



Università
degli Studi
di Ferrara

Dipartimento
di Scienze Chimiche,
Farmaceutiche ed Agrarie



PhD Program in Chemistry

University of Ferrara-Italy

Katowice - January 29-30, 2026



- The PhD Program in Chemistry is organized into two curricula:
 - **Chemical Sciences**
 - **Pharmaceutical and Food Sciences**

- **Inorganic chemistry:** synthesis of metal complexes for medical applications; synthesis of semiconductors and new materials for solar energy conversion; study of redox properties and electronic structure of molecular systems, extended solids, and surfaces through quantum-mechanical calculations and experimental electrochemical and spectroscopic methods; photocatalysis and development of photoelectrochemical solar cells
- **Physical chemistry:** synthesis and characterization of crystalline and amorphous composites for technological applications; development of new materials for electrical energy storage and conversion systems within the context of the sustainable energy transition
- **Analytical chemistry:** development of sustainable methods for the purification of biopharmaceuticals through chromatographic techniques, including continuous processes; development of advanced chromatographic methods for separating analytes from complex mixtures; study of emerging contaminants and development of environmental remediation methodologies; fundamental studies of molecular recognition and metal–protein systems or metal complexes used as drugs; characterization of microporous and nanostructured materials



- **Organic chemistry:** design of sustainable synthesis processes catalyzed in batch mode and in continuous flow (metal-, organo-, photo-, bio-catalysis); synthesis of high value-added molecules for fine chemicals starting from waste materials; CO₂ utilization; synthesis of chiral molecules with biological activity
- **Industrial chemistry:** development and characterization of polymeric materials; valorization of biomasses in industrial processes

- **Pharmaceutical chemistry:** design, synthesis, and characterization of potentially therapeutic molecules targeted to biological targets involved in diseases
- **Cosmeceutical chemistry:** ecofriendly synthesis or extraction of natural bioactive molecules or compounds useful as cosmetic ingredients/carriers; recovery of cosmeceutical ingredients from plant sources and biomass; new approaches to formulation and qualitative-quantitative analysis of cosmetics; analysis and evaluation of raw materials, cosmetic formulations, and finished products
- **Pharmaceutical technology:** design, formulation, and characterization of i) solid dosage forms and drug delivery systems for oral, nasal-inhalation, and loco-regional use; ii) topical cosmetics and medical devices; iii) micro-/nanocarriers for non-invasive administration and targeting of drugs/prodrugs to cells/organs; cellular/tissue models of physiological barriers; pharmacokinetic studies and evaluation of carriers' efficacy and safety



- **Food chemistry:** characterization of functional, organoleptic, and bioactive components in food matrices; valorization of local agri-food products with respect to quality, safety, traceability, and protection of productions
- **Nutraceutical chemistry:** synthesis of molecules and application of green extraction methods to recover high-value compounds from agri-food by-products for use as ingredients or nutraceuticals; identification of molecular/ biomolecular markers as indicators of raw-material processing; study of the bioaccessibility of nutritional and functional food components



First year (60 credits)

Second year (60 credits)

Third year (60 credits)

Research activities

Educational activities

Thesis-related research activity certified by the Supervisor

1st and 2nd year up to 30 credits
(1 credit = 25 hours)

3rd year not less than 30 credits

Attendance at conferences/seminars as an audience member

1 credit per day (6 hours)

Participation in conferences/seminars as a speaker

3 credits

Poster presentation at conferences

1 credit

Journal publication

2 credits

Q1 journal publication

3 credits

Book chapter contribution with ISBN

2 credits

Mobility abroad

5 credits per month (maximum 12 months over the three-year period)

First year (60 credits)

Second year (60 credits)

Third year (60 credits)

Research activities

Educational activities

	1	2	3
Transversal training: IUSS courses 1–4	5 credits per course	20 credits mandatory over the three-year period	not less than 40 credits over the three-year period
Subject-specific training: courses in 6-hour modules	2 credits per module		
Subject-specific training: seminars	1 credits per seminar		
Inter-/multi-/transdisciplinary training: courses	5 credits per course		
Inter-/multi-/transdisciplinary training: seminars	1 credits per seminar		
Subject-specific and inter-/multi-/transdisciplinary training: maximum 20 credits per year			
Academic training: secondment to companies/public administration	5 credits per month		maximum 12 months over the three-year period
Academic training: teaching tutoring	1 credit every 4 hours		maximum 40 hours per year, 10 credits
Academic training: supplementary teaching	1 credit every 4 hours		maximum 40 hours per year, 10 credits

Subject-Specific Training: Advanced Courses and Seminars



Università
degli Studi
di Ferrara

Dipartimento
di Scienze Chimiche,
Farmaceutiche ed Agrarie

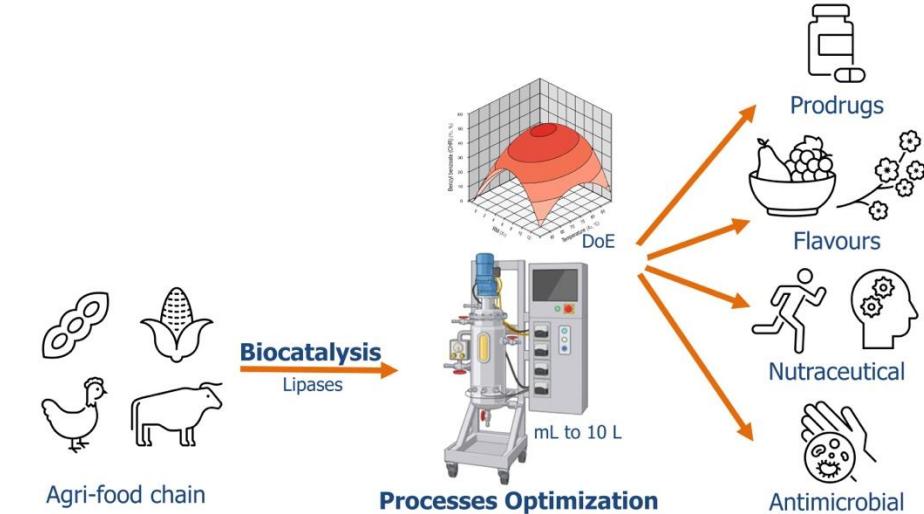
Course	Hours	Credits
New strategies in organic synthesis	12	2
Design and optimization of bioprocesses for sustainable chemistry	12	2
Click chemistry in the development of innovative drugs	12	2
Modern chromatographic techniques for the separation and purification of therapeutic and bioactive molecules	12	2
Advanced analytical methods for studying complex molecular systems in solution	12	2
Sustainable catalytic strategies for organic synthesis	12	2
Synthesis and characterization of nanostructured materials for solar energy conversion	12	2
Electron paramagnetic resonance spectroscopy: principles and applications in scientific research	12	2
Inorganic Chemistry of Radiometals	18	3
Nanotechnological systems: design, characterization and biological targeting	12	2
Introduction to REACH and CLP Regulations for the management of chemical substances and mixtures	6	1
Design of experiments (DoE) in pharmaceutical development and chemistry	12	2
Computational methods for studying reaction mechanisms: from organic chemistry to advanced materials	12	2
Seminars	1-2	1



Course	Hours	Credits
Academic English	12	5
English language (B2, C1)	21	5
English for STEM: communication in science and technology	15	5
Artificial Intelligence in Scientific Research: Methodologies, Applications and Tools	10	5
Third mission and social impact (technology transfer and intellectual property)	24	8
European project design; basic course + advanced course	22	5
Etica / Ethics and research integrity	16	5
Communicating (for) researchers; Modules 1–3	28	5
PhD, innovation and the world of work; Modules 1–3	16	5
Advanced computing and IR language; basic course + specialized course	32	10
Seminars	1-2	1

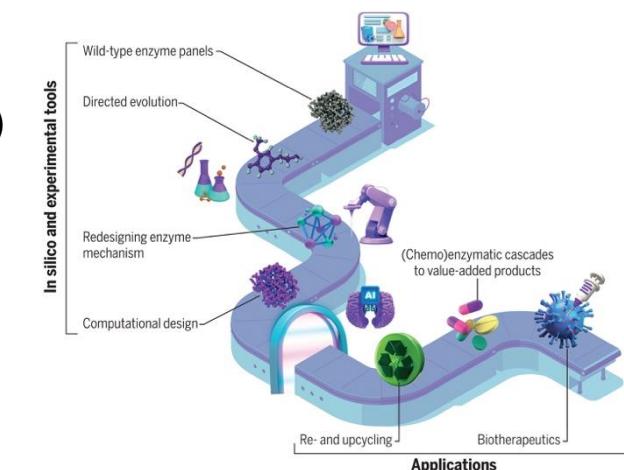
❖ Optimization of Sustainable Enzymatic Bioprocesses: From the Laboratory to Pilot Scale

