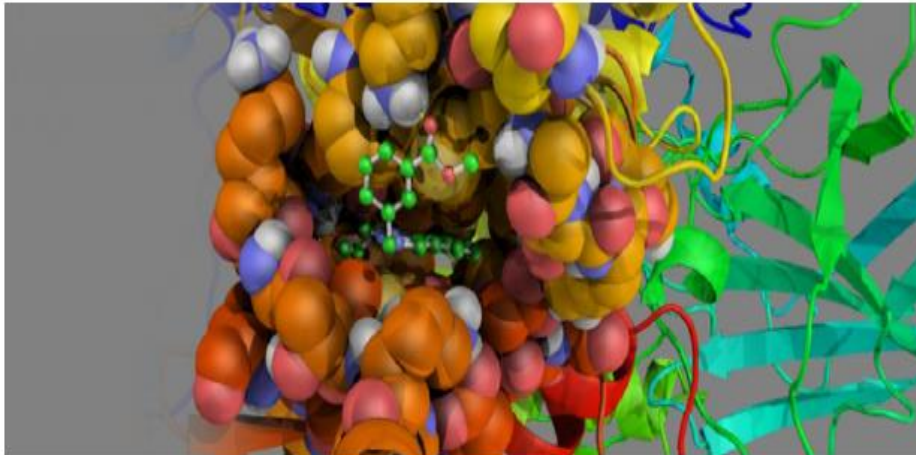
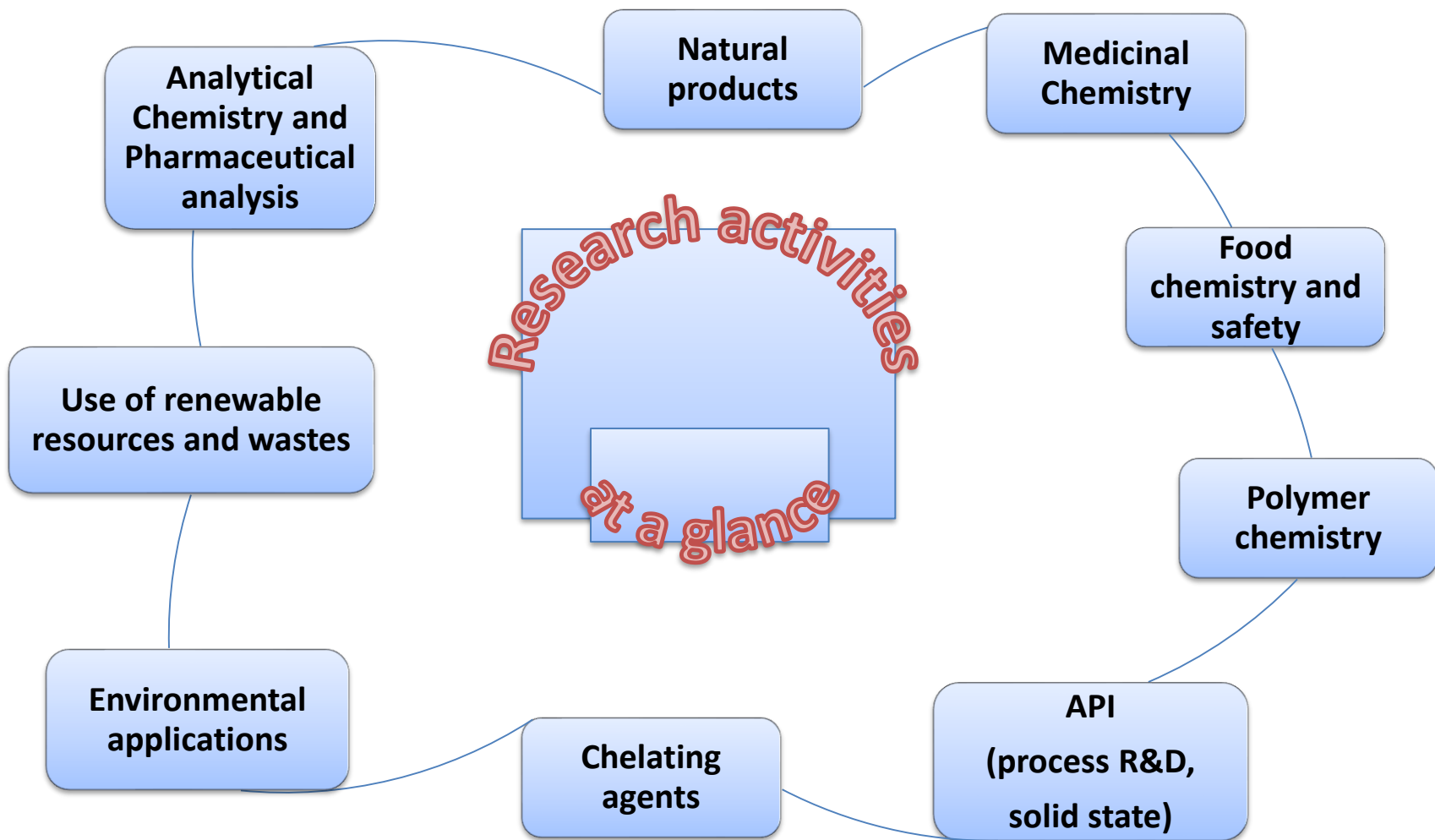


DEPARTMENT OF SCIENCE AND TECHNOLOGICAL INNOVATION



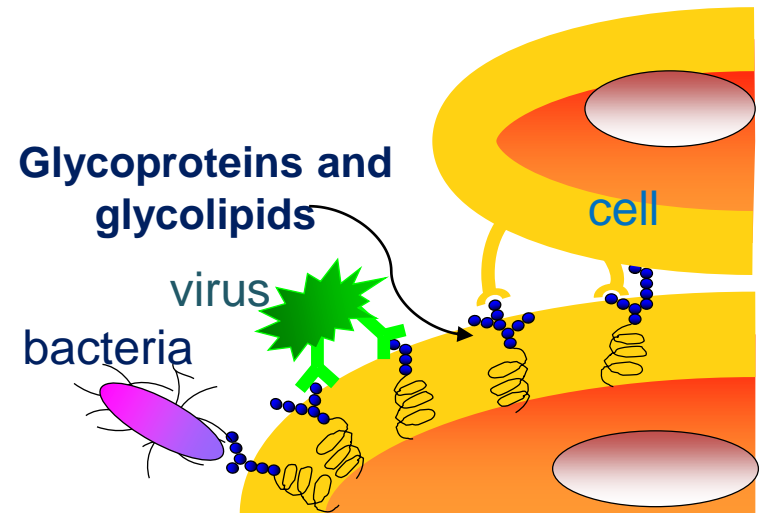
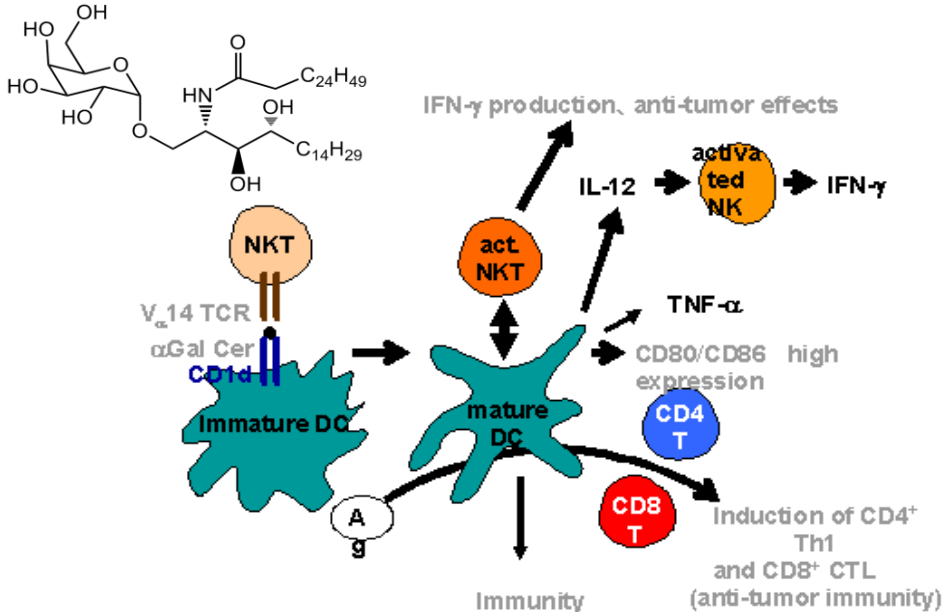
DEPARTMENT OF PHARMACEUTICAL SCIENCES



