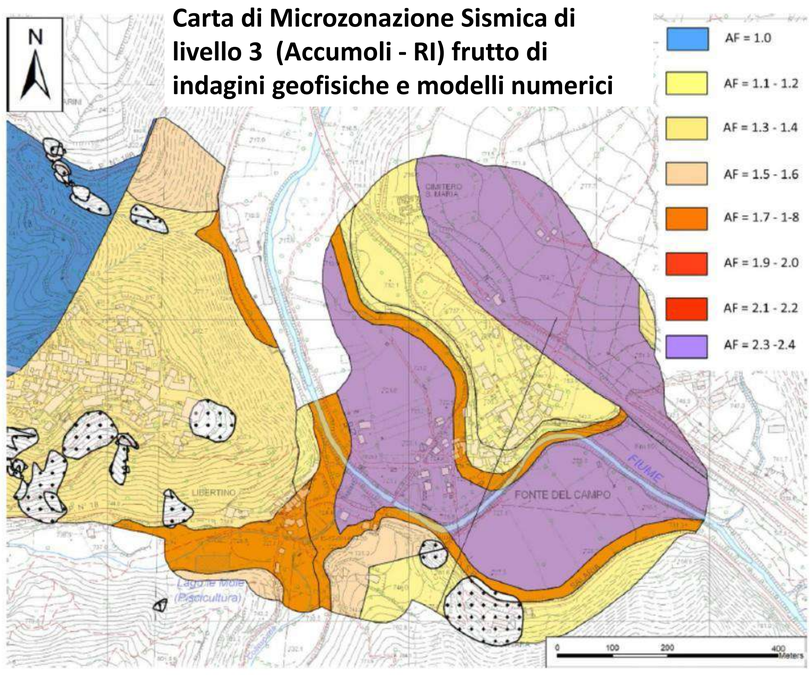


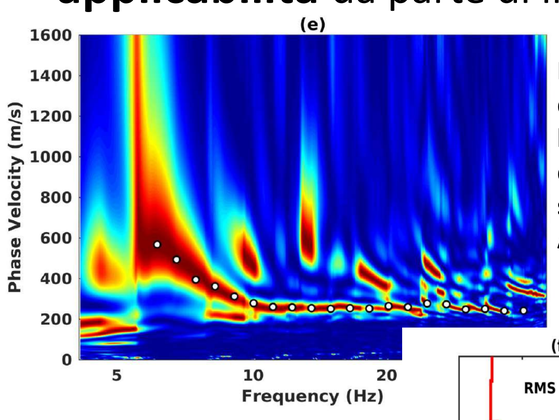


Completa distruzione della città di Accumoli (RI) dopo i sismi del 2016-2017

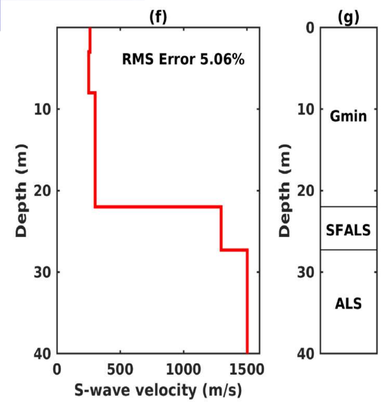
La **geologia e la geofisica** costituiscono strumenti imprescindibili per garantire la corretta realizzazione dei prodotti di MS del territorio, grazie ad un approccio multidisciplinare nell'ambito del settore ERC-PE (Matematica, scienze fisiche, informazione e comunicazione, ingegneria, scienze della terra e dell'universo). I prodotti degli studi di MS sono oggi adattatati alle **esigenze della normativa tecnica vigente ed alla loro applicabilità** da parte di ingegneri, pianificatori urbanistici ed architetti.

Carta di Microzonazione Sismica di livello 3 (Accumoli - RI) frutto di indagini geofisiche e modelli numerici





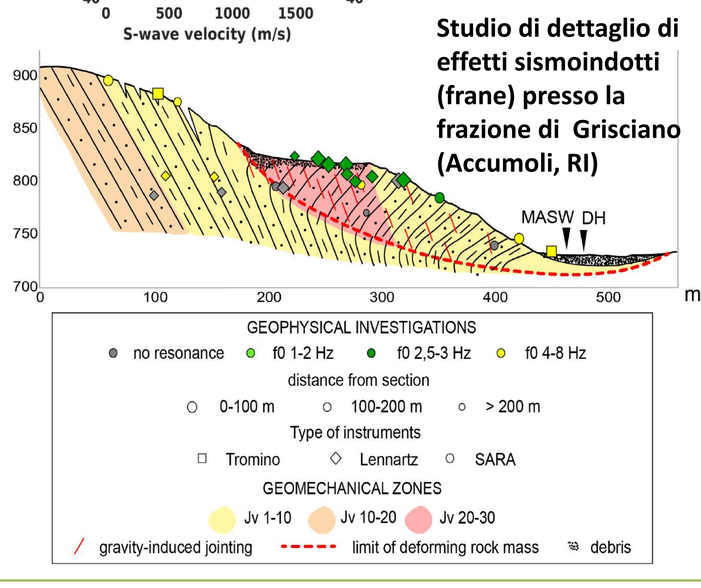
Indagini geofisiche di tipo MASW per la caratterizzazione dinamica del sottosuolo ad Accumoli (RI)



A seguito dei **recenti eventi sismici che hanno coinvolto l'Appennino Centrale nel 2016-2017** La Sapienza, insieme a numerose altre Accademie, Istituzioni ed Enti di ricerca nazionali ed internazionali, è stata impegnata in un'operazione a tutt'oggi unica nel suo genere, per investimento di risorse ed estensione degli areali coinvolti.

Tale operazione è stata finalizzata a definire gli aspetti geologici, geomorfologici, geotecnici e geofisici di **oltre 130 territori comunali terremotati dell'Appennino Centrale** nelle regioni Abruzzo, Lazio, Marche ed Umbria.

Grazie a questa ricerca multidisciplinare è stato possibile **affinare ulteriormente gli strumenti di diagnosi del territorio, finalizzati alla quantificazione degli effetti sismici locali** (intesi sia come risposta amplificativa che come instabilità sismoindotte del terreno). Questi studi di microzonazione sismica hanno portato alla **redazione di cartografie tematiche di alto dettaglio alla scala sub-comunale** (propriamente le carte di microzonazione sismica), rafforzando l'interdisciplinarietà e la complementarietà tra le competenze tecniche coinvolte ed aprendole al mondo dei liberi professionisti e degli amministratori locali.



Studio di dettaglio di effetti sismoindotti (frane) presso la frazione di Grisciano (Accumoli, RI)

Riferimenti recenti

Martino et al. (2019). Earthquake-induced landslide scenarios for seismic microzonation. Application to the Accumoli area (Rieti, Italy)., doi: 10.1007/s10518-019-00589-1

Pergalani et al (2019). Seismic microzoning map. Approaches, results and applications after the 2016–2017 Central Italy seismic sequence. doi: 10.1007/s10518-019-00640-1

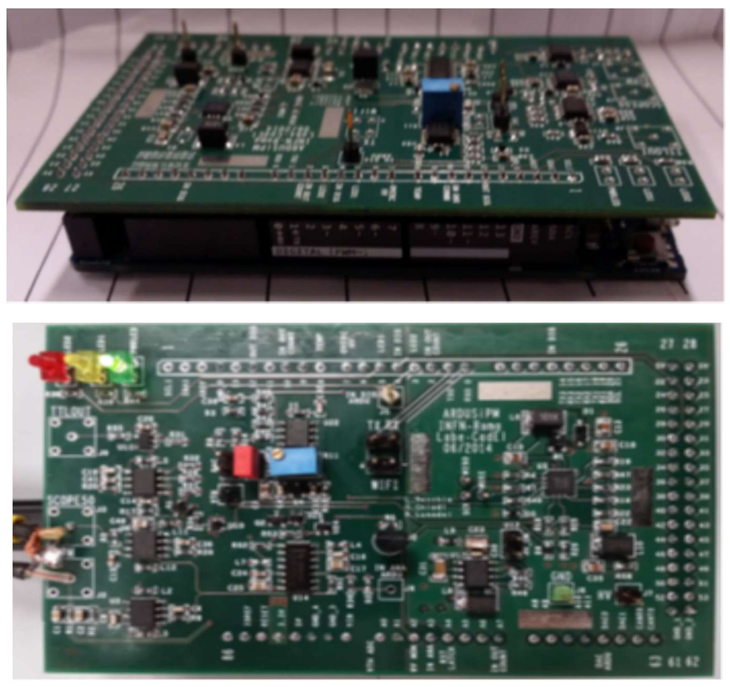
Caprari et al.(2018). Upgrade of the CEDIT database of earthquake-induced ground effects in Italy. doi: 10.4408/IJEGE.2018-02.O-02

ArduSiPM a small, battery-operated, All-In-One particle detector

Valerio Bocci , Giacomo Chiodi, Francesco Iacoangeli, Luigi Recchia

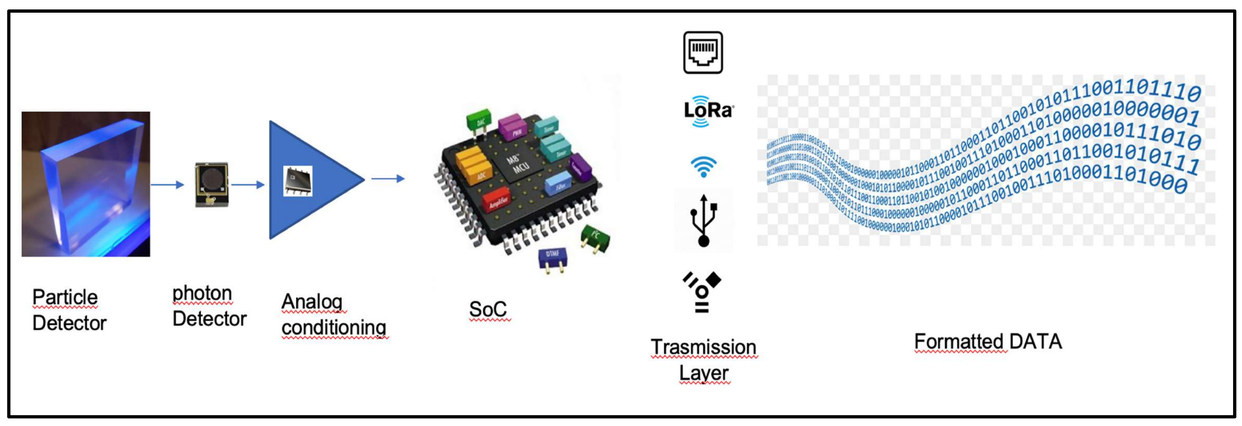
INFN Roma, Piazzale A.Moro, 2 - 00185 Roma
valerio.bocci@roma1.infn.it

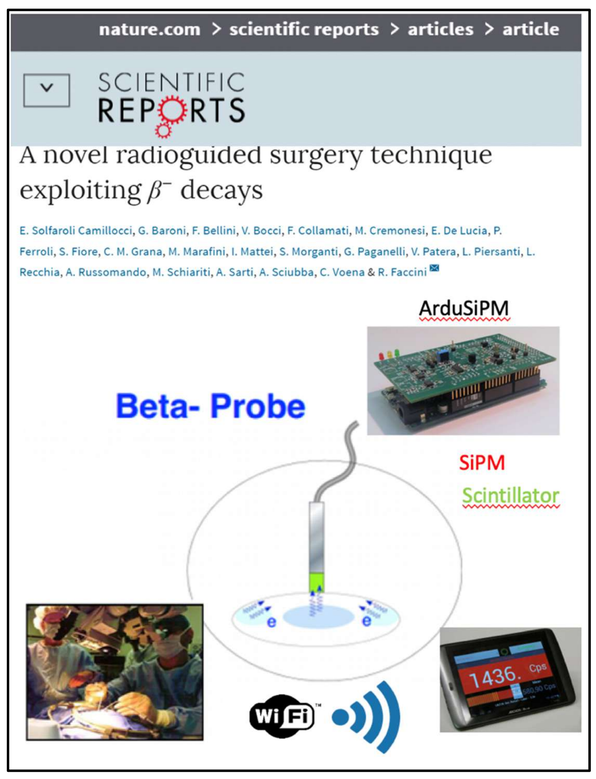
ArduSiPM, developed within the INFN, is the first particle detector in the scientific literature to use a microcontroller and a limited number of external components to control and acquire a scintillation detector using the new high sensitivity photodetector : the Silicon Photomultiplier (SiPM).