- Commercial enzymes – free and immobilized
- Bio-based feedstock
- Processes optimization – Design of Experiments (DoE)
- Products with biological activity
- Laboratory scale to 10 L reactor



❖ Development of Chemo-Enzymatic Routes for Asymmetric Synthesis of Advanced Building Blocks and Biologically Active Compounds

- Expression and purification of recombinant enzymes (ligases, oxidoreductases, others)
- Enzyme immobilization - organic and inorganic solid supports
- Batch and flow enzymatic reaction
- Multi-step synthetic pathways combining enzyme-catalyzed and conventional chemical reactions



❖ Equipment

- Instruments for microbiology and molecular biology
- Gas Chromatograph (FID and MS detectors)
- Orbital shaker – 30 to 80 ° C
- STR – 0.5 to 10 L reactors
- NMR



Prof. Pier Paolo Giovannini

❖ Staff



Dr. Lindomar Alberto Lerin



Dr. Federico Zappaterra

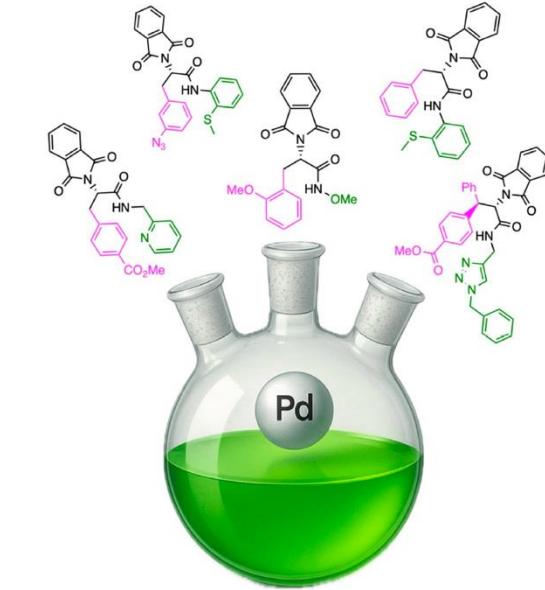


Dr. Francesco Presini

❖ Research theme 1: TM Catalyzed reaction

- Project 1, Development of TM catalyst,
- Project 2, Synthesis of non-natural AA via Pd catalysis

Recent publication: DOI: 10.1002/chem.202502272



❖ Research theme 2: Synthesis of med chem related heterocycles

- Project 1, Synthesis of chiral imidazoline as anticancer drugs,
- Project 2, Synthesis of piperidine structures in opioid receptors,

Recent publication: DOI: 10.3390/molecules29143267

❖ Equipment

- **Isolera 1 and Isolera LS (Biotage) for small to large scale purification.**
- **Biotage initiator microwave synthetizer**
- **H-Cube Pro in flow hydrogenator**

❖ Staff

- **Prof. Claudio Trapella**
- **Dr. Anna Fantinati**

<https://orcid.org/0000-0002-6666-14>



❖ Organocatalysis

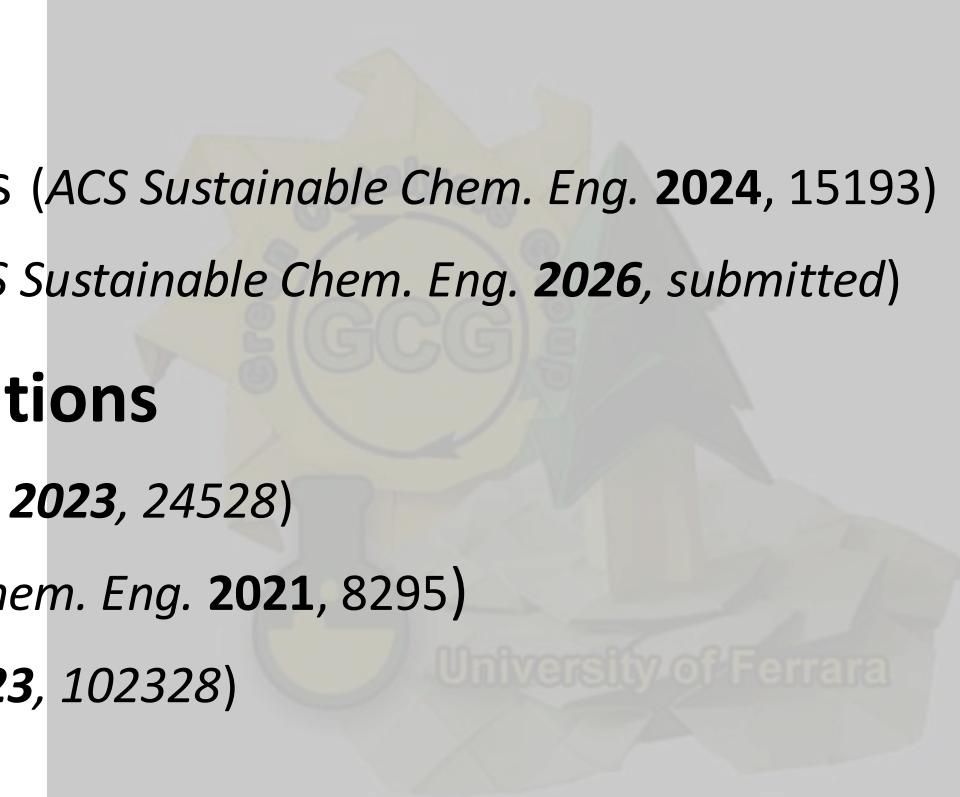
- Immobilization of (chiral) organocatalysts (*ACS Sustainable Chem. Eng.* **2024**, 12482)
- Natural porous materials as heterogeneous supports (*Adv. Sustainable Syst.* **2025**, e01169)
- Synthesis of APIs (*Adv. Synth. Catal.* **2025**, e202500058)
- Synthesis of bio-based polymers (*ACS Appl. Polym. Mater.* **2025**, 1979)

❖ Photocatalysis

- Synthesis of unnatural amino acids and glycoconjugates (*ACS Sustainable Chem. Eng.* **2024**, 15193)
- Fabrication of photoactive materials and utilization (*ACS Sustainable Chem. Eng.* **2026**, submitted)

❖ Process Intensification and Mechanistic Investigations

- NMR relaxation measurements (*ACS Appl. Mater. Interfaces* **2023**, 24528)
- Flow Chemistry – packed-bed reactors (*ACS Sustainable Chem. Eng.* **2021**, 8295)
- Microdroplet chemistry for CO₂ utilization (*J. CO₂ Util.* **2023**, 102328)



❖ Equipment

- Nuclear Magnetic Resonance (Varian 400 MHz, Bruker 500 MHz/HR MAS)
- HPLC-MS (Agilent 1260 Infinity II LC, DAD and RI + Agilent Ultivo LC/TQ)
- Flow (Photo) Chemistry equipment (H-CUBE® PRO, photoreactors, MFC, 3D-printer)
- Microwave Synthesizer – Biotage Initiator

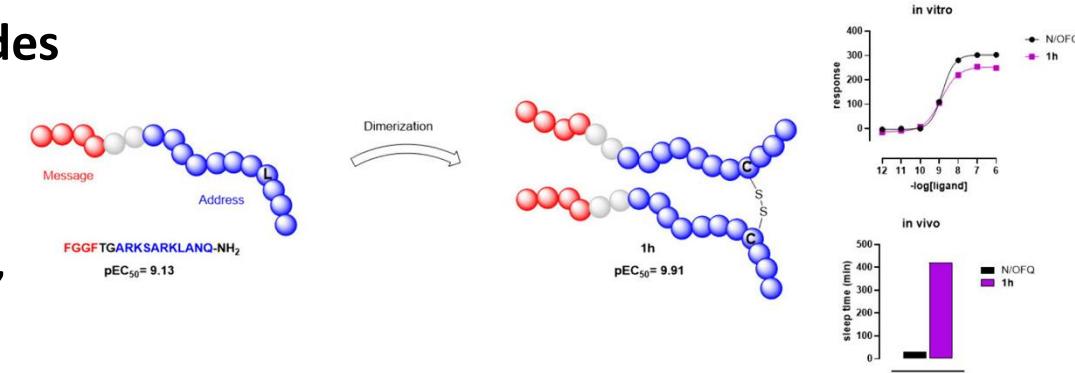
❖ Staff

- Prof. Alessandro Massi
- Prof. Daniele Ragno
- Dr. Graziano Di Carmine
- Dr. Carmela De Risi