Research Topics/1

- Synthesis of glycoconjugates with potential applications as immunomodulators
- Synthesis of carbohydrate analogues as metabolic interferents
- Use of sugars from natural sources and wastes as raw material to obtain high value derivatives

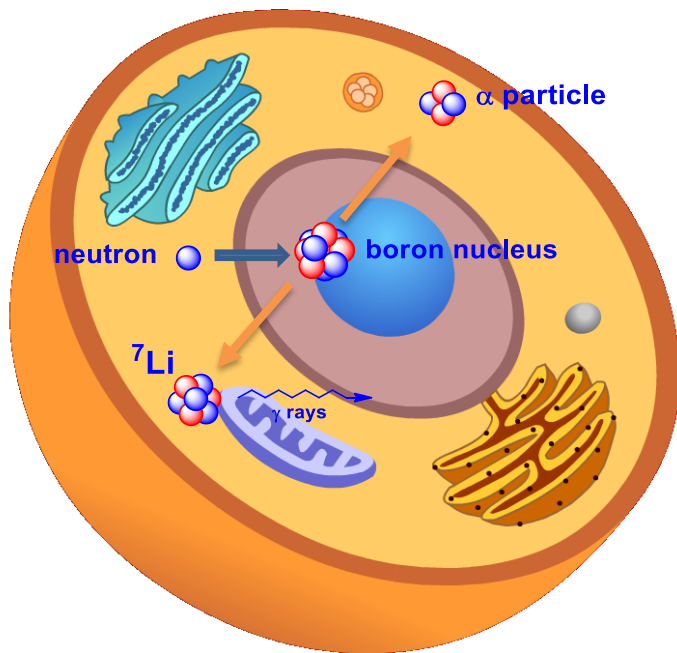
Glycoconjugates play a major role in cell interactions and in immune system surveillance. It is of paramount importance to have tools to gain insight into these phenomena and for various applications. Our group has expertise in handling sugar containing natural compounds and analogs thereof non only using classical synthetic methods but also exploiting renewable sources and "green" approaches



Among the various projects we are developing glycolipids as immunomodulators with application as antitumor agents, in self-immune diseases and as adjuvants in vaccines with a patent on the field:
WO2009060305A2

Research Topics/2

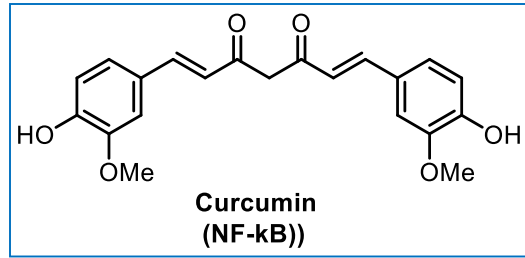
- Synthesis of boronated molecules for application in boron neutron capture therapy
- Development of new synthetic methods



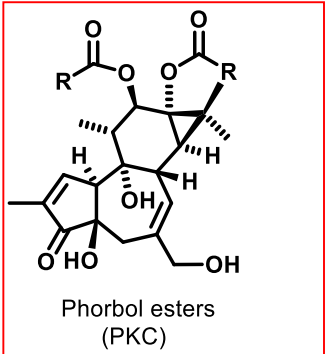
Boron Neutron Capture Therapy (BNCT) is an experimental binary radiotherapy, based on thermal neutron irradiation of the tumour previously enriched with ^{10}B . The thermal neutron capture reaction ($^{10}\text{B}(n,\alpha)^7\text{Li}$), gives rise to two high LET particles that lose all their energy within a cell causing irreversible damages to the DNA, killing the cell. The tumor cells uptake higher ^{10}B concentrations compared to the normal tissues, provided that proper boron containing compounds are administered. Hence, the irradiation with thermal neutrons delivers a potentially therapeutic dose to the malignancy, with a substantial sparing of the healthy surrounding tissues. This selective effect is a promising novelty in the field of the cancer therapy.

We are developing new molecules/delivery systems (nanoparticles) potentially able to selectively accumulate boron in tumor cells.

Our work is directed not only towards the synthesis of new boronated compounds but also to the development of new approaches to them

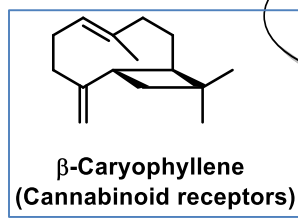
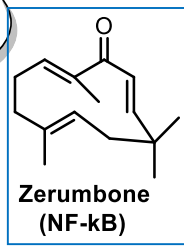
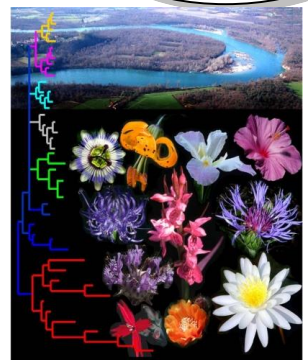
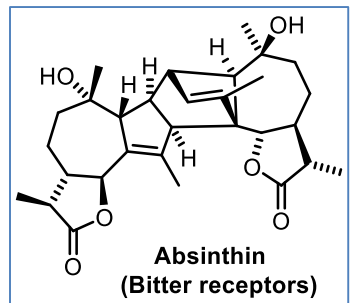


Diversità Chimica legata a composti naturali

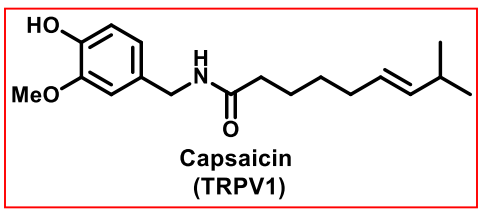
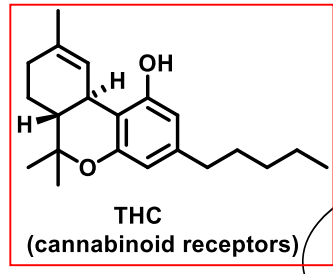


Biodiversità

Sintesi



Modulazione di processi di rilevanza biologica



Drug Discovery

Nutrizione

Tossicologia

Prof. Marco Arlorio
 Prof. Jean Daniel Coisson
 Dott. Fabiano Travaglia
 Dott.ssa Monica Locatelli
 Dott. Matteo Bordiga
 Dott. Cristiano Garino

Contatti:

marco.arlorio@uniupo.it

Tel: 0321375772, 0321375774

Skills & techniques...