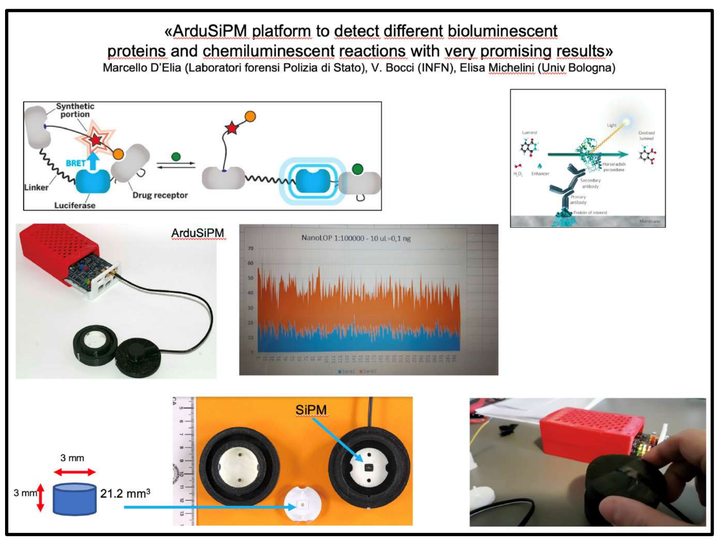


The necessity to use Photo Multipliers (PM) as light detector limited in the past the use of crystals in radiation handled device preferring the Geiger approach.
The Silicon Photomultipliers (SiPMs) are very small and cheap, solid photon detectors with good dynamic range and single photon detection capability, they are usable to supersede cumbersome and difficult to use Photo Multipliers (PM). A SiPM can be coupled with a scintillator crystal to build efficient, small and solid radiation detector. A cost effective and easily replicable Hardware software module for SiPM detector readout is made using the ArduSiPM solution.
The ArduSiPM is an easily battery operable handled device using an Arduino DUE (an open Software/Hardware board) as processor board and a piggy-back custom designed board (ArduSiPM Shield), the Shield contains all the blocks features to monitor, set and acquire the SiPM using internet network.

The peripheral card can connected piggyback using the same form factor of the Arduino, in the Arduino world this pluggable boards are called Shields.
Looking to the potentiality of the SAM3X8E ARM Cortex-M3 CPU, we decide to build up a custom shield to acquire Silicon photomultiplier.
The ArduSiPM Shield is our custom designed board with all electronics interface from Arduino DUE and a SiPM photodetector. The ArduSiPM Shield plugged in the Arduino DUE create an easily transportable system including Front end electronics and data acquisition system.
The global architecture of the system is in the right figure.







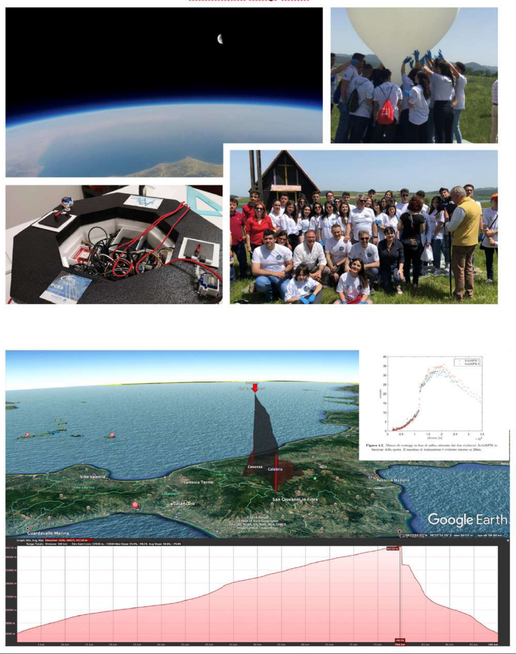
INFN Istituto Nazionale di Fisica Nucleare
MICROCHIP

A scientific collaboration agreement was signed with Microchip Technology (third world microcontroller manufacturer), for the development of particle detectors for Space, using ArduSiPM technology.



Outreach

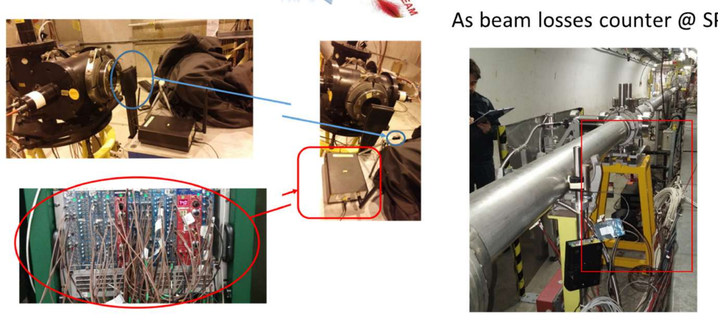
The Scholar Project Mocris. The launch of the ArduSiPM up to **34 000 m** with Balloon to measure Stratospheric Cosmic Ray flux.



Use of ArduSiPM in the CERN UA9 and CRYSBEAM activity

(substitute old Scintillator and electronics for PM)

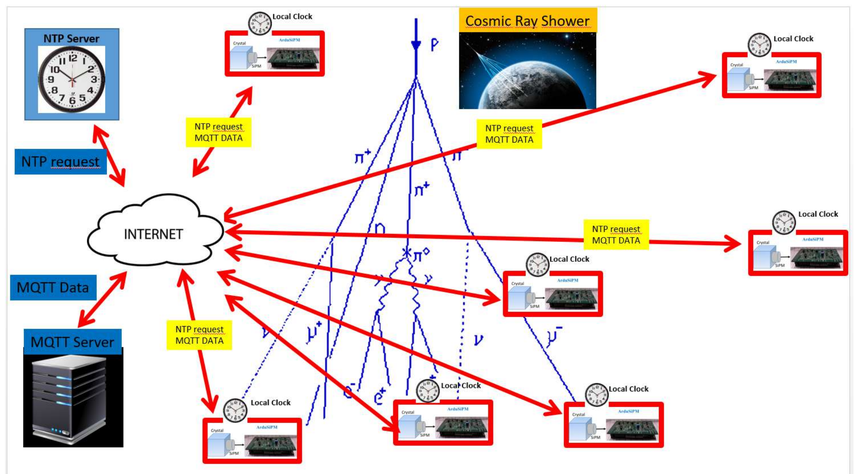
As beam losses counter @ SPS



As beam trigger @ extracted beam line H8 (CERN)

- *This work has been supported by the ERC Ideas Consolidator Grant*
- *No.615089 "CRYSBEAM".*

A distributed Cosmic Ray detector network based on ArduSiPM



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Selective Methyltransferase Activity Reduces Trimethylation of H3K27 in Arabidopsis Seeds

P. Vittorioso*, V. Ruta, C. Longo, R. Dello Ioio, S. Sabatini, P. Costantino
Dipartimento di Biologia e Biotecnologie C. Darwin, Edificio Fisiologia generale, CU026, piano 1 stanza 4
Email: paola.vittorioso@uniroma1.it

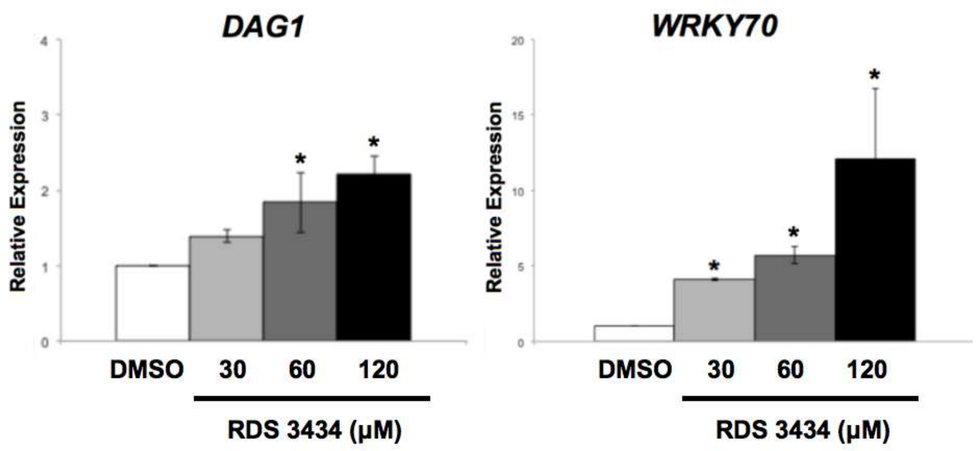
Background: Polycomb repressive complex 2 (PRC2) is an epigenetic transcriptional repression system, whose catalytic subunit (ENHANCER OF ZESTE HOMOLOG 2, EZH2 in animals) is responsible for trimethylating histone H3 at lysine 27 (H3K27me3). In mammals, gain-of-function mutations as well as overexpression of EZH2 have been associated with several tumors; accordingly, highly specific small-molecule inhibitors of EZH2 have been reported. In plants, mutations in some PRC2 components lead to embryonic lethality, but no trial with any inhibitor has ever been reported.

Aim: To develop a pharmacological approach to inhibit EZH2 activity of PRC2 in *Arabidopsis.*
In collaboration with Dip. di Chimica e Tecnologia del Farmaco- Proff. R. COSTI, R. DI SANTO – LS3

Methods: Arabidopsis genetics and molecular tecniques: Wblot, ChIP, qPCR, germination assays, Root Meristem Analysis (Confocal laser scanning Microscope)

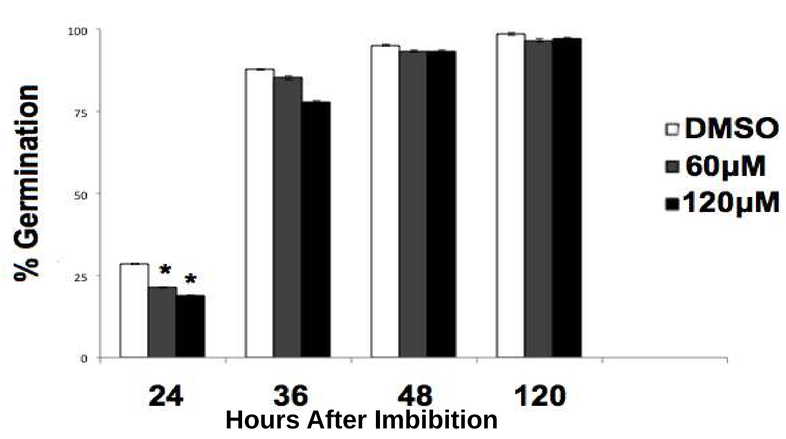
Results: We have developed a methodology for inhibiting in plants the activity of EZH2, the catalytic subunit of PRC2, and show the effects of this inhibition on seed germination and root growth.

Since PRC2 is a transcriptional repression system, inhibition of EZH2 and consequent decrease of H3K27me3 levels should result in the transcriptional derepression of PRC2 target genes.