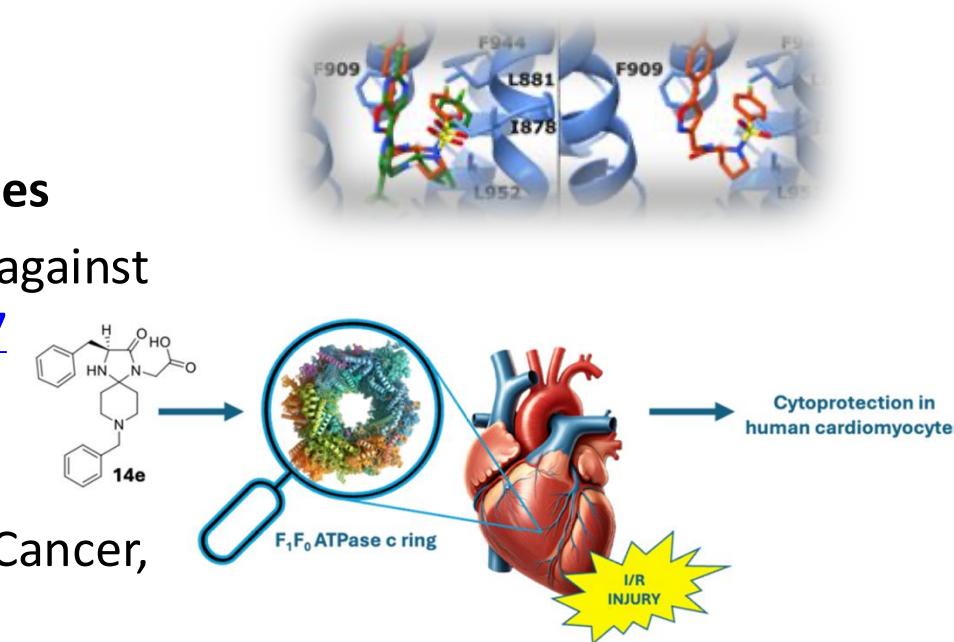
❖ Research theme 1: Design and synthesis of bioactive peptides

- Project 1, Nociceptin/Orphanin FQ Dimeric Ligands, [10.1021/acs.jmedchem.5c02350](https://doi.org/10.1021/acs.jmedchem.5c02350)
- Project 2, Mixed NOP/Opioid Receptor Peptide Agonists, [10.1021/acs.jmedchem.0c02062](https://doi.org/10.1021/acs.jmedchem.0c02062)
- Project 3, Biased Agonists at Nociceptin/Orphanin FQ Receptors, [10.1021/acs.jmedchem.9b02057](https://doi.org/10.1021/acs.jmedchem.9b02057)



❖ Research theme 2: Design and synthesis of bioactive small molecules

- Project 1, Mitochondrial permeability transition pore inhibitors against ischaemia/reperfusion injury , [10.1080/14756366.2025.2505907](https://doi.org/10.1080/14756366.2025.2505907)
- Project 2, TRPA1 inhibitors with analgesic effects, [10.1016/j.ejmech.2025.117732](https://doi.org/10.1016/j.ejmech.2025.117732)
- Project 3, NLRP3 Inflammasome Inhibitors for the Treatment of Cancer, [10.1021/acs.jmedchem.3c00175](https://doi.org/10.1021/acs.jmedchem.3c00175)



❖ Equipment

- Syro I Biotage® automatic synthesizer
- Analytical HPLC Agilent 1200 Series
- Preparative HPLC Agilent 1260 Infinity I
- ESI-MS mass spectrometer ZQ 2000

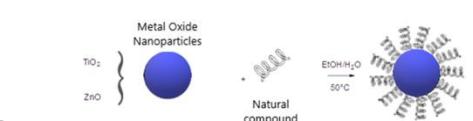
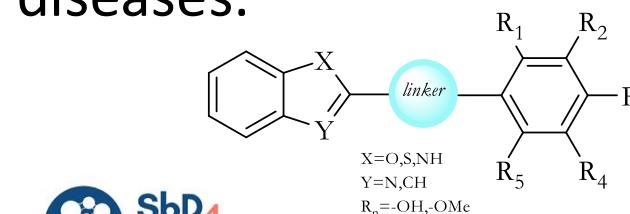
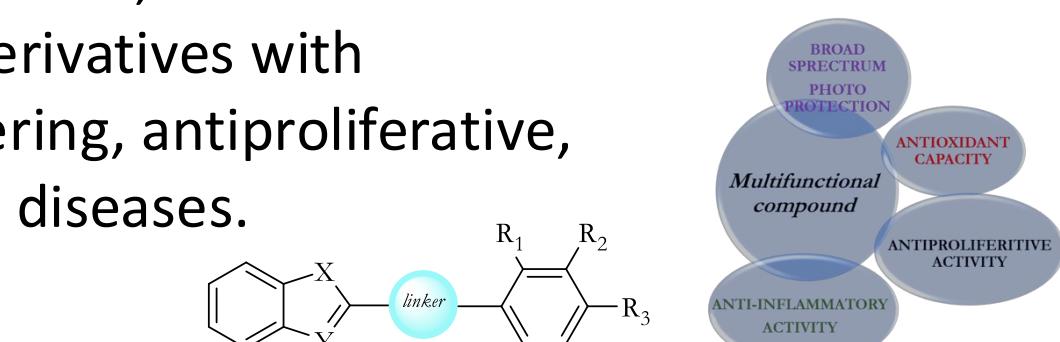
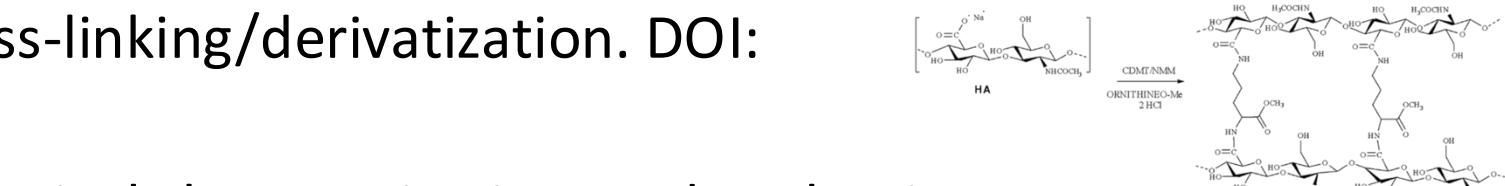
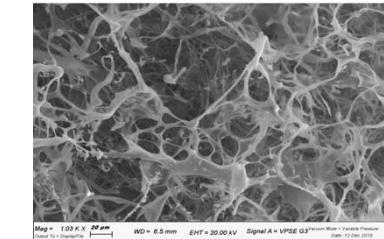
❖ Staff

- Prof. Remo Guerrini
- Dr. Delia Preti
- Dr. Salvatore Pacifico
- Dr. Valentina Albanese



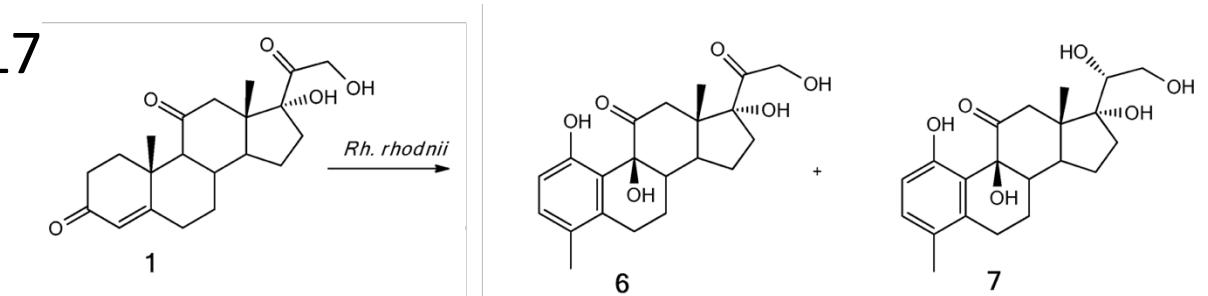
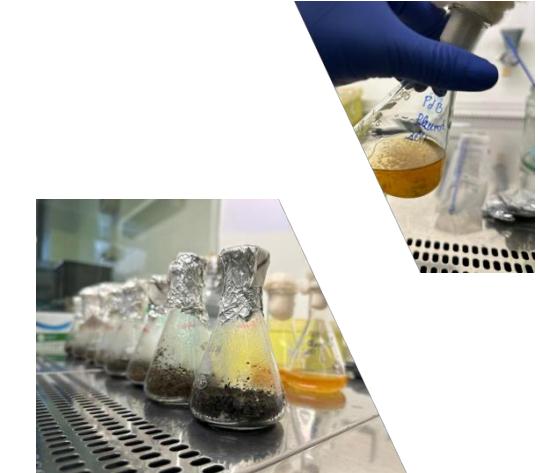
❖ PHARMACEUTICAL-COSMETIC FIELD

- Design, synthesis, characterization, and evaluation of the influence on the antimicrobial and anti-inflammatory properties of new cross-linked or grafted derivatives with high biocompatibility of hyaluronic acid at different degrees of cross-linking/derivatization. DOI: [10.3390/ph16030431](https://doi.org/10.3390/ph16030431)
- Design, synthesis, chemical-physical characterization, and evaluation of the biological activities of new heterocyclic derivatives with multifunctional activity and antioxidant, UV-filtering, antiproliferative, and anti-inflammatory potential for skin-related diseases.
<https://doi.org/10.1016/j.biopha.2025.118511>.
- Safe by Design of Effective and Safe Sunscreen
<https://doi.org/10.1016/j.jcis.2025.138823>.