- **Food chemistry:** (HPLC, HPLC-MS, GC)
- **Food biotechnology:** tecniche PCR e Real-time, elettroforesi/microelettroforesi Lab-on-chip (DNA, proteine)
- **Design/formulazione di nutraceutici e ingredienti funzionali** (spray-dry, microincapsulazione, ultrafiltrazione)



Principali linee di ricerca nell'ambito della *Circular Economy e della Green Chemistry...*

▣ **Caratterizzazione di by-products e scarti delle filiere agroalimentari e loro valorizzazione**

- caratterizzazione delle componenti primarie e secondarie di by-products alimentari (es. siero di latte, perisperma di nocciola, bucce di fave di cacao, frazioni fibrose da cereali, vinacce e vinaccioli....)
- estrazione e caratterizzazione di oligosaccaridi prebiotici
- estrazione e caratterizzazione di sostanze ad azione antiossidante e antiinfiammatoria
- estrazione e caratterizzazione di pigmenti di interesse alimentare

▣ **Formulazione di ingredienti e loro valutazione in modelli alimentari e nutraceutici**

- formulazione di ingredienti (a livello laboratorio e pilota)
- microincapsulazione di ingredienti
- test di proprietà nutrizionali/tecnologiche durante la shelf-life di prodotto

Alcuni esempi di collaborazioni Accademiche internazionali



WAGENINGEN UNIVERSITY
WAGENINGENUR



HACETTEPE UNIVERSITY
To the leading edge... Toward being the best...



iceta

Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares



Academisch Medisch Centrum
Universiteit van Amsterdam

Alcune collaborazioni con Aziende e partnerships...



PROGE FARM®



MB Med.



FERRERO



FIORIO COLORI
... a member of **AromataGroup**



Thermo
SCIENTIFIC



Finanziamenti da.....



PHARMACEUTICAL ANALYSIS

info@symech.it



Giorgio Grosa
Associate professor



Gianna Allegrone
Associate professor



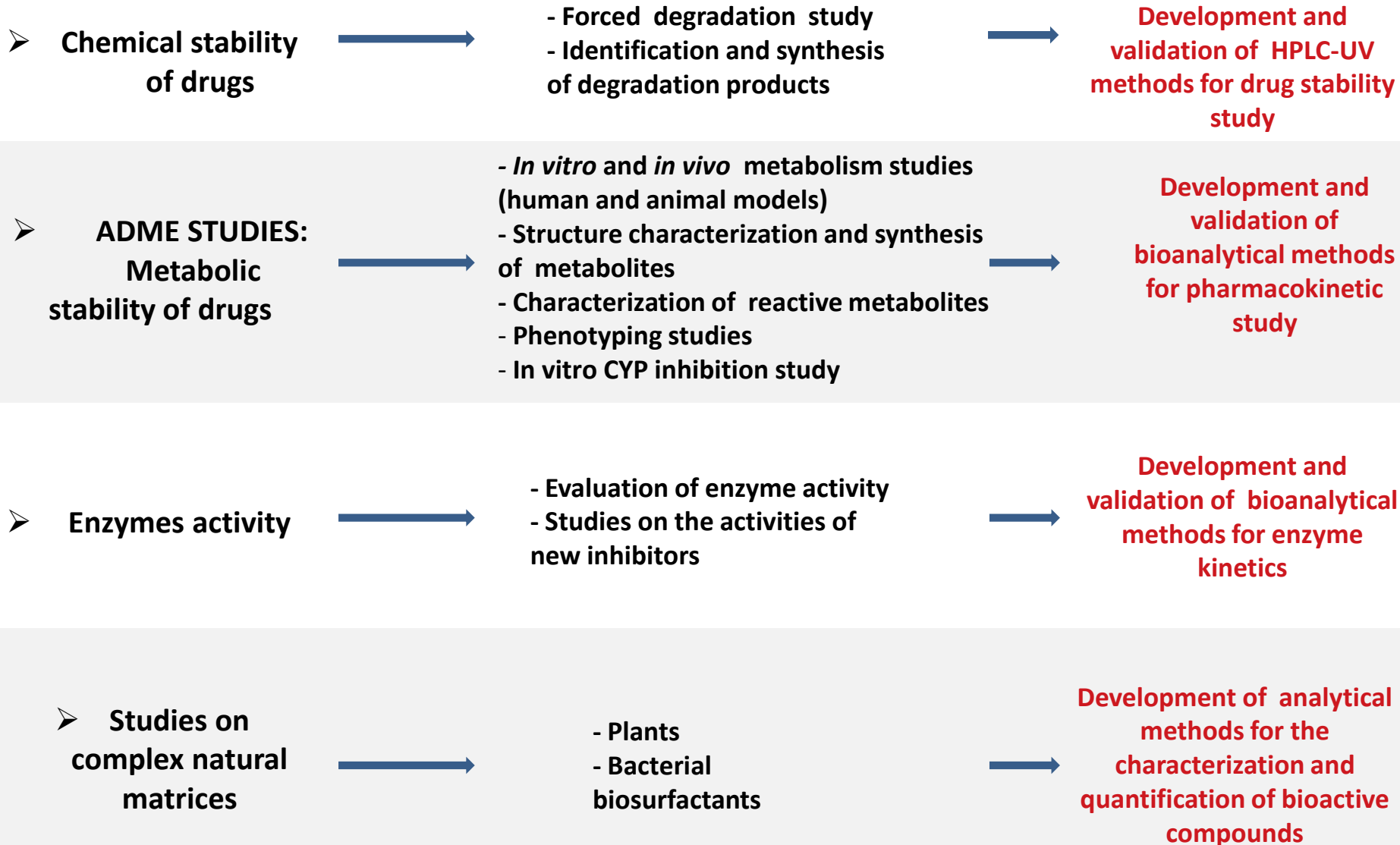
Erika Del Grosso
Assistant professor

Skills

- + Sample preparation: biological and/or natural matrices
- + Development and validation of analytical methods
- + Chemical stability of drugs
- + ADME studies: metabolic stability of drugs
- + Enzymes activity
- + Studies on complex natural matrices

Techniques and instrumentations

- + Chromatography, SPE, LLE, preparative HPLC, etc
- + UV-Vis, HPLC-UV, HPLC-FL, HPLC-MS, GC-MS