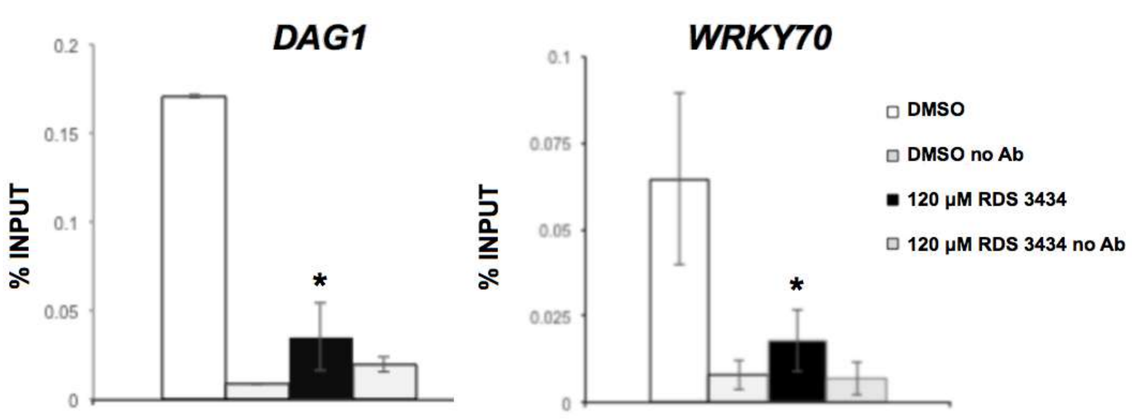


Expression level of DAG1 and WRKY70 in WT seedlings grown on RDS 3434

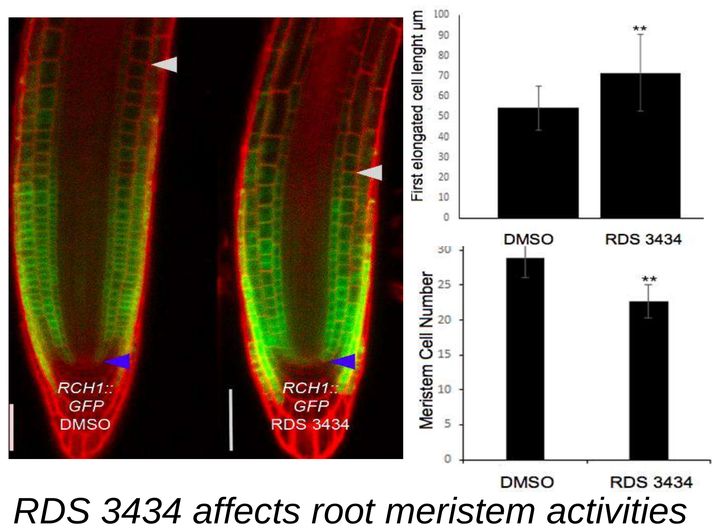
Treatment with the inhibitor caused a significant reduction of the germination rate at 24 hours after imbibition (HAI).



Treatment with the inhibitor caused a reduction of the germination rate at 24 HAI



Treatment with the inhibitor result in loss of the H3K27me3 repressive mark in the PRC2 target loci



RDS 3434 affects root meristem activities controlling the elongation/differentiation potential

Conclusions: This study is of significant interest for the community studying PRC2 activity in plants RDS 3434 could represent a powerful tool to further investigate the effects of the transcriptional control mediated by PRC2 in plants.

Ruta V., Longo C., Boccaccini A., Madia V.N., Saccoliti F., Tudino V., Di Santo R., Lorrai R., Dello Ioio R., Sabatini S., Costi R., Costantino P., Vittorioso P. 2019. Inhibition of polycomb repressive complex 2 activity reduces trimethylation of H3K27 and affects development in Arabidopsis seedlings. *BMC Plant Biology* doi: 10.1186/s12870-019-2057-7.

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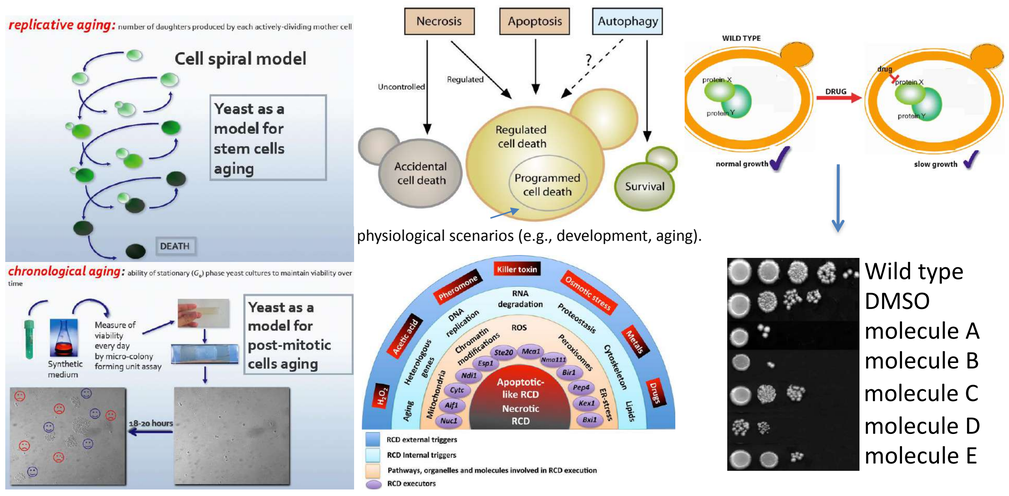
Uso del lievito come modello e strumento per lo studio dell'invecchiamento e delle malattie ad esso correlate

***, Valentina Vapore, Elisa Mancini Cristina Mazzoni**
Dipartimento di Biologia e Biotecnologie «C. Darwin» Edificio Fisiologia generale CU026, piano rialzato stanza 25-26
Cristina.mazzoni@uniroma1.it:

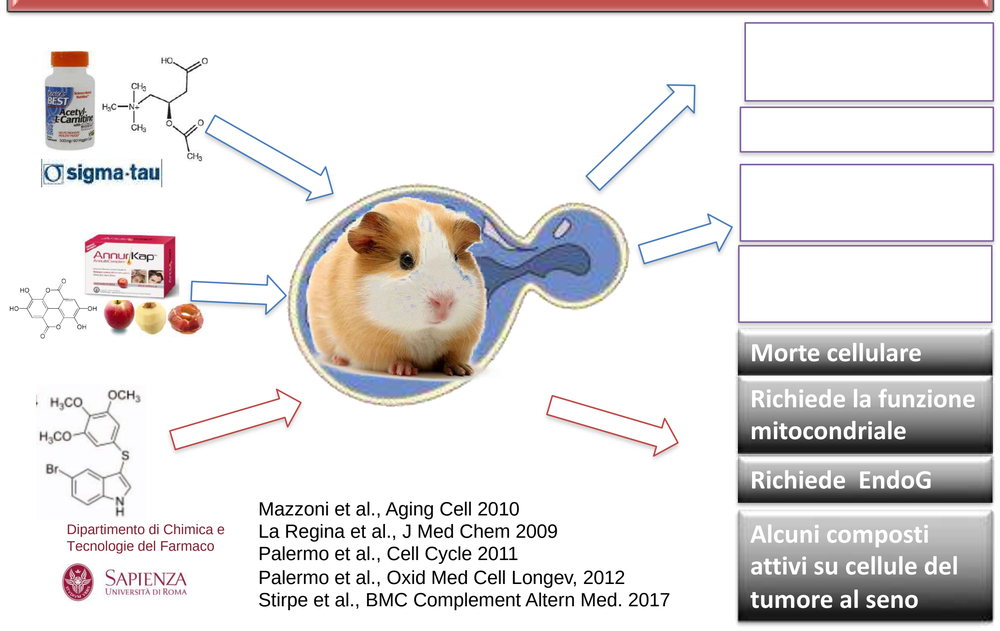
- **Attività di ricerca**
- L'invecchiamento può essere descritto come un processo multifattoriale derivante dall'interazione di fattori sia genetici che ambientali, ed è caratterizzato dall'insorgenza di diverse malattie. I costi e le problematiche etiche legate agli studi sull'invecchiamento umano spingono all'impiego di sistemi modello in grado di fornire risposte facilmente traslabili all'uomo.
- In *S. cerevisiae* lo studio dell'invecchiamento cronologico (CLS), definito come la capacità di una cellula di sopravvivere nel corso del tempo, è estremamente utile se si vuole verificare l'effetto dell'accumulo di danni alle macromolecole durante il tempo.
- Nei nostri laboratori si verifica l'effetto sulla longevità e la morte cellulare a livello molecolare-cellulare in presenza di proteine umane, molecole di sintesi o di nutraceutici. A questo proposito, sono stati studiati diversi interventi genetici, farmaceutici e nutrizionali che diminuiscono o promuovono la longevità nel tentativo di tradurli in trattamenti per la salute e il benessere.
- **Settori ERC**
- LS1_10 - Molecular mechanisms of signalling pathways
- LS2_1 - Molecular genetics, reverse genetics, forward genetics, genome editing
- LS9_1 - Applied biotechnology (including, transgenic organisms, applied genetics and genomics, biosensors, bioreactors, microbiology, bioactive compounds)
- **Strumentazioni e metodologie**
  - Laboratorio delle Fermentazioni (bioreattore a 4 vessel da 1 litro, bioreattore da 2 litri, bioreattore da 30 litri, cappa sterile, autoclave da pavimento, centrifuga fino a 6 litri)
  - Laboratori di ricerca (piccola strumentazione: termocilatori, centrifughe da bancone, sistemi di elettroforesi, cappe sterili, elettroporatore, incubatori, microscopi ottici, micromanipolatore, lettore di micropiastre)
  - Coltivazione e manipolazione dei microrganismi, estrazione e manipolazione di acidi nucleici e proteine, ingegneria genetica e metabolica dei microrganismi, analisi qualitativa e quantitativa degli acidi nucleici e delle proteine, microscopia ottica e fluorescenza

Il lievito come modello/strumento per

Invecchiamento | Morte cellulare | Screening molecole



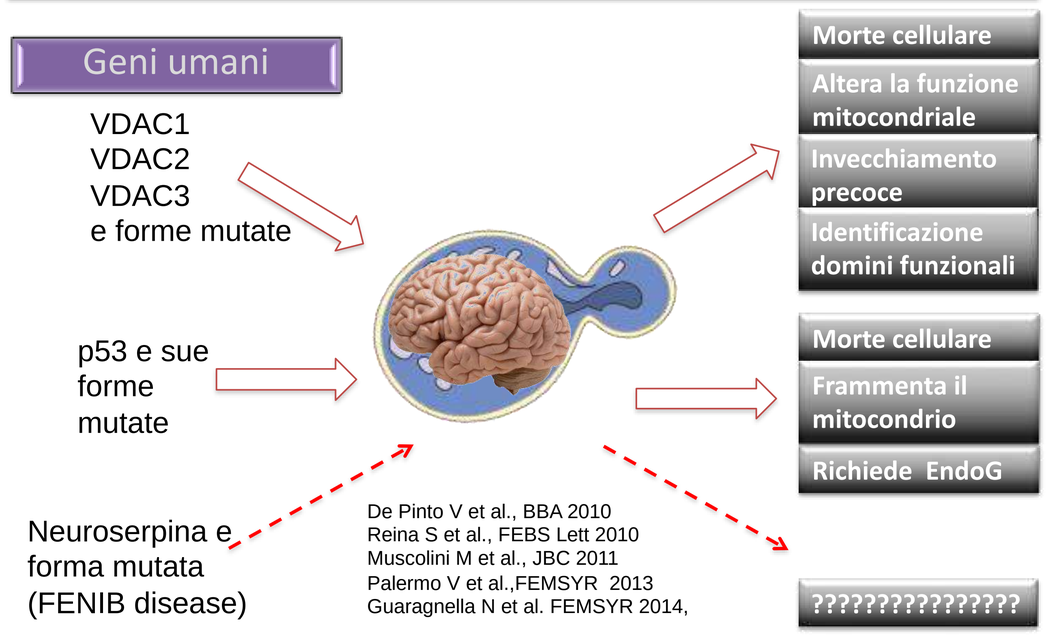
Molecole o nutraceutici



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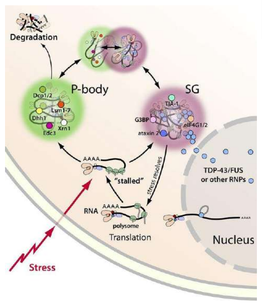
Mazzoni et al., Aging Cell 2010
La Regina et al., J Med Chem 2009
Palermo et al., Cell Cycle 2011
Palermo et al., Oxid Med Cell Longev, 2012
Stirpe et al., BMC Complement Altern Med. 2017

Espressione geni eterologhi



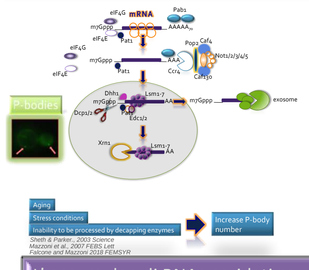
De Pinto V et al., BBA 2010
Reina S et al., FEBS Lett 2010
Muscolini M et al., JBC 2011
Palermo V et al.,FEMSYR 2013
Guaragnella N et al. FEMSYR 2014,