❖ BIOTECHNOLOGY

- Valorization of agri-food by-products for biotechnological production using the SMF (submerged fermentation) approach of: Lactic acid, Biosurfactants, Hyaluronic acid.
<https://doi.org/10.1016/j.ijbiomac.2025.148203>.
- Valorization of industrial by-products using an SSF (solid state fermentation) approach for the biotechnological production of: Lovastatin, Polyphenols, Bittering molecules. DOI: 10.3390/antiox13081014
- Production of second-generation bioactive steroids.
<https://doi.org/10.1016/j.biopha.2025.117>



❖ Equipment

- HPLC Agilent 1100 series
- Suntest CPS+ solar simulator
- Thermo Fluoroskan Ascent FL® Microplate Fluorometer and Luminometer
- Applikon biotechnology bioreactor



❖ Staff

- Prof. Anna Baldisserotto
- Prof. Stefano Manfredini
- Prof. Silvia Vertuani
- Dr. Gaia Bellonzi, Dr. Erika Baldini, Dr. Silvia Boreale, Dr. Stefania Costa, Dr. Elisa Durini, Dr. Ilaria Gugel, Dr. Irene Gugel, Dr. Filippo Marchetti, Dr. Leonardo Montani, Dr. Caterina Rossi



❖ Prodrugs of neuroactive agents

- Synthesis and pharmacokinetic characterization of prodrugs of neuroprotective agents

Botti G, et al. Dimeric ferulic acid conjugate as a prodrug for brain targeting after nasal administration of loaded solid lipid microparticles. *Expert Opin. Drug Deliv.* 2023; 20(11):1657-1679. doi: [10.1080/17425247.2023.2286369](https://doi.org/10.1080/17425247.2023.2286369)

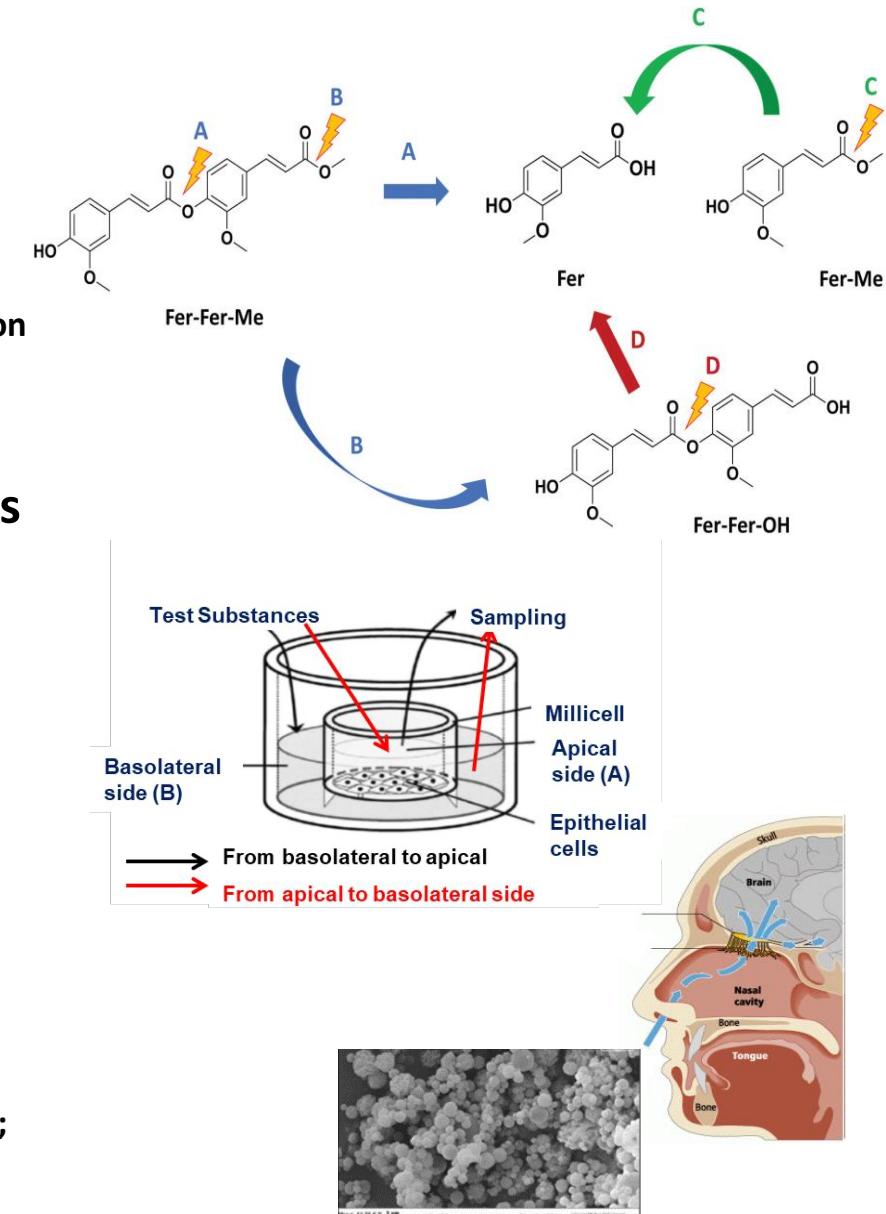
- Cellular models for permeation and activity studies of the prodrugs and their neuroactive agents

Lerin LA et al. Characterization and hydrolysis studies of a prodrug obtained as ester conjugate of geraniol and ferulic acid by enzymatic Way. *Int J Mol Sci.* 2024; 25(11): 6263. doi: [10.3390/ijms25116263](https://doi.org/10.3390/ijms25116263)

❖ Brain targeting of neuroactive agents

- Nasal administration of neuroactive agents as prodrugs encapsulated in micronized or nanonized systems

Botti G, et al. Nasal administration of a nanoemulsion based on methyl ferulate and eugenol encapsulated in chitosan oleate: uptake studies in the central nervous system. *Pharmaceutics*, 2025; 17(3):367. doi: [10.3390/pharmaceutics17030367](https://doi.org/10.3390/pharmaceutics17030367)



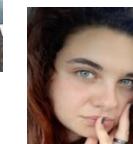
❖ Equipment

- HPLC-UV-diode array
- Laminar flow hood and CO₂ incubator for cell culture
- Contrast phase microscope



❖ Staff

- Prof. Alessandro Dalpiaz
- Prof. Barbara Pavan
- Dr. Giada Botti
- Dr. Anna Bianchi





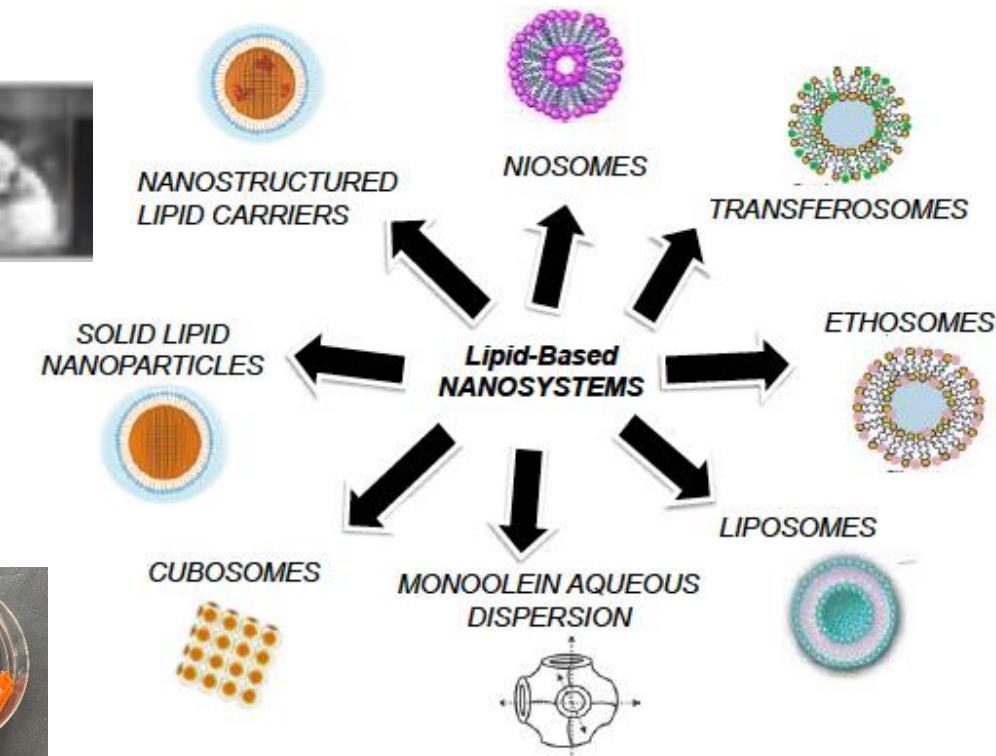
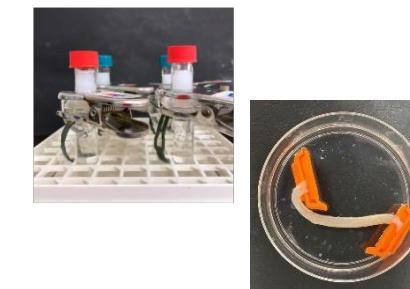
❖ Research in Pharmaceutical Technology