MEDICINAL CHEMISTRY

www.symech.it
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Giovanni Sorba
Full professor



Gian Cesare Tron
Associate professor



Tracey Pirali
Associate professor



Ubaldina Galli
Assistant professor



Alberto Massarotti
RTD-B



Synthesis

- + Multicomponent reactions
- + Isocyanide chemistry
- + Aryne chemistry
- + Click chemistry

In silico

- + ZINC database (virtual cmp)
- + ZINClick database (virtual cmp)
- + *In house* compounds (2000 real cmp)
- + *In silico* MCR deconvolution
- + Molecular simulations

Our group philosophy: *use ideal reactions*

- | | |
|--------------------------------------|---------------------|
| + One Pot | + Efficiency |
| + Simple | + Atom economy |
| + High yields | + Versatility |
| + Resource effective | + Exploratory power |
| + Environment friendly | + Selectivity |
| + Ready available starting materials | |

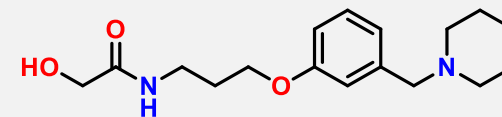


Drugs syntheses using new multicomponent reactions developed by our group

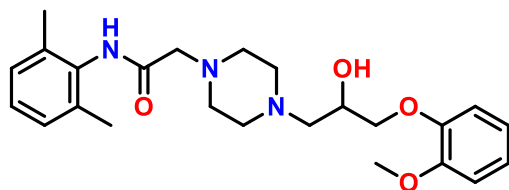
The use of 2-hydroxymethyl benzoic acid as an effective water surrogate in the Passerini reaction: A straightforward access to α -hydroxyamides

Serafini M., Griglio A., Oberto E., Pirali T., Tron G.C.

Tetrahedron Lett., **2017**, 58, 4786-4789



Roxatidine



Ranolazine

An efficient synthesis of symmetric and unsymmetric bis-(β -aminoamides) via Ugi multicomponent reaction

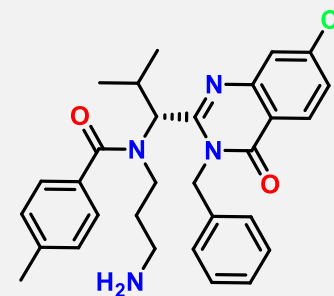
La Spisa F., Feo A., Mossetti R., Tron G.C.

Org. Lett., **2012**, 14, 6044-6047

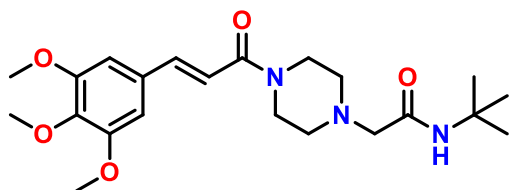
Imides: Forgotten Players in the Ugi reaction. One pot multicomponent synthesis of quinazolinones

Mossetti R., Pirali T., Saggiorato D., Tron G.C.

Chem. Comm., **2011**, 47, 6966-6968



Ipsinesib



Cinpropazide analogue

Split the primary amine in two: secondary diamines may play the role of the primary amine in the Ugi 4CR

Giovenzana G.B., Tron G.C., Di Paola S., Menegotto I.G., Pirali T.

Angew. Chem. Int. Ed., **2006**, 45, 1099-1102



TRPV1 Modulator Compounds

Devesa G.I., Genazzani A.A., Pirali T., Fernandez-Carvajal A., Ferrer-Montiel A.V.
EP17382266.9, 2017, EP17382266



Modulators of SOCE, compositions, and uses thereof

Pirali T., Genazzani A.A., Riva B.
PCT Int. Appl., 2017, WO20172124



TRPM8 receptor agonist compounds and uses thereof

Ferrer Montiel A., Fernandez Carvajal A., Belmonte M.C., Gallar M.J., De La Torre R., Genazzani A.A., Tron G.C., Mercalli V.
PCT Int. Appl., 2017, WO20171256



Inhibitors of nicotinamide phosphoribosyltransferase, compositions, products and uses thereof

Genazzani A.A., Tron G.C., Galli U., Travelli C., Cuzzocrea S., Grosa G., Sorba G., Canonico P.L.
PCT Int. Appl., 2014, WO2014178001 (A1)



Quinolin-4 (1h)-one derivatives as inhibitors of phosphatidylinositol 3-kinases

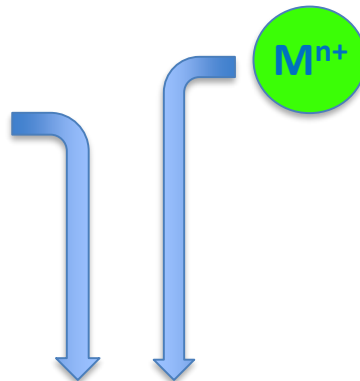
Sorba G., Tron G.C., Galli U., Massarotti A., Hirsch E., Ciraolo E., Pirali T.
PCT Int. Appl., 2012, WO 2012073



Research Topics 1/2

Chelating agents

- Analytical Chemistry
- Textile Finishing
- Paper pulp treatment
- Water hardness treatment
- Stabilization of formulations
- Metal extraction/separation
- Metal etching
- Detoxification/Metal Ion Removal



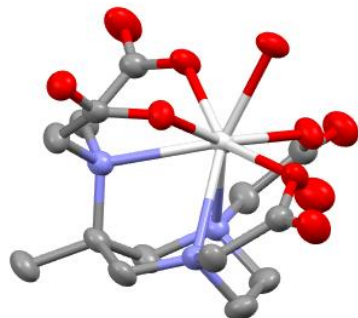
Metal ions

- Magnetic
- Luminescent
- Therapy
- Radioactive
- Endogenous
- Toxic



Metal chelates

- Contrast agents (MRI)
- Nuclear tracers (PET, SPECT)
- Therapy
- Metallopharmaceuticals
- Radiotherapy
- Agricultural supplement
- Catalysis



Diagnostics

- Diagnostic probes

(Bio)conjugation

- Techniques and reagents



Research Topics 2/2

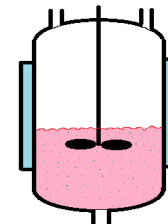
Chemistry of nitrogen-based functional groups

- Synthetic methods
- Nitrogen containing (bio)active compounds
- Surface functionalisation



APIs

(Active Pharmaceutical Ingredients)



Process Chemistry & Technology

- Route design&selection
- Optimisation
- Catalysis
- Sustainability
- Scale-up
- Polymorphism/Solid state
- Related compounds



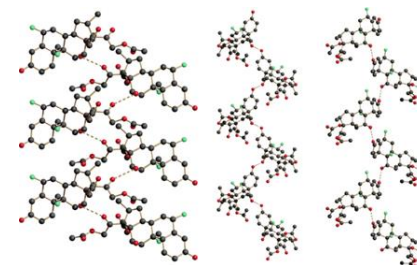
Metal ions

- Metal-based diagnostics
- Metallo-therapeutic compounds
- Interactions

Analysis



- NMR
- IR
- XRD



DISIT Dept. of Science & Technological Innovation



Prof. Leonardo Marchese
(Full Professor)