Rimodellamento dei complessi RNA-proteine: P-bodies e Stress Granules

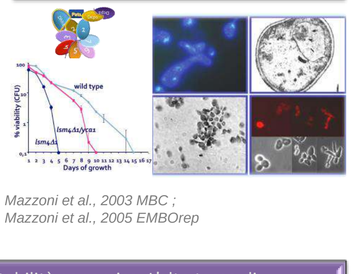


SGs and P-bodies are sites of RNA triage. Exposure to cellular stress can trigger a stress response that stalls translation initiation, resulting in the formation of SGs. SGs are dynamic cytoplasmic RNA–protein complexes that contain RNA-binding proteins, mRNAs, and translation initiation factors. When stress exposure dissipates, SGs disassemble and mRNA translation resumes. Nontranslating mRNAs can also be directed to P-bodies, distinct RNA-protein granules that are sites of stalled translation and mRNA degradation. SGs and P-bodies are differentially regulated and form independently, but they can and often do interact with each other.
From Yun Li et al., 2013 The Journal of Cell Biology 201(3):361-72

La via di degradazione degli mRNA è conservata

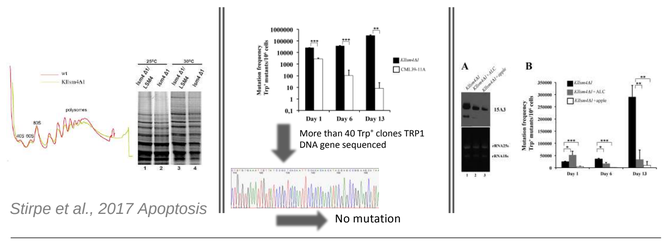


Mutanti del decapping sono short-lived e pro-apoptotici



Mazzoni et al., 2003 MBC ;
Mazzoni et al., 2005 EMBOrep

L' accumulao di RNAs ossidati causa instabilità genomica. L'alto tasso di reversione è associato a difetti post-traduzionali . Questi mutant sono utili per comprendere gli effetti del danno all'mRNA alla risposta allo stress lifespan



Stirpe et al., 2017 Apoptosis

- **Conclusioni**
- Come eucariote, il lievito condivide i meccanismi molecolari e cellulari altamente conservati con le cellule umane. Pertanto è un modello inestimabile per studiare i meccanismi molecolari fondamentali coinvolti in diverse malattie umane
- *S. cerevisiae* fornisce risposte chiare sulla risposta cellulare a induttori e/o protettori di stress. Grazie alla facilità di manipolazione genetico-molecolare e alla disponibilità di tecniche genomiche, i risultati ottenuti, coadiuvati anche da altri studi, sono stati traslati con successo all'uomo

- **Potenzialità applicative**
- Il lievito si presenta come uno strumento/modello per

- Sscreening di banche di molecole
- Identificazione dei bersagli di molecole
- Clean-box per l'espressione di geni umani
- Selezione di ceppi con proprietà applicabili alle produzioni industriali
- Costruzione di ceppi in grado di esprimere pathways biosintetici per produrre molecole di interesse (ingegneria metabolica)
- Costruzione di ceppi in grado di produrre proteine eterologhe di interesse

Riferimenti recenti:

Guaragnella et al., Oxid Med Cell Longev. 2019; Giannattasio and Mazzoni FEMS Yeast Res. 2018 , Giannattasio et al., Front Oncol. 2018 Jun 25;8:236 : Falcone and Mazzoni FEMS Yeast Res. 2018 Sep 1;18(6).; Carmona-Gutierrez et al., Microb Cell. 2018 Jan 1;5(1):4-31; Stirpe et al., Complement Altern Med. 2017 Apr 5;17(1):200Falcone and Mazzoni Cell Mol Life Sci. 2016 Jun;73(11-12):2237-50

Riciclo di Batterie Litio Ione a Fine Vita e Produzione di Nuovi Materiali Elettrodici

P.G. Schiavi, P. Altimari, A. Rubino, M.A. Navarra, F. Pagnanelli
Dipartimento di Chimica, Edificio Cannizzaro, CU014, piano secondo, stanza C.I. 11
Email: francesca.pagnanelli@uniroma1.it

Gruppo di Teoria dello Sviluppo dei Processi Chimici

Il gruppo di ricerca sviluppa processi innovativi per il recupero di materia da rifiuti tecnologici con lo scopo di ottenere nuovi materiali che possano essere direttamente reimpiegati nel campo della catalisi e dell'accumulo di energia.
Settore ERC: SH3_1 Ambiente, risorse e sostenibilità

Strumentazioni e metodologie

In Figura 1 è riportato lo schema del processo idrometallurgico sviluppato per il recupero dei materiali che compongono le batterie litio ione a fine vita [1,2].
Il frantumato di pile (ottenuto mediante criomacinazione in impianto pilota), è stato trattato per l'estrazione dei metalli di interesse (Li, Co, Ni, Mn) e della grafite.
I metalli sono stati impiegati per la sintesi di nuovi catodi ($LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$, NMC) e la grafite purificata per essere riutilizzata come anodo.
I materiali recuperati sono stati caratterizzati tramite XRD, XPS, SEM, EDX, BET e testati come elettrodi in semicelle al litio.

Risultati

In Figura 2 sono riportati i valori di capacità specifica registrati durante la ciclazione galvanostatica della grafite (Fig.2-A) e dell'ossido misto NMC (Fig.2-B) che sono stati recuperati dal processo sopra descritto.
I valori ottenuti sono prossimi a quelli teorici rispettivamente di 372 e 160 mAh/g per grafite ed NMC e confrontabili con valori dei corrispondenti materiali elettrodici commerciali.
Inoltre, in Figura 2-B, è riportato il confronto tra l'NMC ottenuto dai metalli recuperati con uno ottenuto da reagenti sintetici.

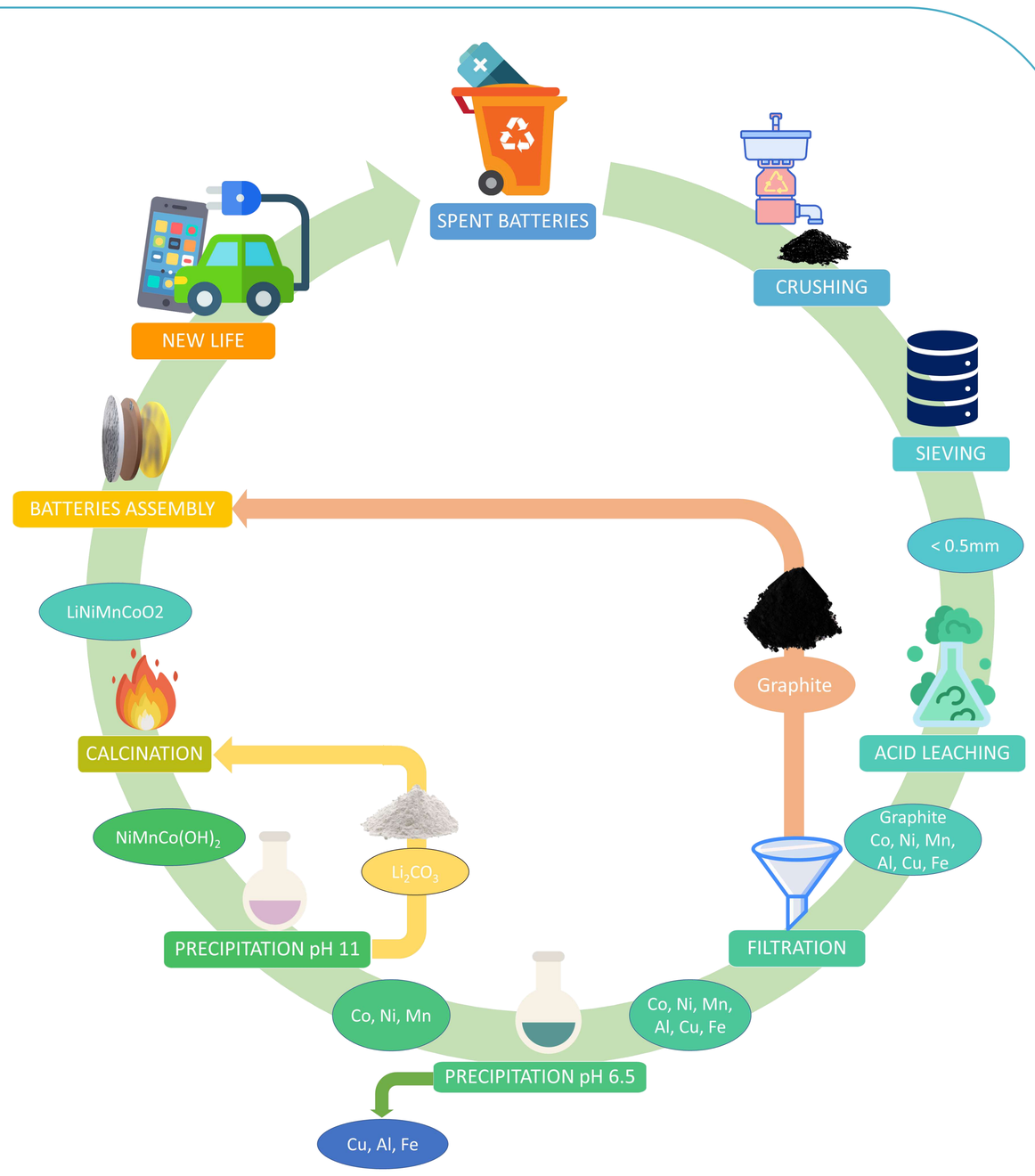


Figura 1: schema del processo idrometallurgico sviluppato per il riciclo di batterie litio ione a fine vita e la produzione di nuovi elettrodi

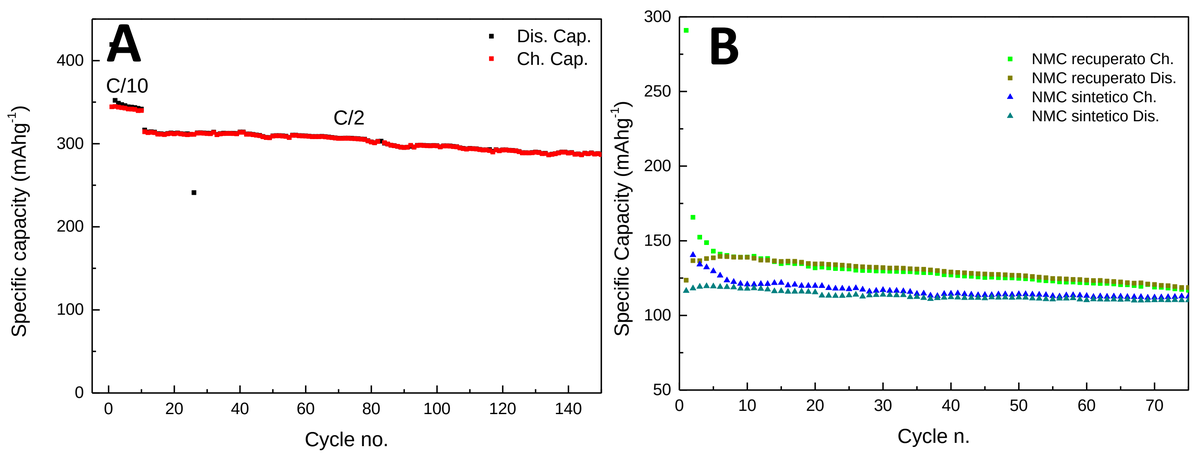


Figura 2: ciclazioni galvanostatiche dei materiali recuperati
A) grafite (1C= 372 mAh/g);
B) $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (1C: 160 mAh/g)

Conclusioni

Il processo sviluppato consente di recuperare i componenti elettrodici delle batterie litio ione a fine vita e di produrre materiali elettrodici per nuove batterie litio ione evitando complesse sequenze di purificazione.
I materiali recuperati presentano particolare rilevanza soprattutto in vista dell'espansione del mercato dei veicoli elettrici che utilizzano preferenzialmente elettrodi di tipo NMC.

Riferimenti recenti

[1] T.A. Atia, G. Elia, R. Hahn, P. Altimari, F. Pagnanelli, Closed-loop hydrometallurgical treatment of end-of-life lithium ion batteries: Towards zero-waste process and metal recycling in advanced batteries, Journal of Energy Chemistry, (2019) 220-227.
[2] P.G. Schiavi, L. Farina, R. Zanoni, P. Altimari, I. Cojocariu, A. Rubino, M.A. Navarra, S. Panero, F. Pagnanelli, Electrochemical synthesis of nanowire anodes from spent lithium ion batteries, Electrochim. Acta, 319 (2019) 481-489.