- development and characterization of drug delivery systems (mainly lipid- or polymeric-based micro- and nanosystems) for bioactive molecules administrable via cutaneous, ophthalmic or oral route
- *in vitro* drug release and bioaccessibility
- pharmaceutical nanosystems for gene therapy
- cosmetic and agricultural nanodelivery systems



FIELDS OF APPLICATION

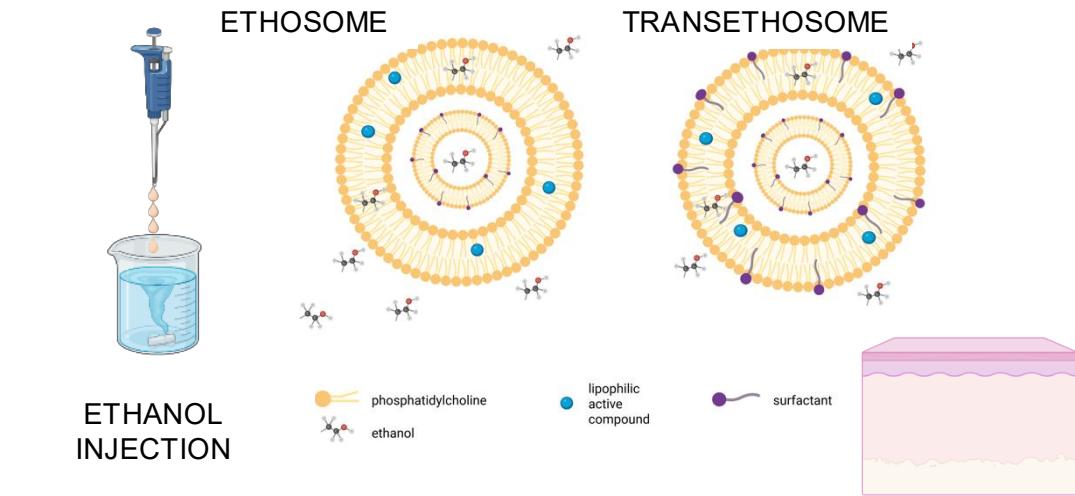
- pharmacy
- diagnostics
- cosmetic
- nutritional
- environment
- agriculture



❖ PRODUCTION AND CHARACTERIZATION OF NANOVESICULAR LIPID SYSTEMS

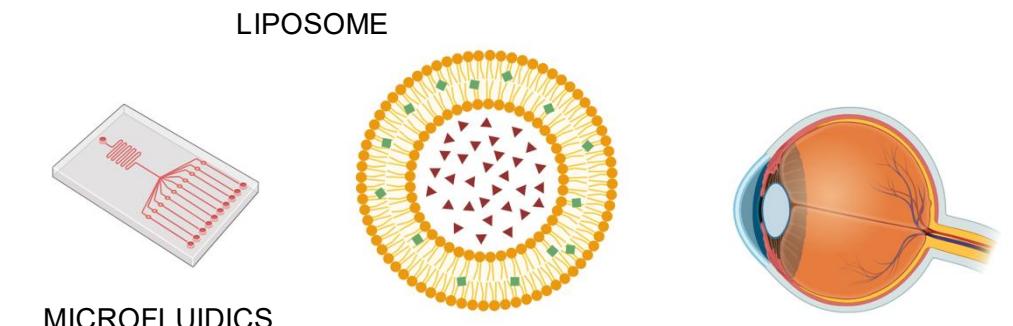
➤ Ethosomes and transethosomes for transdermal drug delivery

Bondi et al. Gossypin-Loaded Ethosome Gel for Cutaneous Administration: A Preliminary Study on Melanoma Cells. *Antioxidants (Basel)*. 2025 Feb 5;14(2):186. doi: 10.3390/antiox14020186.



➤ Liposomes for ocular drug delivery

Esposito et al. Microfluidic Fabricated Liposomes for Nutlin-3a Ocular Delivery as Potential Candidate for Proliferative Vitreoretinal Diseases Treatment. *Int J Nanomedicine*. 2024;19:3513-3536. <https://doi.org/10.2147/IJN.S452134>





❖ Equipment and TECHNIQUES

- extrusion, spray drying, freeze-drying
- cell culture, wound healing
- optical, fluorescence, electronic microscopy
- PCS, UV, IR, HPLC
- Franz cell, dialysis
- *in vitro* digestion, bioaccessibility

❖ Staff

Rita CORTESI
Associate professor

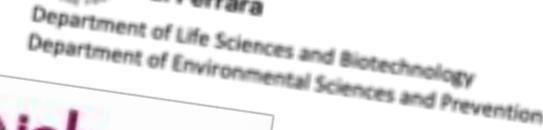
Maddalena SGUZZATO
Assistant professor

Francesca FERRARA
Researcher

Sara Vita ASMUNDO
PhD Student

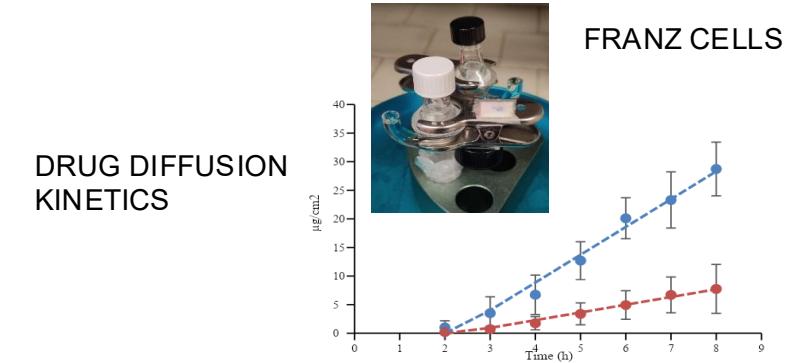


COLLABORATIONS NETWORK



❖ Equipment

- HPLC
- Photon Correlation Spectroscopy
- Franz cells



❖ Staff

- Prof. Elisabetta Esposito (Associate Professor)
- Dr. Federico Santamaria (Research fellow)
- Dr. Nicholas Castaldini (PhD Student)

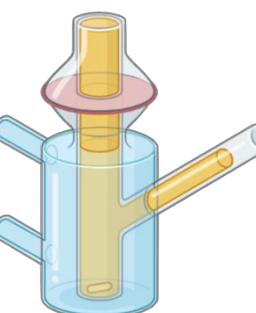
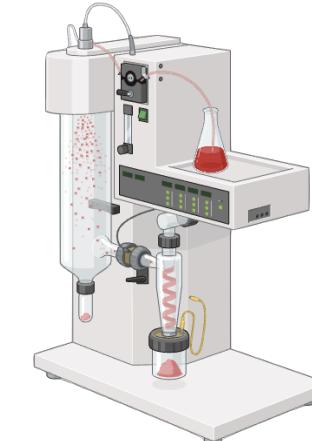
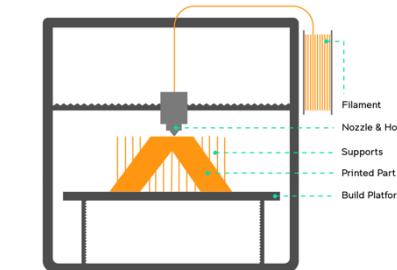


❖ Research

1. NASAL DRUG DELIVERY BY POWDER DOSAGE FORMS

- 1.a Nose-to-brain
- 1.b Loco-regional action

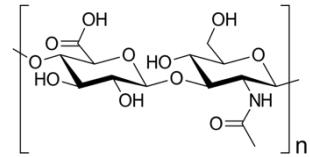
- Microparticle manufacturing by **spray drying** and characterization
- In vitro/ex vivo **dissolution/permeation**
- In vitro powder deposition (nasal model)
- Delivery device optimization by 3D printing (FDM)



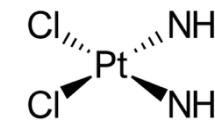
❖ Research

2. LOCO REGIONAL CHEMOTHERAPY

Sodium Hyaluronate
(NaHA)