Prof. Maurizio Cossi
(Full Professor)



Prof. Enrica Gianotti,
(Associate Professor)



Prof. Chiara Bisio
(Associate professor)



Dr. Giorgio Gatti
(Researcher)



Dr. Ivana Miletto
(Researcher)



Dr. Marta Corno
(Researcher)



Dr. Alberto Fraccarollo
(Technician)

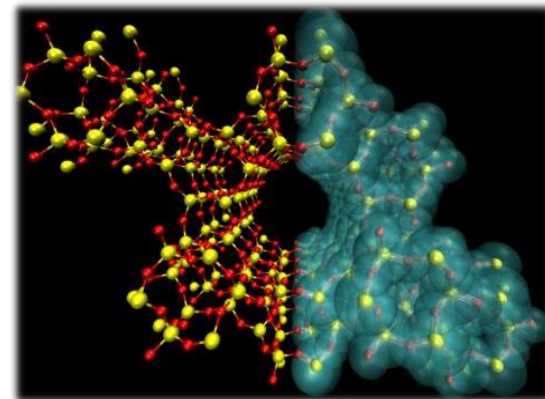


Dr. Geo Paul
(Post-doc)

Chemistry for the Future

Role in the Grand Challenges

- ✓ Sustainable energy
- ✓ Cleaner drinking water
- ✓ Health care
- ✓ CO₂ capture
- ✓ Renewable Fuels



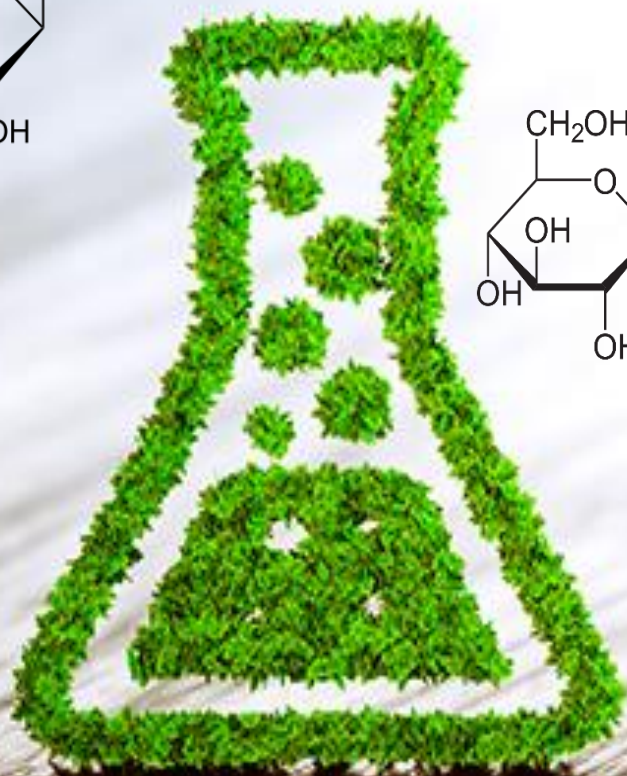
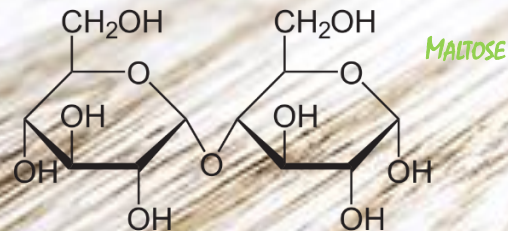
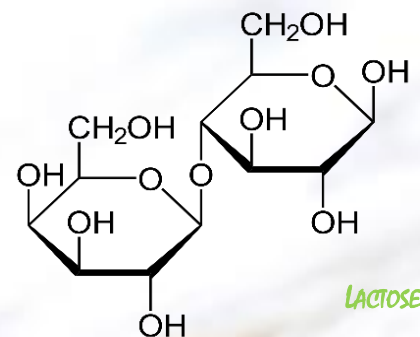
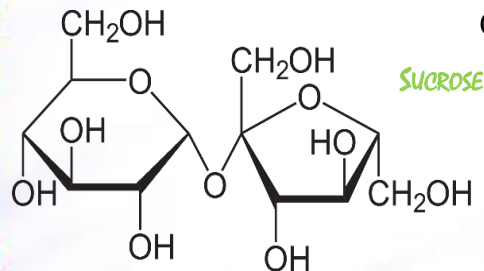
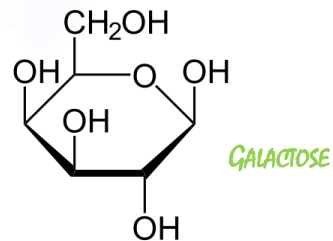
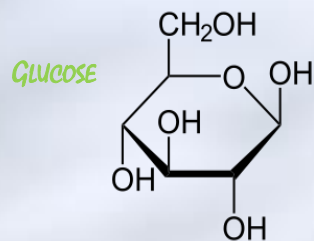
SUSTAINABLE HETEROGENEOUS CATALYSTS & CATALYTIC PROCESSES

Engineering and Tailoring the catalytic properties of heterogeneous porous catalysts

- ✓ Photochemistry
- ✓ Photoelectrochemistry
- ✓ Atom efficiency
- ✓ High selectivity
- ✓ Waste minimization
- ✓ Environment