Dipartimento di Biologia e Biotecnologie Charles Darwin
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CANTHARIDIN IN BLISTER BEETLES: *from biodiversity to biotechnology*

Emiliano Mancini[1]*, Silvia Gisondi[1], Maurizio Muzzi[2], Andrea Di Giulio[2], Emiliano Fratini[2], Manuela Cervelli[2], Paolo Mariottini[2], Fabrizio Lombardo[3], Tiziana Persichini[2], Tecla Gasperi[2], Marco Alberto Bologna[2]

*1 **Dipartimento di Biologia e Biotecnologie «C. Darwin», Sapienza, Ed. Zoologia, CU 008, piano II, stanza L001***
2 Dipartimento di Scienze, Roma Tre, Viale G. Marconi 446, 00146, Roma;
3 Dipartimento di Sanità Pubblica e Malattie Infettive, Sapienza, Piazzale A. Moro 5, 00185, Roma;
* ***email: emiliano.mancini@uniroma1.it***

Background

- **Cantharidin** (CA) **is a toxic terpene** produced by **blister beetles** (Coleoptera: Meloidae, ~ 3000 species). It is used both as a defensive agent and nuptial gift [1,2] and accumulated in large quantities in body compartments of these insects, such as male accessory glands [3].
- This blistering substance - traditionally used as an aphrodisiac - is **a promising bio-compound for several medical applications** (e.g., dermatology and cancer treatment) [4]...
- ... however the **metabolic pathway**, **site of production** and **storage**, **transport** and **detoxification** mechanisms of CA in blister beetle are still unclear.

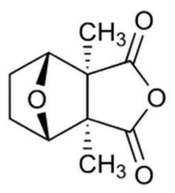


Fig. 1 *– The cantharidin molecule.*



Fig. 2 *– A big droplet of hemolymph containing cantharidin is exuded from a blister beetle (Berberomeloe majalis) as a "reflex-bleeding".*

Aims

*The **'CANBBIO'** Project*

CANTARIDINA: dalla BIODIVERSITA' alle BIOTECNOLOGIE

is an interdisciplinary effort to:

1) **identify** and **quantify CA** and **related compounds (CRCs)** in natural populations of Meloidae;
2) describe the **morphology of CA-producing/storing organs**;
3) detect the **expression of genes involved in CA transport** and **production**;
4) build novel **drug-delivery tools** for a safe therapeutic use of CA and CRCs in oncology and dermatology.

from biodiversity...



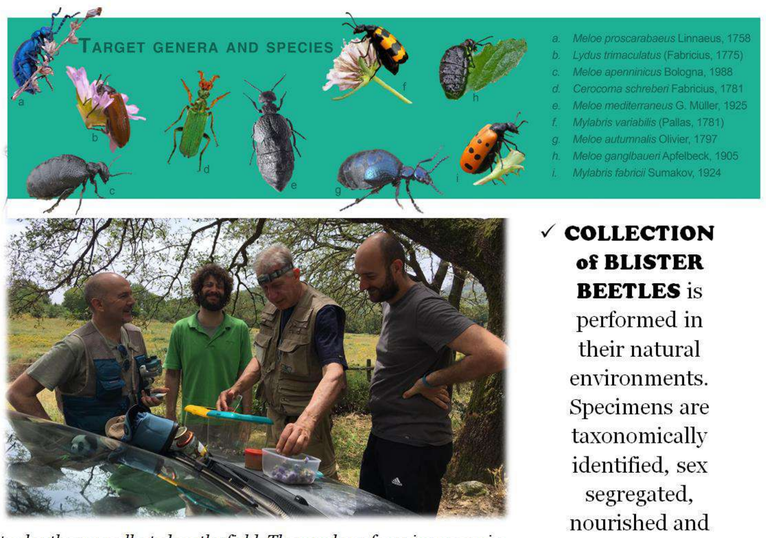


Fig. 3 *– Targeted species of blister beetles are collected on the field. The number of specimens varies from ~5 to 50 individuals per site, depending on the requirements for the subsequent analyses.*

✓ **COLLECTION of BLISTER BEETLES** is performed in their natural environments. Specimens are taxonomically identified, sex segregated, nourished and kept alive...

✓ **ULTRASTRUCTURAL MORPHOLOGY** of dissected males' reproductive organs (e.g. accessory glands, testis etc.) are compared among species using electron microscopy techniques...

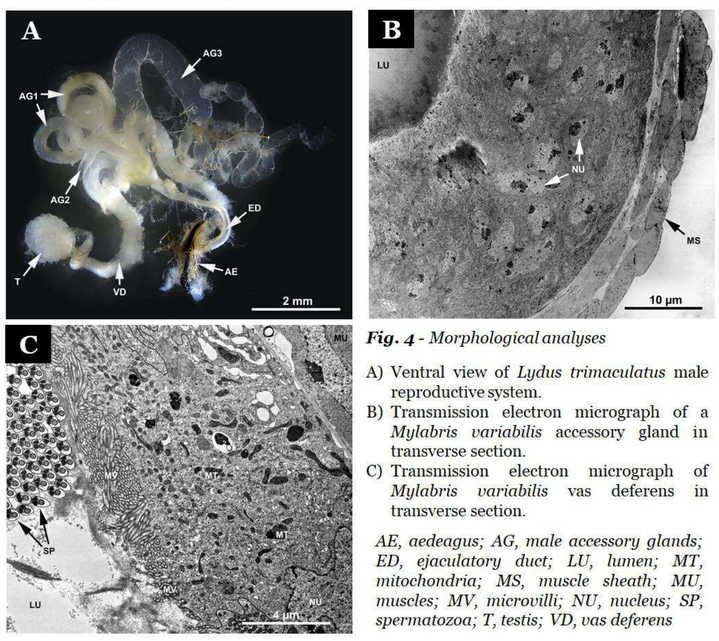


Fig. 4 *- Morphological analyses*

A) Ventral view of *Lydus trimaculatus* male reproductive system.
B) Transmission electron micrograph of a *Mylabris variabilis* accessory gland in transverse section.
C) Transmission electron micrograph of *Mylabris variabilis* vas deferens in transverse section.

AE, aedeagus; AG, male accessory glands; ED, ejaculatory duct; LU, lumen; MT, mitochondria; MS, muscle sheath; MU, muscles; MV, microvilli; NU, nucleus; SP, spermatozoa; T, testis; VD, vas deferens

✓ **CHEMICAL ANALYSES** through GC-MS are conducted on different species to reveal potential differences in presence and quantity of CA and CRCs in males and females in order to give clues on any potential role in blister beetle biology...

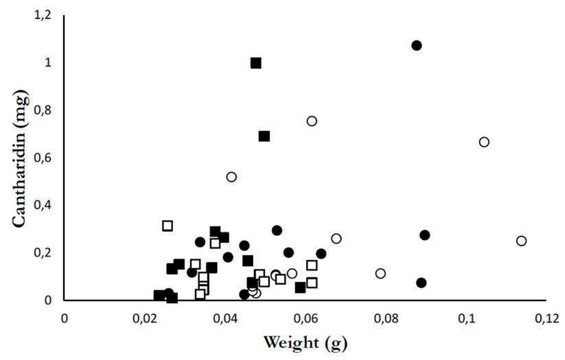


Fig. 5 *- CA content (in mg) is linearly and positively related to individual dry weight (in g), a proxy of beetle size [3].*



Mylabris variabilis (■) *males;* (□) *females*

Lydus trimaculatus (●) *males,* (○) *females*

✓ **TRANSCRIPTOMIC** characterization of male reproductive organs and of the secreted hemolymph will reveal candidate genes responsible for CA production and transport...

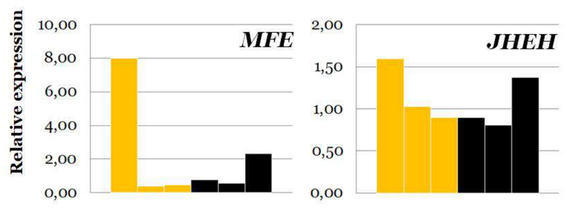


Fig. 6 *– CA production is strictly related to the synthesis of the juvenile hormone (JH).*

The final enzymes of the JH pathway, such as MFE (left) and JHEH (right) are in fact expressed in the male reproductive organs (in yellow, 3 replicates), as well as in corpora allata + the rest of the body (in black, 3 replicates) in Mylabris variabilis.

... to biotechnologies!



The 'CANBBIO' project involves 5 research groups from 'Roma Tre' and 'Sapienza' with different - but complementary - expertise. Our industrial partners are 'TAKIS s.r.l.', a biotech focused on the development of therapeutic cancer vaccines against tumor antigens and 'IDI FARMACEUTICI', a company manufacturing medical devices in dermatology.

✓ **CELL BIOLOGY** assays are carried out to detect the effects of CA on tumor cells ...

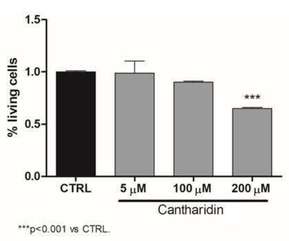


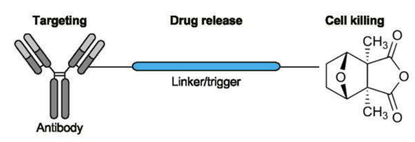


Fig. 7 *– Effects of CA on U373 (human neurogliablastoma astrocytoma) cells.*

Left: Cell viability measured by MMT assay on U373 cells treated with 5, 100 or 200 µM of CA for 24 h. Cell viability was significantly decreased after the treatment with 200 µM of CA.

Right: Trypan blue exclusion test of cell viability: U373 cells were treated with 200 µM CA for 24 h; dead cells are visualized by Trypan blue staining, whereas viable cells exclude the dye.

The final aim of the Project is to produce a novel ADC (**Antibody-Drug Conjugate**) to specifically deliver CA or CRCs to cancer cells, paving the way for more effective therapeutic applications



References

[1] Bologna MA 1991. *Coleoptera Meloidae*. Fauna d'Italia. XXVIII. Calderini, Bologna; [2] Carrel JE et al. 1993. *Cantharidin production in a blister beetle*. Experientia 49 (2): 171–174; [3] Gisondi S et al. 2019. *Cantharidin content in two Mediterranean species of blister beetles, Lydus trimaculatus and Mylabris variabilis (Coleoptera: Meloidae)* Entomological Science 22, 258–263; [4] Moed L. et al. 2001. *Cantharidin revisited: a blistering defense of an ancient medicine*. Archives of Dermatology 137 (10) 1357–1360.

Fundings

This work is developed in the frame of the project "***CanBBio – Cantaridina: dalla Biodiversità alle Biotecnologie***" (prot. n° 85-2017-14967) granted by Regione Lazio (Progetti Gruppi di ricerca – Conoscenza e Cooperazione per un Nuovo Modello di Sviluppo, L.R. Lazio 13/08).

Scienze della Vita

Functionalized nanoparticles for advanced applications: from nanomedicine to optoelectronics

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Introduction

Nanoparticles (NPs) play a significant role in the advancement of scientific and engineering technologies at the nanoscale. Within the ERC panel PE5 (PE5_1. PE5_6; PE5_10), the research for new functional and advanced nanostructured materials, their structural and applicative properties has elicited much interest because of their distinct characteristics that influence physical, electrical, chemical, biological, and optoelectrical properties. NPs bear several advantages such as tuneable size, high surface to volume ratio, ease of surface functionalization and stability jointly with electrical conductivity, catalytic activity, light absorption and scattering, resulting in enhanced performance over their bulk counterparts. There are different application areas of interest that led to the exploration of different NPs: from polymeric NPs (**PNPs**) to metal-based NPs (**MNPs**) capped with mono- and bi-functional hydrophilic/hydrophobic thiols which allow their dispersion in both polar/nonpolar solvents.

PNPs

Polymeric NPs can be obtained starting from acrylate monomers, i.e.: methyl methacrylate (MMA), acrylic acid (AA) and N,N-dimethylacrylamide. (DMAA).

Co-polymeric P(MMA-co-AA), and P(MMA-co-DMAA) nanoparticles are obtained via an emulsion water/toluene polymerization technique using different MMA/AA or MMA/DMAA molar ratios.

Surface functionalities and charge can be tuned by a proper choice of the functional groups.

Dyes, antibodies, enzymes, drugs and recently Y^{3+} salts are loaded on the PNPs, for applications ranging from optics, photonics to nanomedicine.