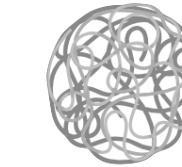
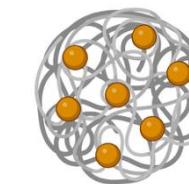
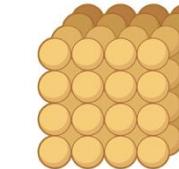
Cisplatin
(cisPt)



Implantable delivery systems (e.g. film)

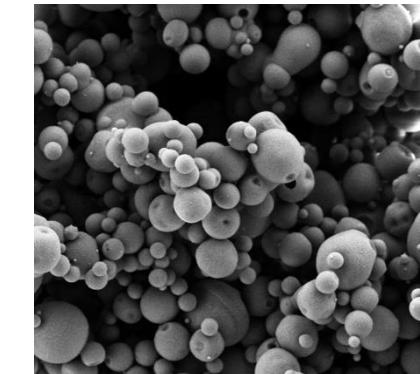
3. FORMULATION OF POORLY WATER-SOLUBLE DRUGS

Crystalline drug



Polymer

Amorphous
Solid
Dispersion



❖ Equipment

- Mini Spray Dryer (Buchi B-191)
- Dynamic Light Scattering for nanoparticle size analysis
- Vertical Franz-type cells
- Alberta Idealized Nasal Inlet equipment
- HPLCs with UV-Vis and RID detectors
- FDM 3D printer
- Tablet press
- Dissolution equipment for solid dosage forms

❖ Staff

- **Dr. Sabrina Banella, Ph.D.** (Tenure-Track Researcher, UniVR)
- **Dr. Fabrizio Bortolotti** (external consulting technician)

❖ Collaborations

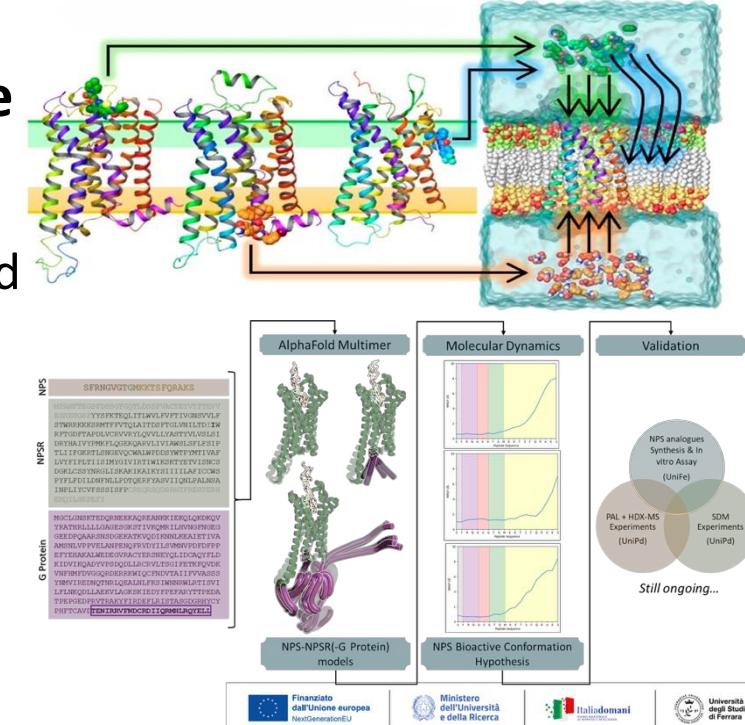
- Prof. N Realdon (University of Verona, IT)
- Prof. F. Sonvico, F. Buttini (University of Parma, IT)
- Prof. P. Russo, P. Del Gaudio (University of Salerno, IT)
- Prof. D. Rekkas, G. Valsami, Dr. P. Papakyriakopoulou (University of Athens, GR)
- Prof. Abu Serajuddin, Prof. Ketan Patel (St. John's University, Queens, USA)
- Prof. P. Colombo (PlumeStars srl, IT)





❖ Development & Application of Computational Methods for the Rational Design of G Protein–Coupled Receptors Modulators

- *Allosteric Modulation*: Identification of biogenic amine (Dopamine D₂ and Serotonine 5HT_{2C}) receptor allosteric binding sites and rational design of novel allosteric modulators. <https://doi.org/10.1021/acscentsci.1c00802>
- *Dimerisation*: Identification of AT₁R-B₂R hetero-dimer interface and rational design of peptide and small molecule dimer disruptors/inducers
- *Deophranisation of peptide GPCRs*: Identification of GPR-151 and GPR-20 orthosteric binding site, endogenous modulator, and exogenous ligands



❖ Rational design of Peptide GPCR modulators

- *Neuropeptide S Receptor*: Receptor 3D models generation and validation, rational design of novel peptide and small molecule (biased) agonists
- *Nociceptin Receptor*: Receptor 3D models generation and validation, rational design of novel peptide and small molecule (biased) agonists
<https://doi.org/10.1039/D4MD00747F>; <https://doi.org/10.1021/acs.jcim.4c00499>





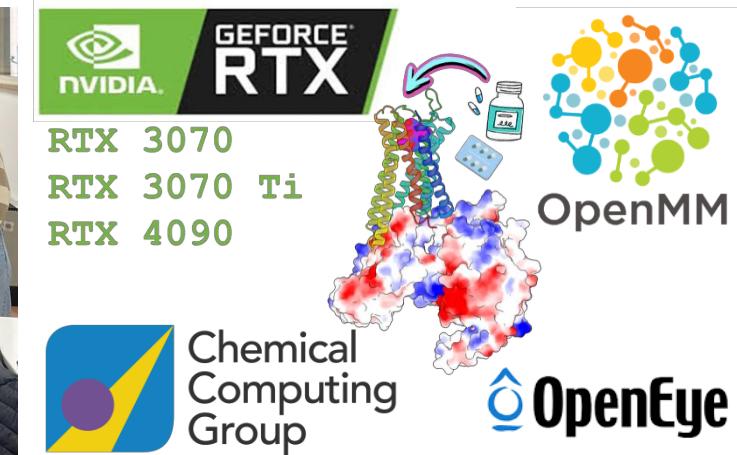
❖ Equipment

- Four workstations equipped with the Ubuntu 22.04 LTS operating system, AMD Ryzen processors, and RTX-series graphics cards
- Open-source and commercial software packages for the application of ligand-based (e.g., ph4 model generation) and structure-based (e.g., docking and molecular dynamics) for the rational design of new bioactive molecules



❖ Staff

- **Prof. Antonella Ciancetta (PI)**
- 4-6 MSc Medicinal Chemistry and Biotechnology Students yearly

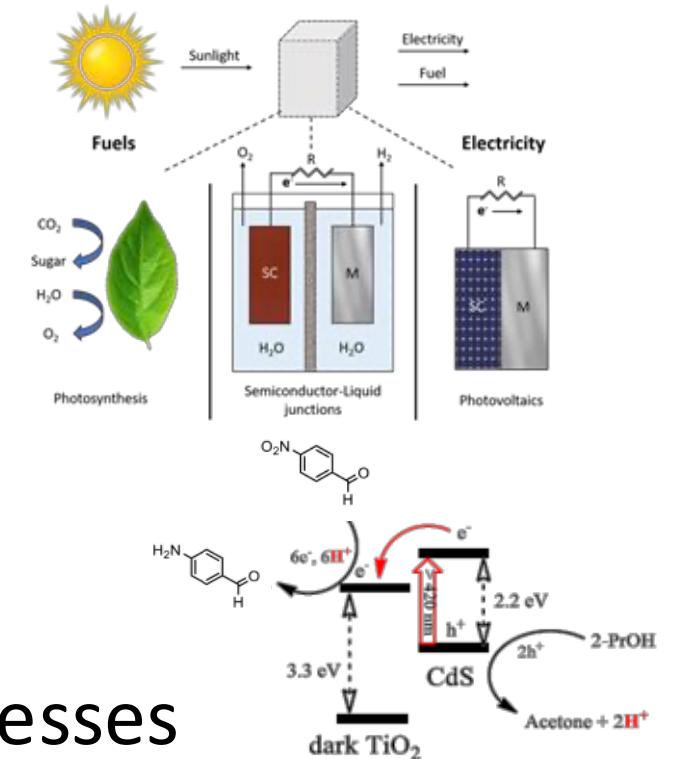


❖ Photoelectrochemistry and Photocatalysis

- Semiconductor Solar Cells and Solar Fuels
- Electrocatalysis
- Semiconductor Nanoparticles for Photocatalysis

Adv. Energy Mater. **2025**, 15, e00253; *ACS Energy Lett.* **2024**, 9, 5, 2193–2200;

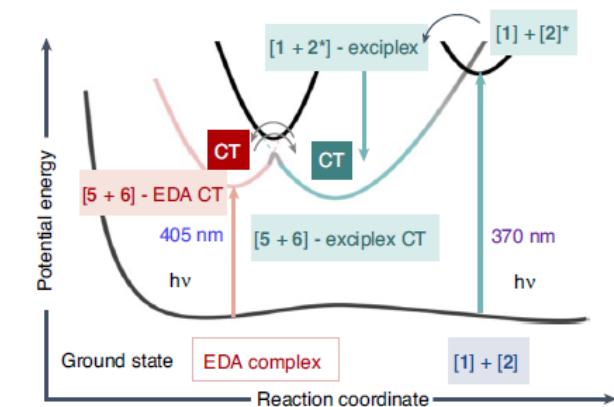
ACS Appl. Energy Mater. **2020**, 3, 5, 4658–4668



❖ Molecular Photochemistry for sustainable processes

- Small Molecule Activation
- Photochemical Reaction Mechanisms

Nature Catal. **2024**, 7, 1223; *Nature Synth.* **2023**, 2, 26; *Nature Chem.* **2025**, DOI: 10.1038/s41557-025-01960-3.