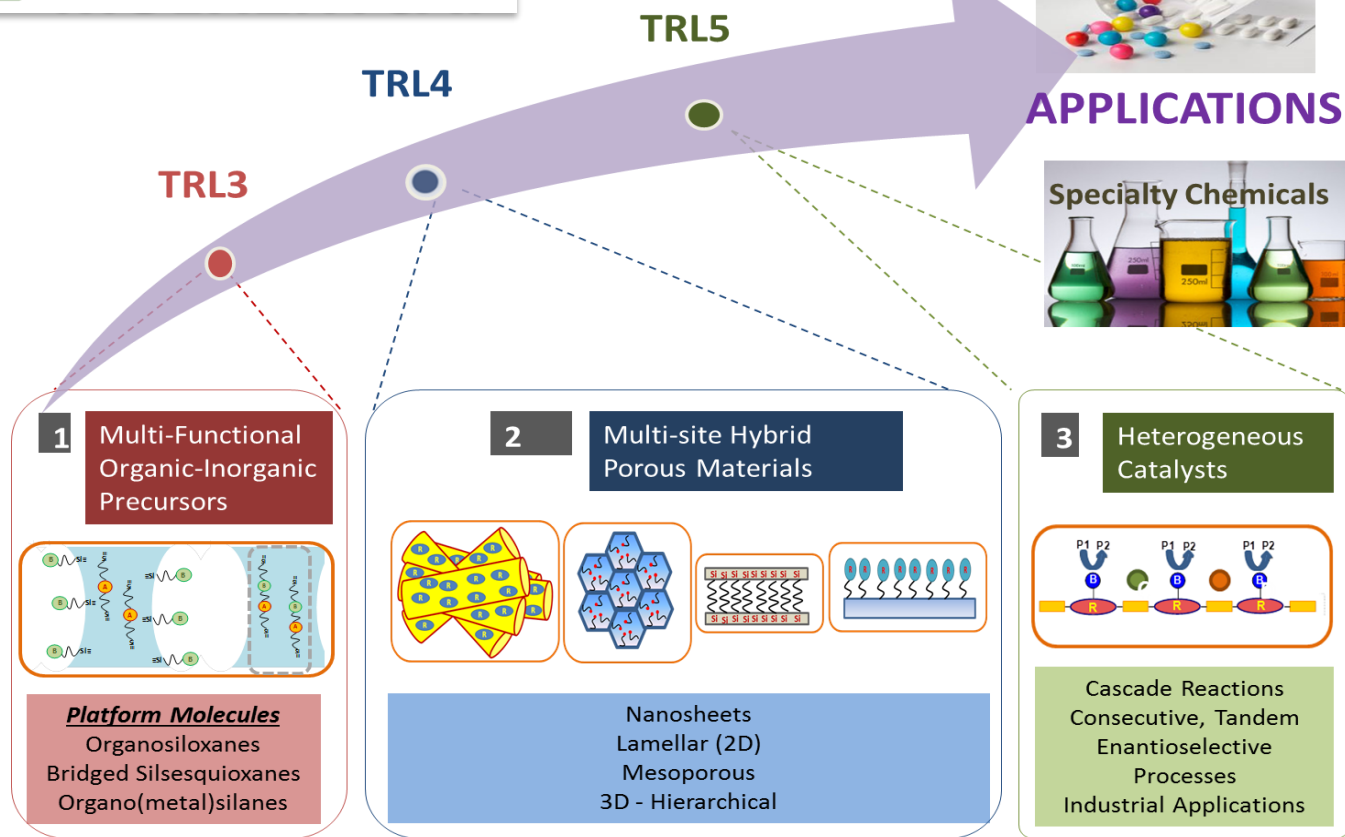
- ***New heterogeneous catalysts for environmentally friendly processes;***
- ***Development of nanoporous materials for storage and activation of gas or adsorption of environmental pollutants;***
- ***Optimisation of luminescent materials for optoelectronic and biomedical applications;***
- ***Synthesis and modelisation of materials for the production of energy with low environmental impact;***
- ***Development and application of theoretical and computational techniques***

Environmentally Friendly Synthesis of Porous Catalysts using GREEN Templates



MULTI-site organic-inorganic Hybrid CATalysts for MULTI-step chemical processes

MULTI2HYCAT



The new hybrid catalysts will allow avoiding the extra-efforts associated with isolation of intermediate products, wastes and solvents elimination and purification processes thus enabling more efficient and sustainable catalytic routes from the economic, energetic as well as the environmental points of view.

Development of Materials and Methods for Environmental Applications



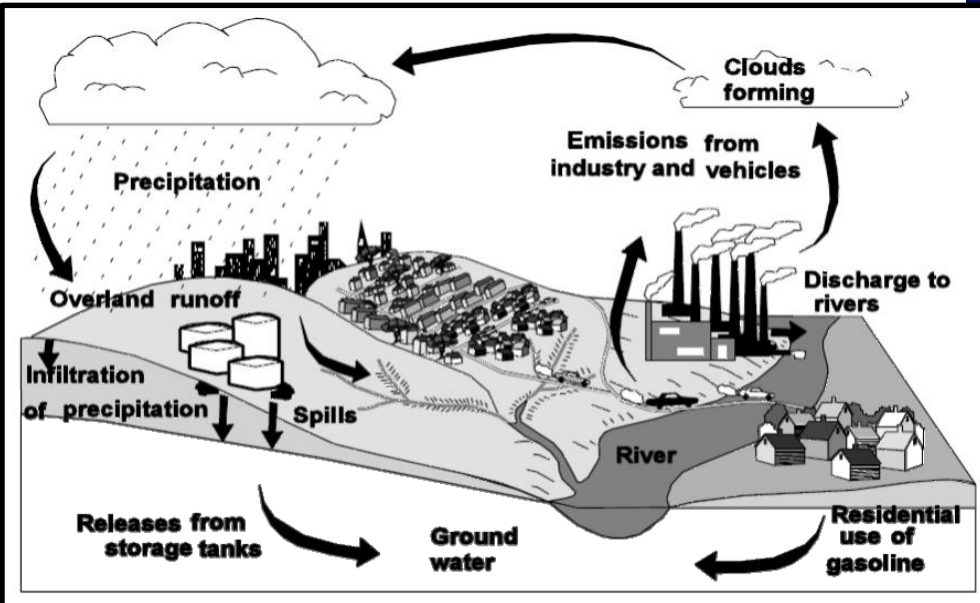
ENVIRONMENTAL POLLUTION

CO₂ capture/ transformation

(PRIN Project n° 2010A2FSS9 :
“Mechanisms of CO₂ activation for the design of new materials for energy and resource efficiency .)

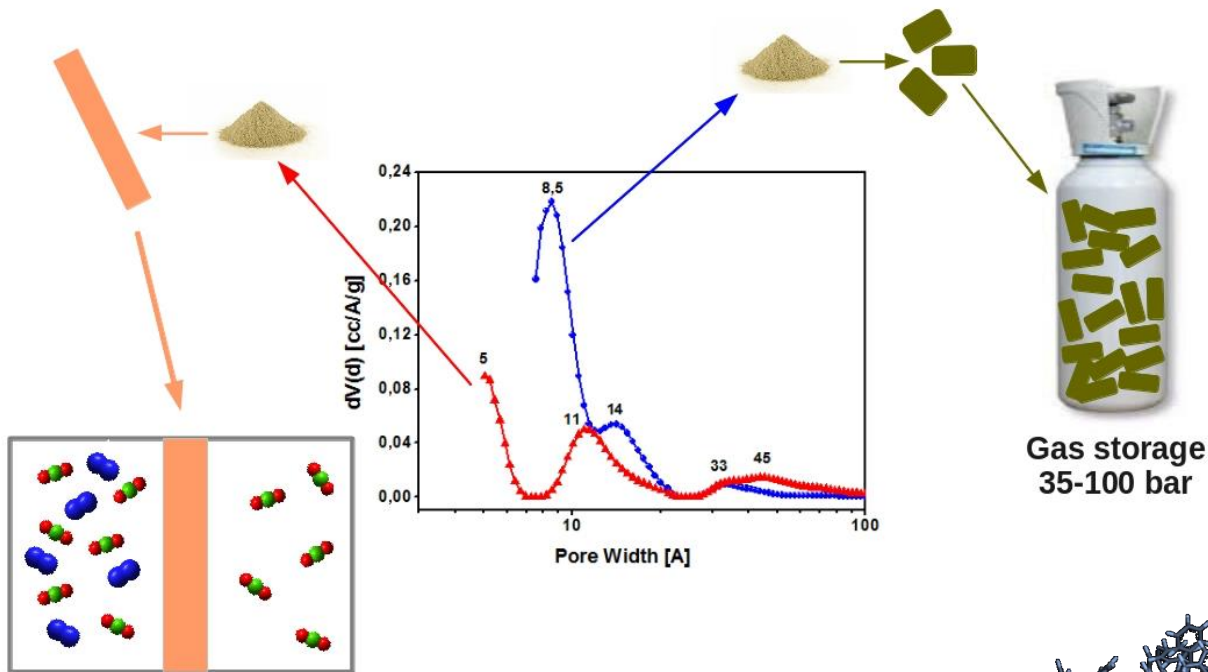
Removal of pollutants from water and gas phase