PNPs with spherical shape and size in the range 50-900 nm are obtained.

AIM

The goal of our work is to synthesize and characterize NPs that are subsequently tested for sensing, biotechnology and nanomedicine applications.

Instruments and methods

Fully equipped laboratory for chemical synthesis of colloidal materials is available. Extensive structural studies are possible through conventional techniques such as UV-Visible and FT-IR/FarIR/ATR spectroscopies, flanked by Dynamic light scattering (DLS), ζ-potential, Gel permeation chromatography (GPC) and electrical measurements. Moreover, the lab is also equipped with a freeze-dryer.

MNPs

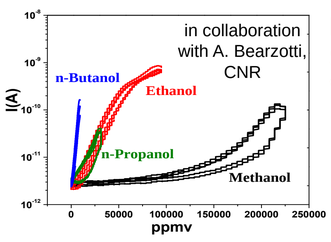
Metal NPs (with M = Au, Ag, Pt, Pd) can be functionalized with different kinds of thiolates, both mono and bi-functional. Ligand choice is crucial to tune the solubility of the particles thus obtaining hydrophilic, hydrophobic and amphiphilic NPs.

Hydrophobic and amphiphilic particles are obtained by a two-phase synthesis (Schiffrin-Brust), whereas hydrophilic NPs are synthesized via an aqueous monophasic approach. Both methods require a metallic precursor compound ($AuCl_4^-$, Ag^+, Pt^{2+}, Pd^{2+}) that is reduced with a reducing agent, i.e. sodium borohydride in the presence of a thiolate as a capping agent. The presence and the stoichiometry of the capping agent are fundamental for the stability of the colloidal suspensions.

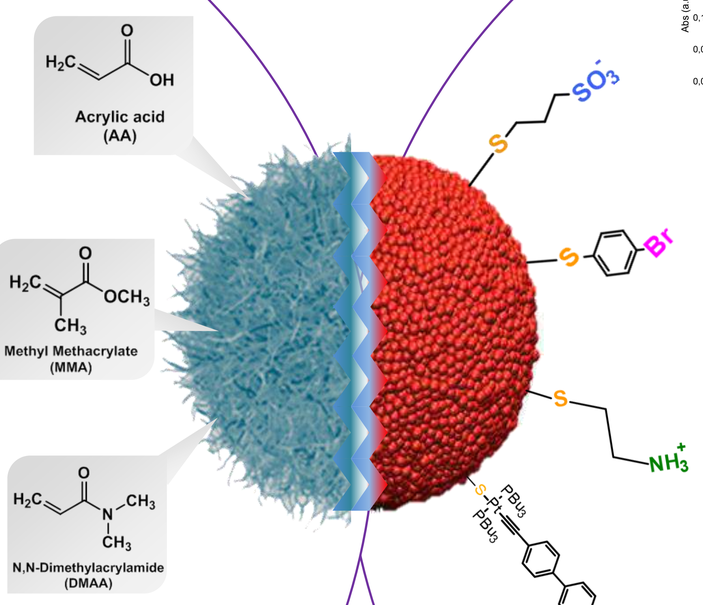
Spherical MNPs with diameter in the range 2-50 nm are isolated and characterized.

OUR MULTIDISCIPLINARY RESEARCH

Sensing



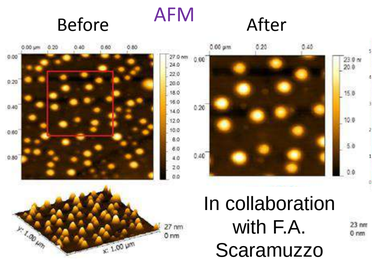
Resistive Sensors for VOCs



Nanomedicine

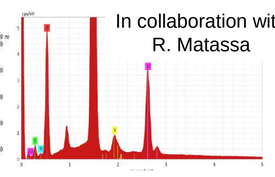
Loading of hydrophobic drugs and Y^{3+}

AFM



In collaboration with F.A. Scaramuzzo

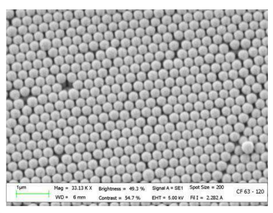
SEM/EDX
P(MMA-co-DMAA)-Y

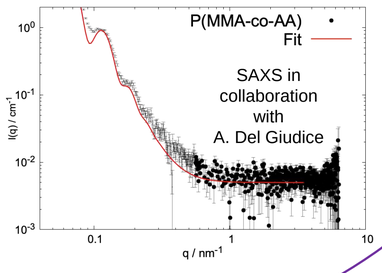


In collaboration with R. Matassa

Radiosurgery project in collaboration with R. Faccini

Photonics

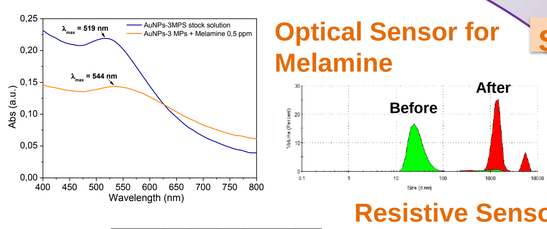




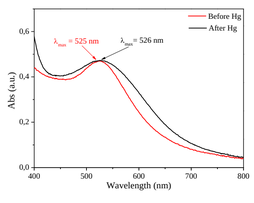
Structural studies

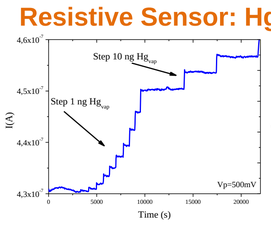
Sensing

Optical Sensor for Melamine



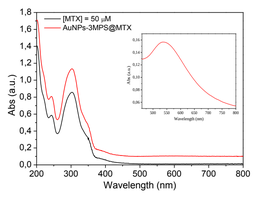
Resistive Sensor: Hg_{vap}



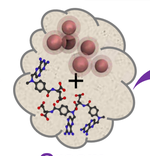


in collaboration with A. Bearzotti, CNR

Nanomedicine

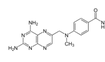


Immobilization of drugs, e.g. methotrexate

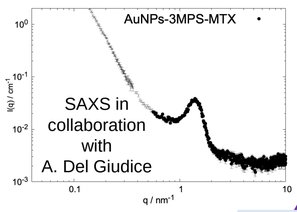


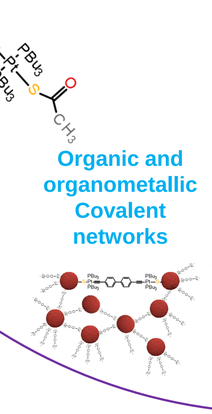
Cream formulation



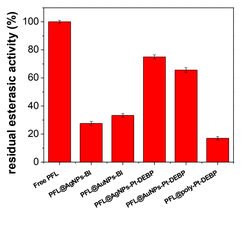


Structural studies for the study of interaction





Organic and organometallic Covalent networks



Lipase enzyme immobilization

In collaboration with. C. Palocci

Biotechnology

Conclusions and perspectives

The methodologies adopted for the NPs synthesis allow us to obtain stable nanostructured materials. Characterization results of the prepared colloids prove that MNPs are promising multi-functional systems, which allow to combine electrical/photoelectrical and localized surface plasmon resonance properties (LSPR) with biological activity. Likewise, PNPs possess properties that can be used in the inorganic field, although the most recent results have been obtained in the field of nanomedicine as nanocarriers, thanks to their stability and cytocompatibility.

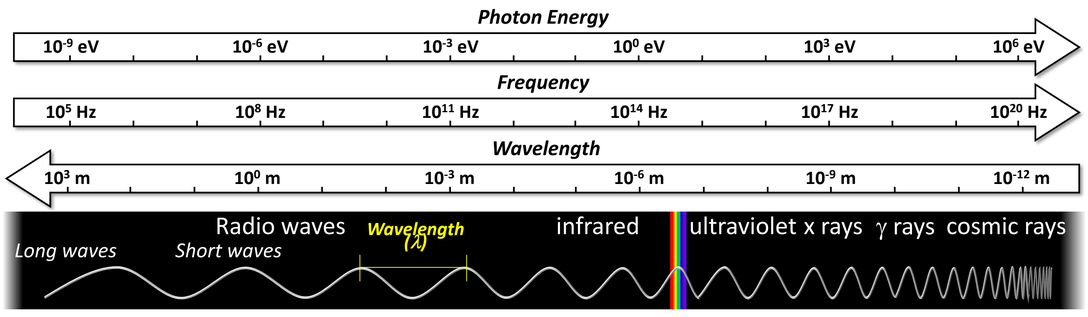
Some references

I. Fratoddi, L. Benassi, E. Botti, et al., Effects of topical methotrexate loaded gold nanoparticle in cutaneous inflammatory mouse model, *Nanomedicine*, 17, 276-286 (**2019**)
I. Fratoddi, R. Matassa, et al., Electronic Properties of a Functionalized Noble Metal Nanoparticles Covalent Network, *J. Phys. Chem. C*,121, 18110-18119 (**2017**)
I. Fratoddi et al., Y^{3+} embedded in polymeric nanoparticles: Morphology, dimension and stability of composite colloidal system, *Colloids Surf. A: Physicochem. Eng. Aspects*, 532, 125-131 (**2017**)

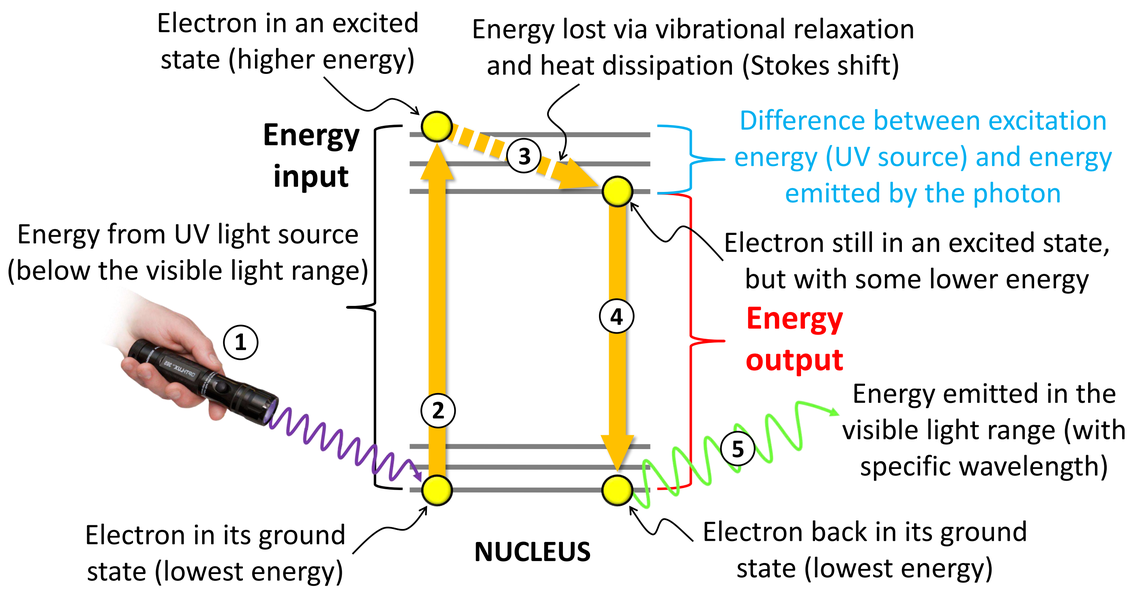
Seeing the invisible: the magic world of fluorescent minerals