❖ Equipment

- **Electrochemical and Photoelectrochemical Workstations (IMPS, EIS, etc.)**
- **Time Resolved Optical Spectroscopy**
- **Surface Characterization (AFM, ATR-IR, Profilometry, etc.)**



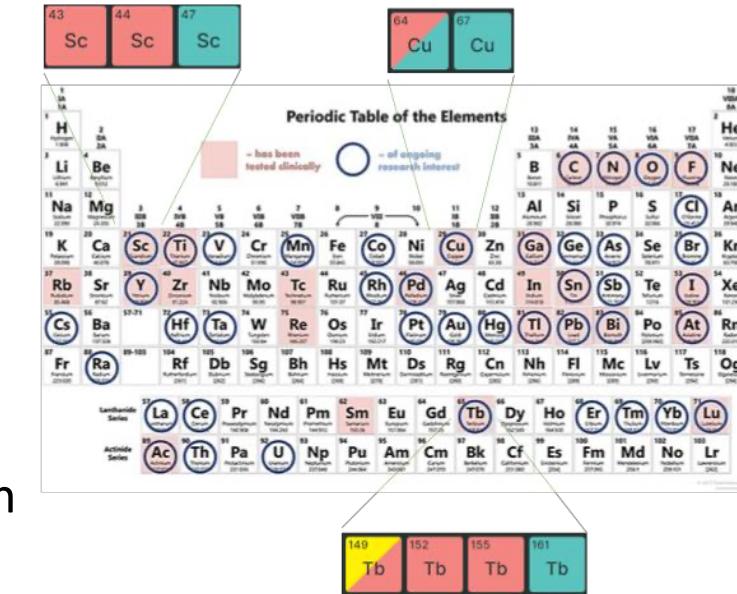
❖ Staff

- **Stefano Caramori, Mirco Natali, Stefano Carli, Alessandra Molinari, Serena Berardi, Vito Cristina, Edoardo Marchini**

Inorganic Chemistry, Radiochemistry and Nuclear Imaging

❖ Development of cyclotron-based radiometal production methods for nuclear medicine

- APHRODITE-155_Accelerator-based Production of tHeranostic radionuclides.
- Cyclotron-driven production of ^{52}Mn for PET/MRI imaging.
<https://doi.org/10.1186/s41181-024-00288-6>
- Automated technologies for the separation of radiometals and production of radiopharmaceuticals. DOI: 10.1007/978-3-031-84632-8_4.



❖ Development of metal complexes for diagnostics and therapy

- Development and evaluation of new metal-based complexes as potential MRI contrast agents. DOI: 10.3390/ijms24043461
- Development of Copper Complexes for Cancer Treatment.

❖ In vivo imaging studies

- pharmacokinetic, biodistribution, therapeutic effect of antitumoral agents or radiopharmaceuticals

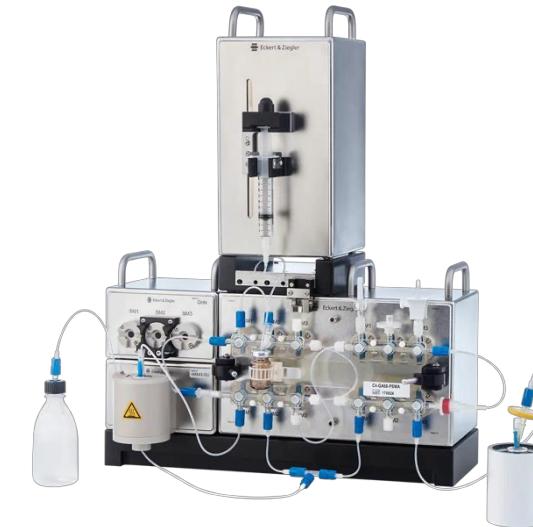


❖ Equipment

- **Modules for the automated separation of radiometals, software and cassettes.**
- **PET, CT, SPECT imaging systems present in the Laboratory for Nuclear Imaging and Computed Tomography (LINC) of University of Ferrara**

❖ Staff

- **Prof.ssa Alessandra Boschi**
- **Prof.ssa Licia Uccelli**
- **Dott.ssa Lorenza Marvelli**
- **Dott.ssa Petra Martini**



**PET, CT, SPECT imaging systems
([©]MOLECUBES)**

❖ Water confined in porous materials

- **Objective 1:** water for energy scavenging: mechanical-to-electric energy conversion via triboelectrification, thermal energy storage - Nano Energy 2025, 111488 – most downloaded article in 2025)
- **Objective 2:** find the mechanism underneath mild confined supercritical water and engineer materials to control/optimize it - JACS, 2024, 13236.

❖ Research theme 2: 3rd-generation photovoltaics & indoor photovoltaics

- **Objective 1:** identify major bottlenecks to enhance efficiency in 3rd generation PV, halide perovskites and beyond, e.g., E/HTM - Joule 2024, 1691 - ~ 600 citations in < 2 yrs.
- **Objective 2:** indoor photovoltaics for powering the IoT - APL Energy 2023, 021502.

❖ Research theme 3: Thermocatalytic methane decomposition → H₂ + value-added carbon

- Objective: understand catalyst structure–performance relationships in methane splitting for CO₂-free hydrogen and solid carbon co-products – Applied Catalysis B 2025, 125817

❖ Equipment/software

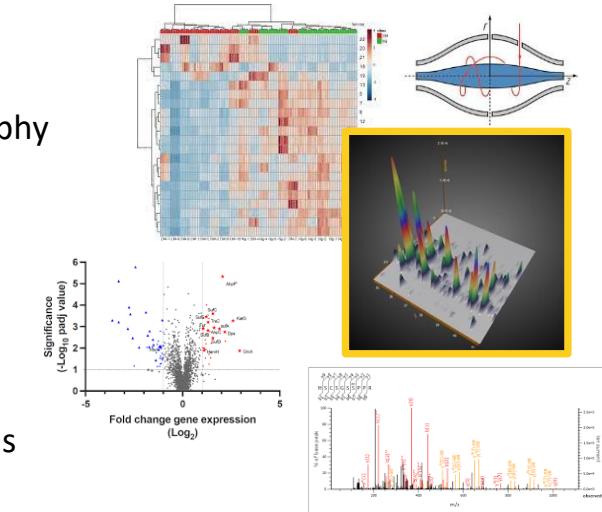
- Molecular simulation software, analysis and visualization:
 - Community codes & workflows: LAMMPS, CPMD, MiMiC, Janus
 - Licensed codes: VASP, CrystalMaker
- HPC: 752 cores Epyc CPU cluster, with 20TB storage + ~1000 cores/3xH100 hybrid cluster

❖ Staff

- Prof. Simone Meloni (PI).
- Dr. Sebastiano Merchiori (Postdoc).
- Ribhu Bhatia (PhD candidate).
- Nicola Verziaggi.
- Matteo Bragagnolo

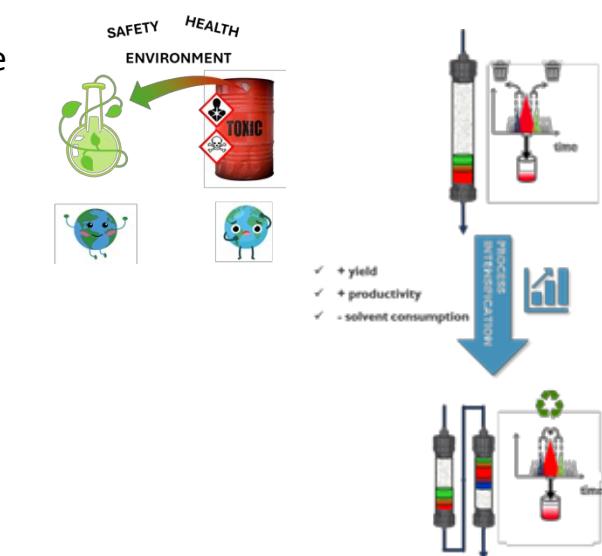
❖ Omics-based approaches for the characterization of complex matrices

- Volatile and non-volatile metabolomic profiling of agri-food waste and industrial by-products using chromatography coupled with high-resolution mass spectrometry to support valorization strategies.
- Proteomic and metabolomic analysis of biological fluids and environmental matrices to explore biomarkers and differential molecular patterns across samples.