(Research supported by ENI in collaboration with the University of Bologna)

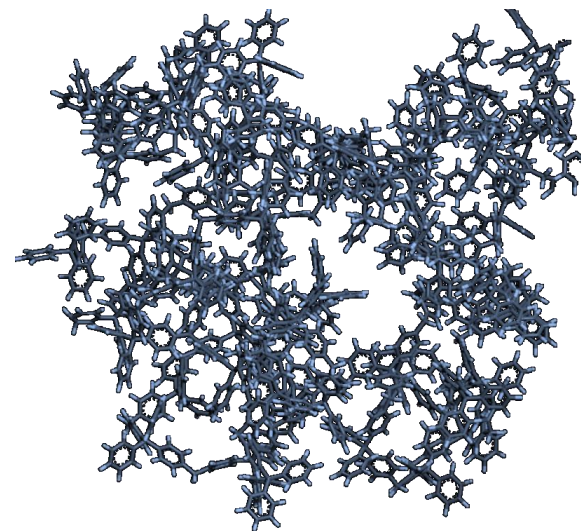
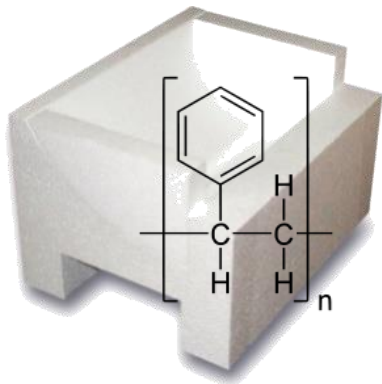


Tailoring porous polymers/carbons for gas storage/separation applications and pollutants removal – recycling waste products

Patented by

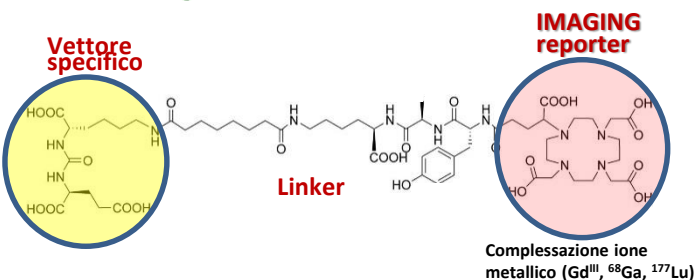
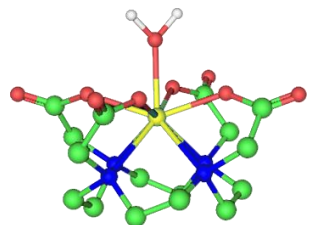
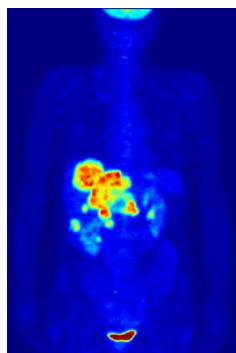
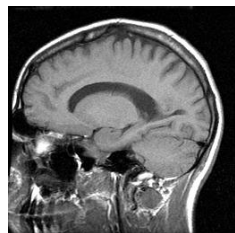


Gas separation/purification
0.1-1 bar



Sonde metalliche per la diagnostica clinica

[Prof. M. Botta, Prof. L. Tei, Dr. F. Carniato, Dr. G. Digilio, Dr. D. Lalli]



- Design, sviluppo e caratterizzazione di complessi metallici paramagnetici quali sonde diagnostiche per MRI; ottimizzazione dei parametri molecolari per aumentare l'efficienza delle sonde ad alti campi magnetici (1.5-3 T).
- Nanoparticelle inorganiche multifunzionali per applicazioni diagnostiche e teranostiche.
- Sintesi di nuovi chelanti ottimizzati per applicazioni in MRI e medicina nucleare (PET, SPECT) e/o teranostica.
- Sintesi di sonde per imaging molecolare: sintesi di chelanti bifunzionali e loro coniugazione a vettori biologici (peptidi, molecole biologicamente attive) o a sistemi nanoparticellari sia di tipo organico (micelle, liposomi) che ibrido organico/inorganico;
- Sviluppo di sonde molecolari responsive al microambiente tissutale per applicazioni in imaging molecolare e cellulare.

Applicazioni di rilassometria NMR

- FFC Relaxometry è una tecnica sperimentale avanzata che aggiunge una nuova dimensione all’NMR.
- Le misure a differenti intensità di campo magnetico “sentono” le diverse frequenze del moto molecolare. La gamma disponibile di campi magnetici, da quasi zero a 3 Tesla (tipica degli scanner medici) implica che si possa investigare, con un singolo esperimento, i processi di moto su una vasta gamma di scale temporali (da ms a ps).
- La FFC Relaxometry è utilizzata nello sviluppo della diagnostica e della terapia medica, dell’industria dei materiali avanzati, degli studi ambientali e della scienza e della tecnologia agroalimentare.





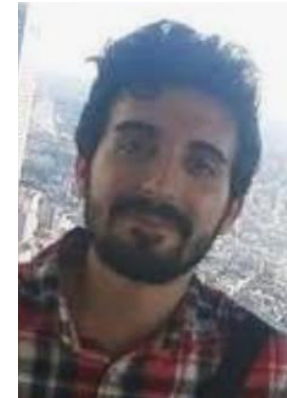
Eleonora Conterosito
Post-DOC



Enrico Boccaleri
Associate Professor
Group leader



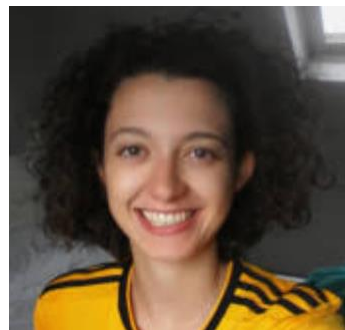
Marco Milanesio
Associate Professor



Mattia Lopresti
PhD student



Luca Palin
Post-DOC



Beatrice Mangilini
Bursary



Giuseppe Rombolà
Post-DOC



Valentina Toson
Post DOC

From waste to fine chemicals toward a circular economy, three cases

Egg shell recovery

- 150,000 tons of this material disposed in landfills each year (US market)
- Italian market: 13 billion eggs produced every year, whose about 40% is employed in egg processing, which lead to the presence of **more than 300000 tons eggshell per year**
- Currently used for Landfilling (associated cost: 0.25 €/Kg, plus the drying step before shipment or ingredient for fertilizers or for feedstock for animals different from chickens (selling price: 15 €/ton, minus plus the drying step before shipment)

Wheat and rice straw and rice husk recovery

- About 600 million tons wheat straw other 600 million tons of rice straw, more than 100 mil tons of rice husk difficult to be disposed in landfills each year (US market)
- **Only about 20% of rice straw is used** in valuable chains, most of the material returned to soil, mixed in manure, burned directly in the fields or in specific plants for power and heat generation

Waste cement recovery

- Cement and concrete are **unsubstitutable materials for infrastructure development**. Its production of them is based on **non renewable mineral resources and environmentally demanding processes**.
- In Europe, about **180 million tons of concrete demolition waste (CDW) are produced every year**, around 31% of all the waste produced in the European Union.
- The way towards a **total recovery of concrete demolition waste (CDW) is a challenge** requiring technological and scientific efforts to upcycle waste materials

CASE 1: Egg shell recovery: ITTO20090644 patent - Use of eggshells as additives composite materials

Using eggshell as an available, inexpensive and light-weight feedstock for a **potential source of different products, organic fractions and raw materials**

A new approach...