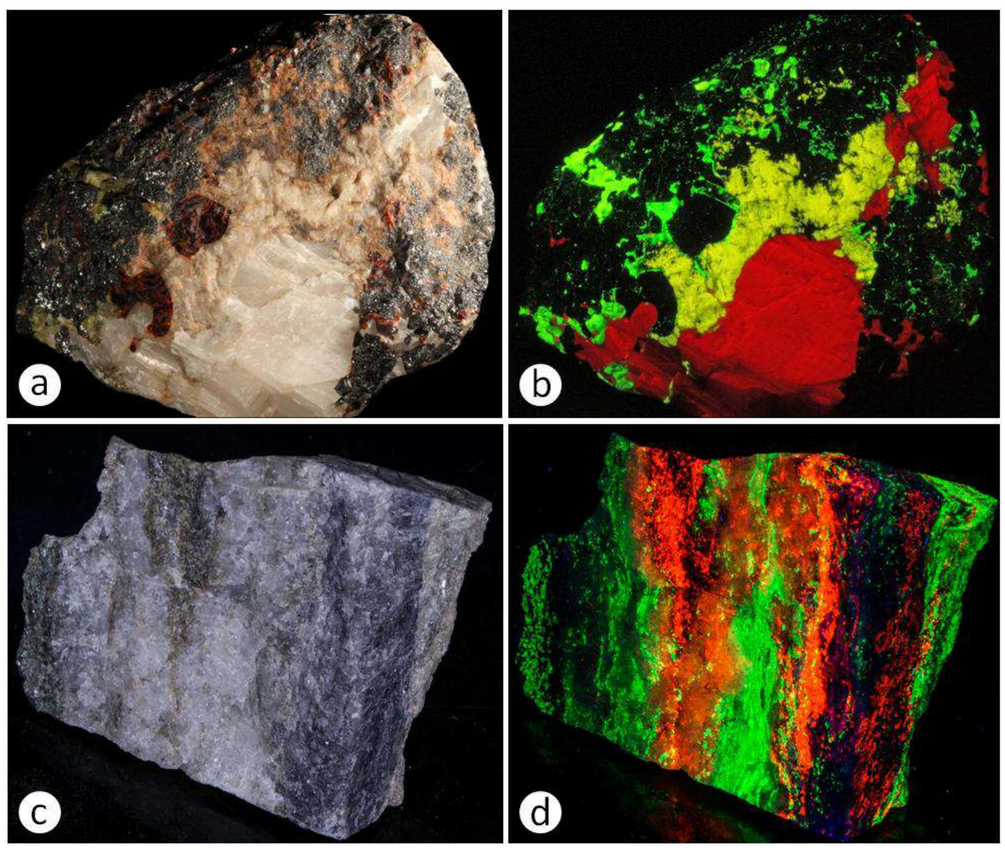
Michele Lustrino
Dipartimento di Scienze della Terra, Edificio MINERALOGIA, CU 009, piano terra stanza n. 114 *Email: michele.lustrino@uniroma1.it*





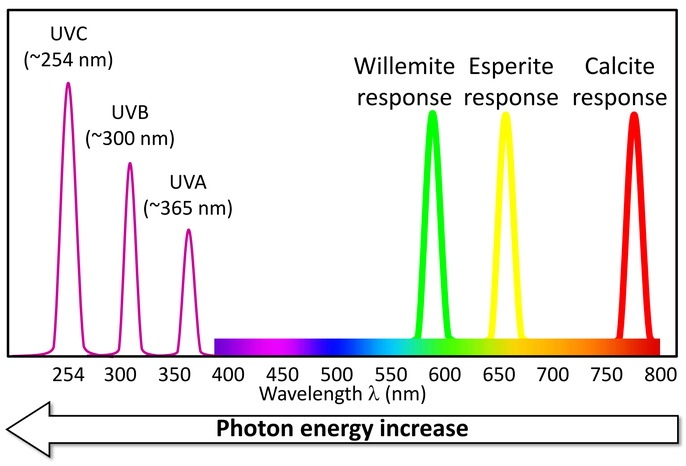
(Electromagnetic spectrum showing the wavelength (in m), the frequency (in Hz) and the energy (in eV). The visible light occupy a very narrow range of the spectrum. *Infra* in Latin means "below". Infrared indicates the frequencies below the red. *Ultra* in Latin means "over". Ultraviolet indicates the frequencies higher the violet.





Rocks observed with natural light (a and c) and under SW light (b and d). Colours in b (Franklin mine, New Jersey, USA) represent: calcite (red), esperite (yellow), green (willemite), black (non fluorescent franklinite). Colours in d (Garpenberg mine, Bergslagen, Sweden) represent: calcite (red and orange), green (willemite), fluorite (blue). Pictures courtesy of www.naturesrainbows.com.

Explanation of fluorescence. (1) A source of high energy electromagnetic radiation (UV) hit the electron of a specific mineral or amorphous phase; (2) the electron is excited and jumps to higher energy orbital; (3) the electron remains in its excited state, but loses some energy by vibrational relaxation and heat dissipation; (4) the excited electron comes back in its ground state, emitting photons with lower energy; (5) the emitted photon has lower energy and, consequentially, lower frequency and higher wavelength, possibly entering in the narrow range of visible light.



Examples of strongly focused UVA (LW), UVB (MW) and UVC (SW) hypothetical electromagnetic sources. The different height of the UV peaks qualitatively indicates the energy of photons. The three curves in the visible light range indicate the response to UVC light to willemite (Zn_2SiO_4), esperite [$PbCa_3Zn_4(SiO_4)_4$] and calcite ($CaCO_3$) as seen in the pictures to the left.

Fluorescence demonstrations have a unique value in teaching.

With simple experiments showing the effects of UV light-sensible minerals, it is possible to start the description of the electromagnetic spectrum, including x- and γ-rays, the visible light and radio waves, the origin of the colours, the discover and origin of radioactivity, the adaptability of the human eyes to the environment, the origin of the solar energy, the principles of the atomic structure, the photon energy and elemental quantum physics including the photoelectric effect.

Riferimenti recenti

Herschel, W., 1800, Experiments on the refrangibility of the visible rays of the sun. Phyl. Trans. Roy. Soc., 90, 284-292.
Patton, D., 1993, Roentgen and the new light - Roentgen's moment. Part 3. The genealogy of Roentgen's barium platynocianide screen. Invest. Radiol., 28, 954-961.
Stokes, G.G., 1852, On the change of refrangibility of light. Phil. Trans. Royal Soc. London, 142, 463-562.

Dipartimento di Biologia
e Biotecnologie
Charles Darwin

SAPIENZA
UNIVERSITÀ DI ROMA

The HoMoLoG project: 3D bioprinting of human induced Pluripotent Stem Cells (iPSCs)

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[1]Dipartimento di Biologia e Biotecnologie "C. Darwin"; [2]Istituto Italiano di Tecnologia - Center For Life NanoScience CLNS@Sapienza; [3]Dip. Fisiologia e Farmacologia "Vittorio Erspamer"

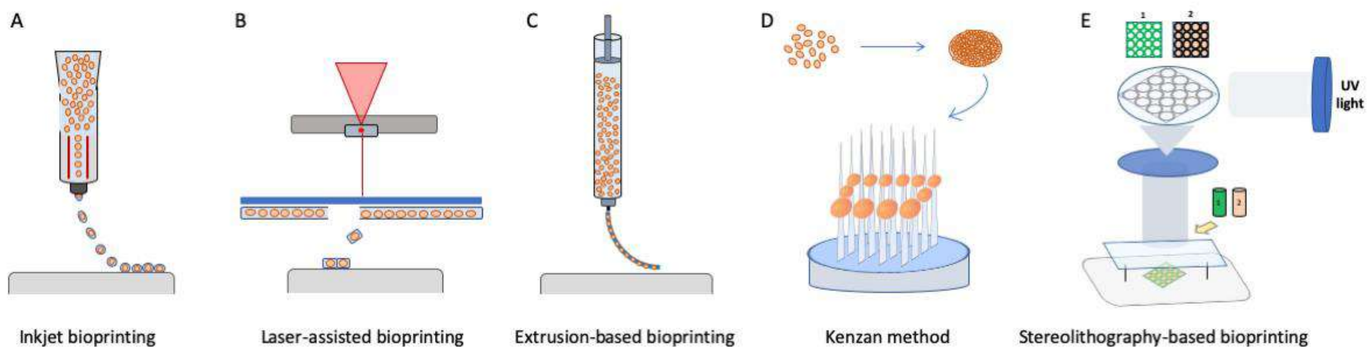
**Email: alessandro.rosa@uniroma1.it*

Three-dimensional (3D) printing of biological material, or **3D bioprinting**, is a rapidly expanding field with interesting applications in tissue engineering and regenerative medicine.

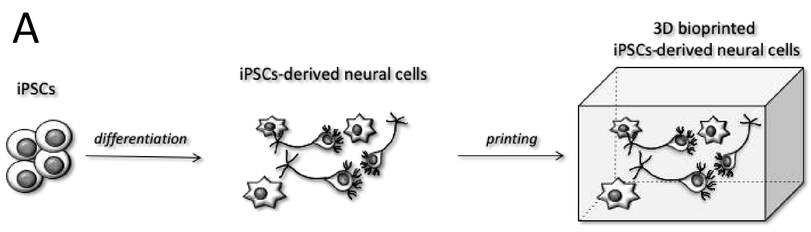
The **HoMoLoG project** stems from a fruitful collaboration between groups of Sapienza University and the Center for Life NanoScience of the Italian Institute of Technology (CLNS@Sapienza), with broad expertise in stem cell biology, neurophysiology and bioengineering. Thanks to these convergent skills and interests, we have been able to develop a novel type of **3D bioprinted cortical construct**, based on human neurons derived from **induced Pluripotent Stem Cells (iPSCs)**, which shows molecular, morphological and functional properties of neuronal networks and can be used for disease modeling and drug screening.

Human iPSCs are derived from adult cells (for instance skin or blood cells) and can be then converted into any cell type of the body, including cardiac cells, neurons and other cell types of biomedical interest. The figure on the right is a schematic representation of the methods used so far for bioprinting human iPSC-derived cells (reviewed in *Salaris and Rosa, 2019*).

Our work exploits extrusion-based bioprinting to obtain 3D constructs from human iPSC-derived cortical neurons and glial precursors.