❖ Green purification strategies, biomass valorization, and adsorption processes

- Development of green analytical methods with eco-friendly solvents and purification workflows based on process intensification using continuous multicolumn chromatography.
- Extraction of bioactive compounds from complex matrices and valorization of waste materials within circular economy frameworks.
- Investigation and modeling of adsorption phenomena on engineered and waste-derived materials to support the development of selective and sustainable purification processes.



❖ Environmental monitoring

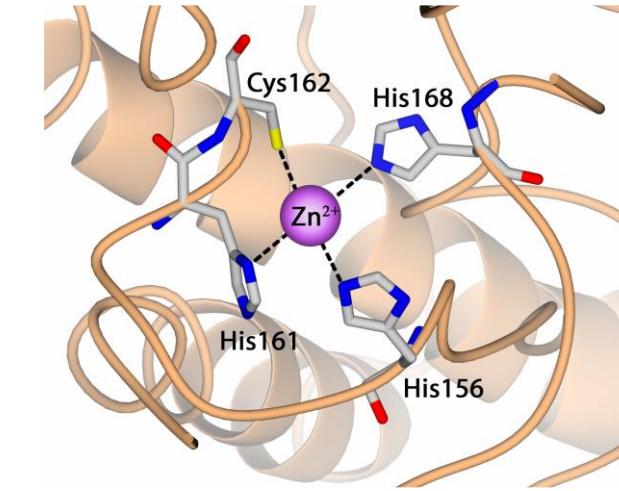
- Non-target screening of persistent organic pollutants in environmental matrices (water, soil, sediment, air, PM).
- Development of unified analytical strategies for the extraction and determination of emerging pollutants.

Selected publications:

- D. Barboni et al., *Anal. Bioanal. Chem.* 2025, *in press*. <https://doi.org/10.1007/s00216-025-06030-8>
- M. C. Corviseri et al., *Talanta*, 2025, 292, 127944. <https://doi.org/10.1016/j.talanta.2025.127944>
- A. Polidoro et al., *J. Chromatogr. Open*, 2025, 8, 100245. <https://doi.org/10.1016/j.jcoa.2025.100245>
- C. De Luca et al., *Green Chem.*, 2025, *in press*. <https://doi.org/10.1039/D5GC01158B>
- N. D. Spadafora et al., *Anal. Bioanal. Chem.*, 2024, 416, 3797-3809. <https://doi.org/10.1007/s00216-024-05321-w>

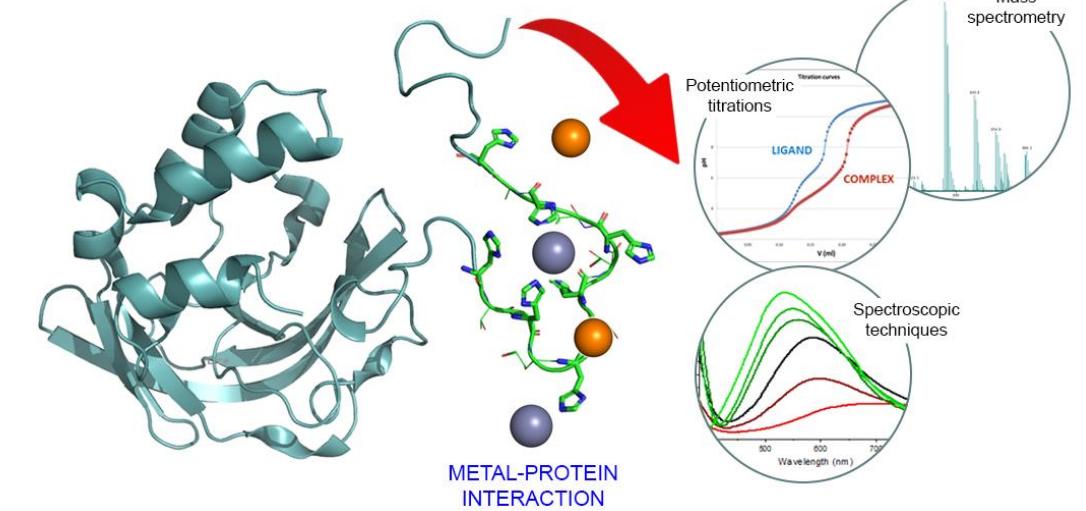
❖ Analytical multi-technique approach to study biological systems

- Development of methods and models for the determination of speciation data and thermodynamic parameters in multicomponent aqueous solutions aimed at the characterization of metal complexes with multifunctional ligands, macromolecules, polyelectrolytes, especially peptides.
- Investigation of metal homeostasis in bacterial and fungal pathogens through chemical thermodynamics.



❖ Next generation therapeutics through metal-chelating peptides

- Design and study of peptide-based metallodrugs and enzyme mimetics to develop next-generation antimicrobial and anticancer therapeutics.



Selected publications:

D. Bellotti et al., *Dalton Trans.*, 2020, 49, 9393-9403. <https://doi.org/10.1039/D0DT01626H>

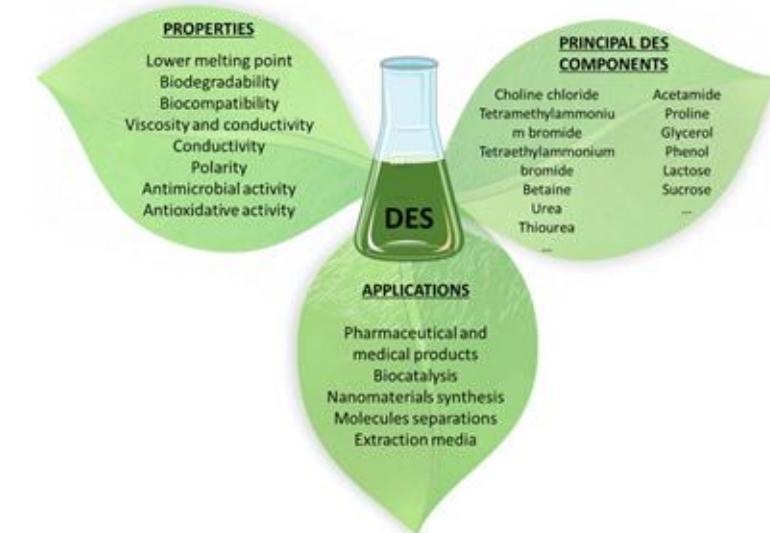
D. Bellotti et al., *Anal. Biochem.*, 2023, 680, 115315. <https://doi.org/10.1016/j.ab.2023.115315>

S. Leveraro et al., *Inorg. Chem.*, 2025, 64, 6751-6760. <https://doi.org/10.1021/acs.inorgchem.5c00672>

A. Caproni et al., *Anal. Biochem.*, 2025, 700, 115784. <https://doi.org/10.1016/j.ab.2025.115784>

❖ Functional Foods:

- enriched & fortified foods with bioactives
- natural bioactives characterization in food matrices
- boosting nutritional properties by food/feed enrichment
- enzyme and ultrasound assisted bioactive extraction
- natural deep eutectic solvents for bioactive recovery from wastes



❖ Functional Foods:

- simulated human gastrointestinal digestion process
- release of bioactives from food matrices
- behavior of delivery/encapsulated systems
- protein & lipid digestibility
- novel food design



Equipment

❖ Our labs are equipped with advanced instrumentation for omics, separation science and solution equilibria studies, including:

- UHPLC or GC coupled with HRMS
- Comprehensive 2D chromatography platforms (2D-GC, 2D-LC)
- Supercritical fluid chromatography (SFC)
- UHPLC coupled with charged aerosol detection (CAD)
- Single-column and multi-column chromatography systems
- Fully automated potentiometric titrators
- Titration calorimeter
- Software for multivariate analysis, big data integration and thermodynamic parameter calculation for solution equilibria
- Bioreactor (also for microbiota fermentation studies)
- Fluorescence Spectrophotometer (e.g. ORAC assay)
- HPIC (pulsed amperometric & conductometric detectors)
- Climatic hood
- Ultrasonics probe



❖ Staff

Prof. Alberto Cavazzini	Dr. Annalisa Maietti
Prof. Luisa Pasti	Dr. Tatiana Chenet
Prof. Maurizio Remelli	Dr. Simona Felletti
Prof. Catia Contado	Dr. Natasha D. Spadafora
Prof. Nicola Marchetti	Dr. Chiara De Luca
Prof. Paola Tedeschi	Dr. Denise Bellotti
Prof. Martina Catani	Dr. Desiree Bozza
Prof. Flavio A. Franchina	Dr. Mirco Cescon
Prof. Marco Beccaria	Dr. Claudia Stevanin
	Dr. Allan Dos Santos Polidoro