Extracting nutrients and materials from eggshell with sustainable methods, avoiding also the use of raw non-renewable materials and the landfilling of by-products

Bio-based products

- Valuable organic fractions (proteins, saccharides, collagen)
- Pure calcium carbonate, used as filler
- Calcium-hydroxyapatite ($\text{HA} - \text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$), to be used as biomaterial
- Heavy metal sorbents for wastewater treatment
- Functional metal oxides



CASE 2: From wheat and rice waste biomasses to fine chemicals: IT102015000044819 patent - A process to extract inorganics from cereal biomass via mild treatment

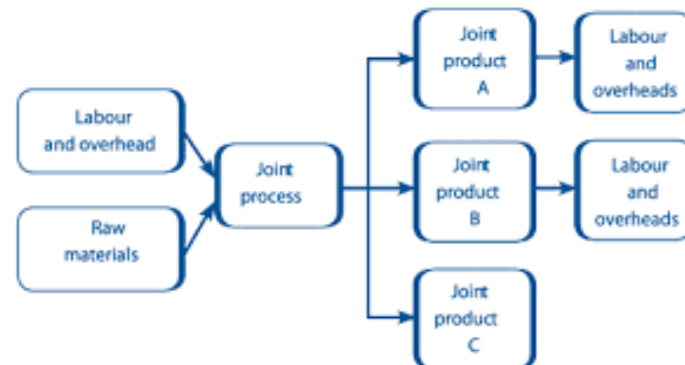
Main hinders are due to **high levels of silica** contained in these biomasses (5-10% wt. dry mass in rice straw, 2-5% in wheat, 10-20% in rice husk and wheat awns)

A new approach...

The silica content of straw and husk can become a benefit, as cereal residues can be raw material to produce several high added value **inorganic and organic materials** for a wide range of applications

New products/value chains....

1. High purity (> 95%) inorganics of natural origin
2. Fibrous organic materials
3. Organic liquid fractions for biorefinery/biofuel processing
4. Fertilisers with mineral components and organic humic fraction



Case 3, cement demolition waste recovery: EP2878586 - Cementitious products obtainable from disposed concrete

There are demonstrated possibilities to:

- **Separate** and selectively collect **non-hydrated and hydrated fractions**
- Employ selected fractions into new **cement burning processes**



A new approach....

The cement production process and the formulation of concrete can move **from a linear "cradle to grave" process to a circular "cradle to cradle" process**

A series of low-impact products....

- Recovered fractions for cement burning
- Recovered fractions for new cement formulations (i.e. geopolymers)
- Recycled aggregates with controlled and stable performances



www.michelelaus.it



Michele Laus
Full professor



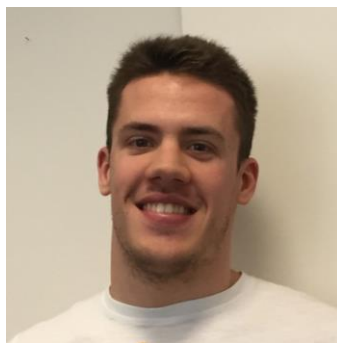
Katia Sparnacci
Associate professor



Valentina Gianotti
Associate professor



Diego Antonioli
Technician

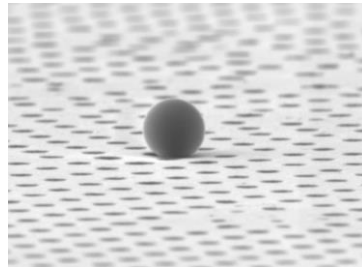


Riccardo Chiarcos
PhD student

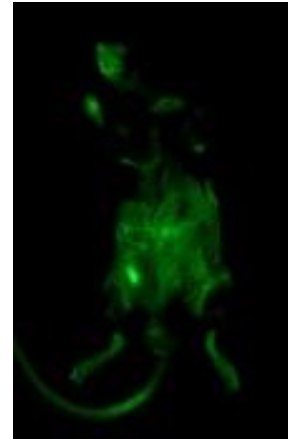


Cristiano Aliberti
PhD student

Materials
for
energy



Biomedical
applications

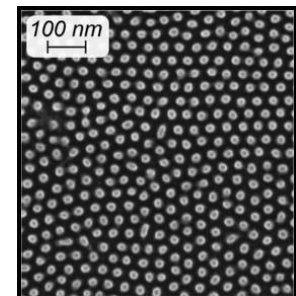
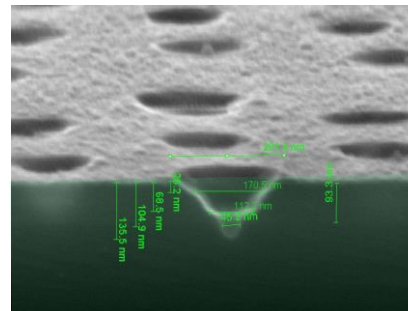
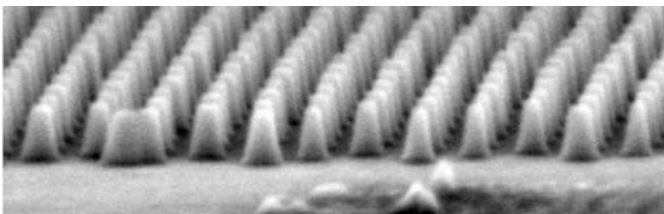


Polymeric Materials

Synthesis
&
Characterisation

Microelectronic
applications

Photonic applications





CO₂ as alternative carbon source to provide building block for the chemical industry



Raw materials

- Cyclic Carbonates and Polycarbonates
- Polyether polycarbonate polyols
- Foams
- Polyurethanes and block copolymers

Valorization and recycling of plastic waste



Chemico-physical characterization of recycled plastics in order to optimize their formulations



*Informazioni sui responsabili dei gruppi di ricerca
(contatti telefonici e e-mail, dettagli delle attività di ricerca,
pubblicazioni, brevetti, ecc.)*

Portale unico per l'Ateneo:

<https://upobook.uniupo.it/>

(ricerca per cognome/nome)

In alternativa, i siti web dei Dipartimenti:

www.dsf.uniupo.it

www.disit.uniupo.it