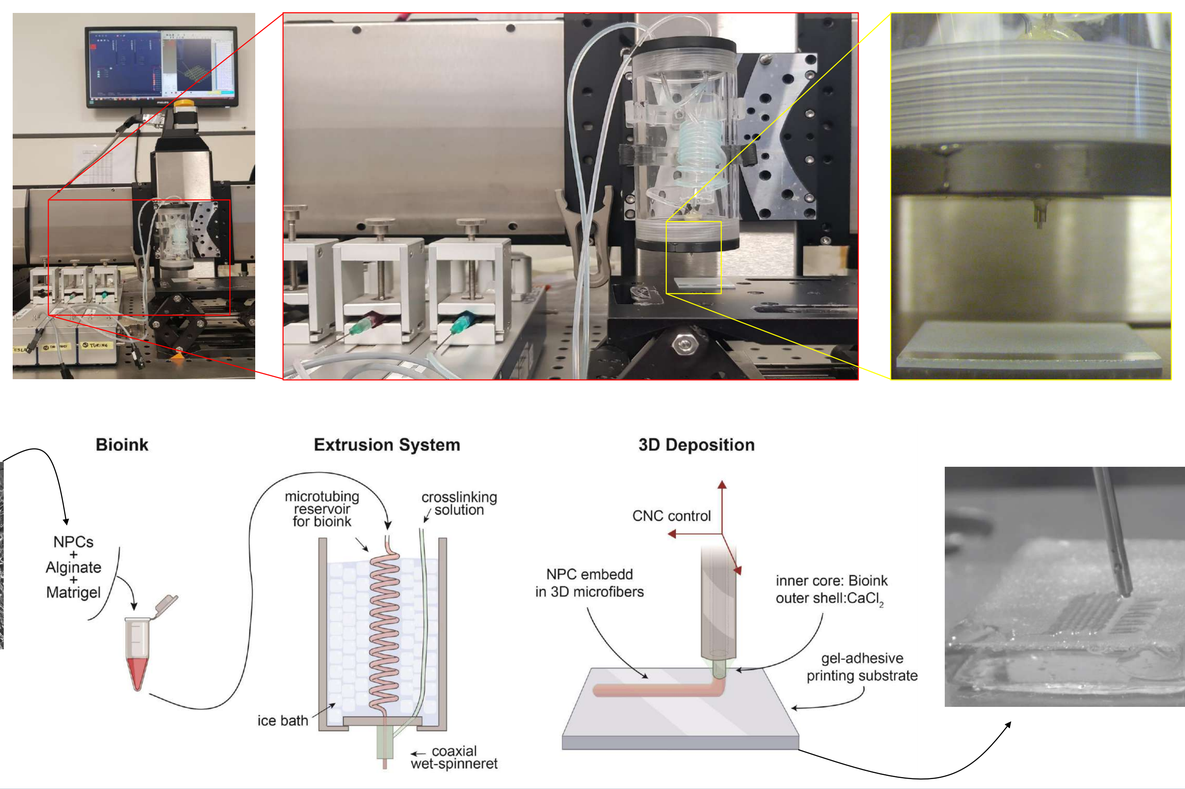
Instruments and methodologies



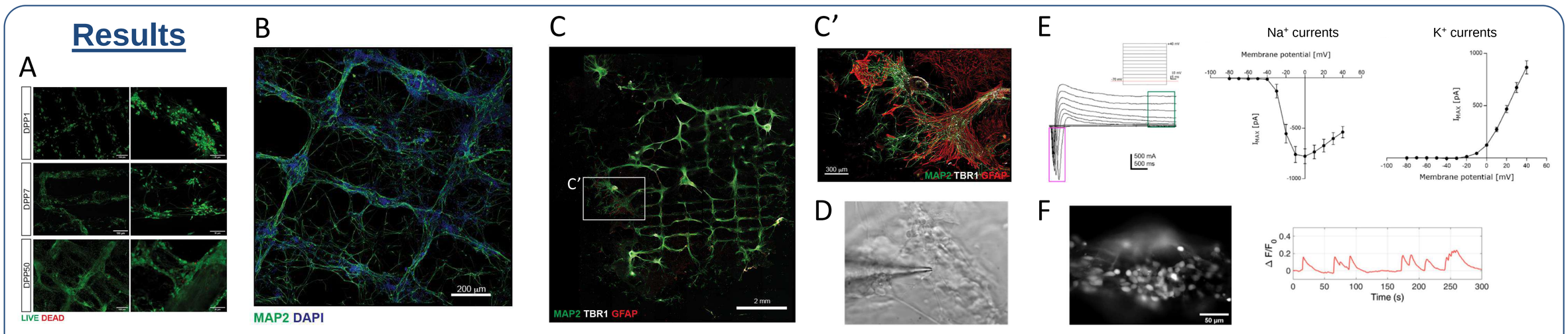
(A) Our method is based on the initial differentiation of human iPSCs into neural cells (cortical neurons and glial precursors), which make the cellular material of the bioink.

(B) Photograph of the 3D-bioprinter machine, a custom-made extrusion-based bioprinter implemented with co-axial wet-spinning microfluidic devices (*Colosi et al., 2017*). Close-up pictures show increasing magnifications of the extrusion system.

(C) Schematic representation of the bioprinting method outline. Human iPSC-derived neural cells are dissociated and mixed with a solution containing 2% w/v alginate and 0.5X Matrigel to make the bioink. During the printing process, bioink and crosslinking solution (calcium chloride) meet at the ending tip of the coaxial extruder, where Ca^{2+} ions trigger the gelation of alginate. A micrometric cell-embedding gel fiber is therefore spun out and deposited in pre-determined positions. Printing instructions are expressed in g-code language, and printing codes were generated using a custom MATLAB algorithm.



Results



We printed the cells as a reticulum, consisting of two alternating perpendicular layers of microfibers with theoretical diameter of 100 µm, separated by gaps of 200 µm, a layer thickness of 100 µm, deposited at a speed of 240 mm/min, forming a squared fiber mesh of 5 mm × 5 mm × 200 µm. (A-C') The great majority of the cells were viable at different days post printing (DPP) and express neural markers (B: DPP7; C-C': DPP70). (D) Bioprinted neurons were then analyzed functionally by single-cell patch-clamp recording. (E) Left: representative scheme of the recording protocol (purple box: inward sodium currents; green box: permanent outward potassium currents); right: average traces of large inward voltage-dependent Na^+ currents and outward voltage-dependent K+ currents. (F) Single action potential evoked in current clamp recording and a representative calcium trace, as a function of ΔF/F0, of cortical neurons isolated within the 3D network at DPP7. Reference: *Salaris et al., Journal of Clinical Medicine (2019)*.

Conclusions and future perspectives

Our work is the result of an extensive effort in the optimization of the bioprinting process and bioink composition, with the goal to define proper conditions for generating **human artificial 3D cortical neural tissues from iPSCs**. Bioprinting neurons and glial cells represents a challenge. Neurons are vulnerable cells in vitro and environmental stress due to the printing process may affect neural cell viability and influence further differentiation and maturation. Our method allows long term survival of human neurons, up to 70 days post printing, without affecting differentiation and maturation. This is the longest time of maintenance of human iPSC-derived neurons in 3D bioprinted constructs. Bioprinted iPSC-derived neurons, similar to 2D cultures, display functional properties typical of immature neuronal networks. We are currently working on strategies to improve the maturation of the cortical neurons in the 3D construct. Moreover, identifying more physiological, standardized and defined alternatives to Matrigel is necessary for basic and translational applications of bioprinted constructs.

This study opens the possibility for generating more complex human neural 3D constructs, for instance by printing mixed populations with precise ratios of neuronal and glial cells and/or printing iPSCs carrying pathogenic mutations associated to neurological diseases. Notably, the bioprinting approach can be further implemented with more sophisticated microfluidic platforms that might allow the deposition of multiple materials and/or multicellular bioink within a single scaffold, by simultaneously extruding different bioinks or by rapidly switching between alternative bioink compositions, with the aim of controlling the localization of individual cell types in predetermined positions of the 3D construct. In the next future we plan to use different specific neuronal subpopulations and other cell types, which can be obtained by iPSC differentiation, as the cellular component of 3D constructs for disease models and drug screening. This would be particularly relevant in the case of complex diseases with clear non-cell autonomous contribution of neural and non-neural cells. In the long term, further development of this technology could provide bioprinted cortical neural constructs that can be exploited as **customized, standardized and scalable pre-clinical models for drug safety and toxicity studies**.

Salaris F., Colosi C., Brighi C., Soloperto A., de Turris V., Benedetti M.C., Ghirga S., Rosito M., Di Angelantonio S., Rosa A. (2019). 3D bioprinted human cortical neural constructs derived from induced Pluripotent Stem Cells. **Journal of Clinical Medicine.** 8(10), 1595.

Salaris F., Rosa A. (2019). Construction of 3D in vitro models by bioprinting human pluripotent stem cells: challenges and opportunities. **Brain Research.** 1723, 146393.

Assembling a setup for infrared multispectral imaging of Medieval codices

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ERC sectors:

- *PE4_2- Spectroscopic and spectrometric techniques*
- *SH5_8- Cultural studies, cultural identities and memories, cultural heritage*

Introduction

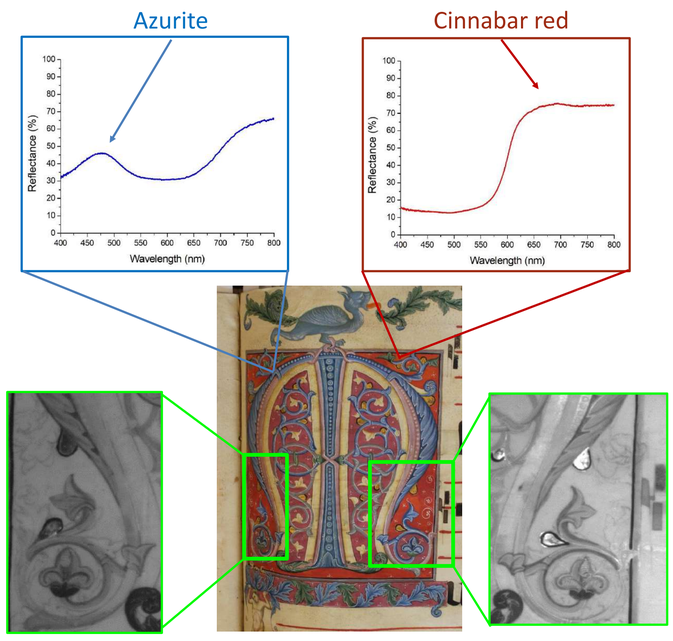
An ongoing collaboration between Departments of Sapienza aimes to build a framework for **infrared imaging of illuminated manuscripts**. The results obtained by these measurements will support the identification of pigments and stilistic analysis, based on previous non-invasive methods such as Fiber-Optics Reflectance Spectroscopy (FORS) and Near-InfraRed (NIR) Imaging.





1 NIR Imaging and FORS spectroscopy

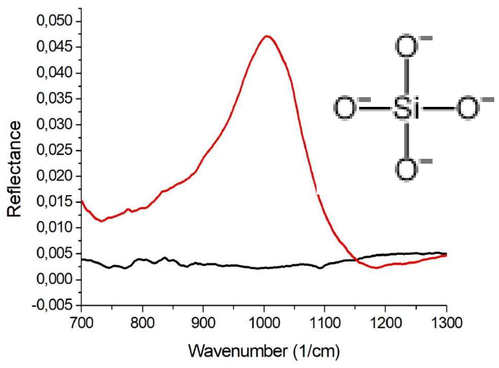
Two techniques, commonly used for manuscripts, have been adopted to characterize the pigments and to reveal the presence of '*pentimenti*' under the final layer, i.e. the Fiber Optics Reflectance Spectroscopy (**FORS**) and the Near-InfraRed (**NIR**) Imaging. Two FORS spectra (*above*) and NIR images (*below*) are here shown.



2 Mid-Infrared (MIR) Microscope

A database of **MIR spectra** has been created in order to investigate the chemical composition of pigments and bindings used in illuminations. Reflectivity spectra were acquired using a Michelson Interferometer coupled with HYPERION FT-IR Microscope (left figure). Comparision between azurite and ultramarine is also shown in the right figure.

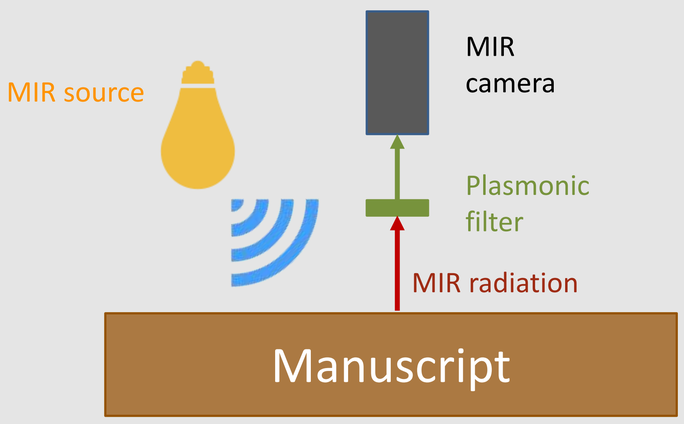




Metal silicate (Ultramarine)
Organic metal (Azurite)

3 Chemical imaging in the MIR region

The extension of imaging to MIR can provide information on the chemical nature of materials used in illuminations (pigments, organic compounds and metals) and will be carried out using **plasmonic filters** (on the right) to select region of interest and a dedicated **MIR camera** (below).

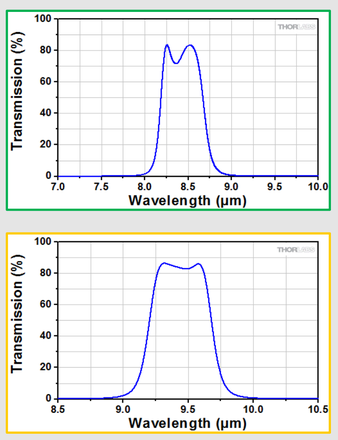


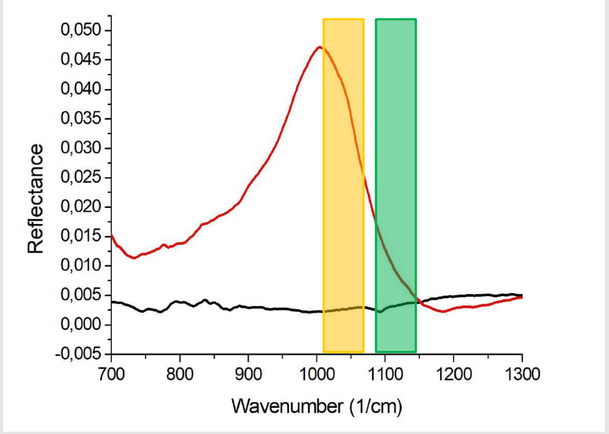
Spectrally resolved images through band-pass filters



$$\frac{\nu}{\Delta\nu} = 20$$

MIR Camera
640x480 pixels
8-14 µm
1250-715 cm^{-1}





Riferimenti recenti

Colours: the art and science of illuminated manuscript (2016)

Nodari and Ricciardi *"Heritage science"* (2019) 7:7