

**Ph. D. School in
Chemical and Pharmaceutical Sciences and Technologies
University of Trieste (Italy)**

Research Lines

Each one of the 5 broad Research Areas of the School comprises several active research lines, listed below. For every new Cycle (i.e. every year), the School proposes some specific research projects, typically one for each fellowship plus some additional projects (see the specific link on this webpage for details), among which the successful candidates will select their own. It is worth stressing that, in most cases, the research projects are being performed within well established national and international collaborations as well as specific European projects.

1. *Inorganic and Bio-Inorganic Chemistry*

- Synthesis and characterization of cobalt compounds as models of vitamin B12.
- Development of new ruthenium compounds as anticancer agents.
- Electrochemistry of metallo-proteins: investigation of the structure-reactivity relationship in cytochrome c.
- Substitution kinetics and electrochemical investigations in coordination compounds.

2. *Catalysis*

- Synthesis and characterization of rhodium and iridium organometallic compounds to be employed as homogeneous catalysts for the production of oligo- and poly-acetylenes.
- Development of cobalt and palladium complexes with chelating nitrogen ligands to be used as catalysts in the polymerisation of olefins and in the CO/olefin co-polymerization.
- Isolation and characterization of intermediates in the catalytic cycles.

3. *Biocrystallography*

- Expression, crystallization and X-ray structural determination of natural and "miniaturized" proteins. A large part of the crystallographic studies are performed at the dedicated X-ray beamline of the synchrotron of Trieste, ELETTRA.

4. *Supramolecular Chemistry*

- Metal-driven synthesis and characterization of supramolecular assemblies of porphyrins and other chromophores for photophysical applications and molecular recognition processes.
- Synthesis, structural determination and functions of supramolecular systems containing porphyrins and/or calixarenes and structural investigations of coordination polymers.
- Synthesis and characterization of supramolecular systems assembled through reversible covalent interactions and coordination to metal centers.
- Supramolecular assemblies of peptides having defined conformations.
- Supramolecular fluorescence sensors.
- Nanoparticles as templates for the construction of supramolecular systems.

5. *Nano-sciences and Nano-technologies*

- Design, preparation and characterization of nanostructured materials for the conversion of gaseous pollutants and for the production of hydrogen.
- Computational studies with atomistic and ab initio techniques of cerium oxides and of their interactions with small adsorbed molecules.
- Organic functionalization of fullerenes and carbon nanotubes.
- Design and preparation of nano-structured materials with high thermo-insulating capacity.
- Design and preparation of nano-structured catalysts for wastewater detoxification.

6. *Theoretical Chemistry*

- Computational studies on the electronic structure of molecules and clusters by ab initio and density functional methods.
- Theoretical description of the photo-emission and photo-absorption processes for molecules in gaseous phase or adsorbed on surfaces.
- Development of algorithms and their implementation in FORTRAN parallel programs for the descriptions of the electronic continuum with DFT and TDDFT methods.

7. *Molecular Spectroscopy*

- Vibrational spectroscopy and reticular dynamic of molecular crystals. Investigation of optical properties in the infrared region of ferro-electrical materials. SERS and SIERA studies concerning the interactions of heterocyclic molecules with metallic surfaces.
- Investigation of lyotropic liquid crystals through NMR spectroscopy of quadrupolar nuclei.
- Determination of the local structure in disordered or non-crystalline materials by EXAFS and XANES spectroscopies using the dedicated beamline at the synchrotron of Trieste, ELETTRA.

8. *Organic and Bio-organic Chemistry*

- Synthesis of amino- and ketoesters and their bio-transformations, mediated by baker's yeast and other microorganisms and commercial hydrolases, for the production of enantiomerically pure lactones and lactams with potential antibiotic and anticancer activities.
- Nitroalkylations and nitroalkenylations of enolates of lactones and lactams as well as of cyclic, acyclic and heterocyclic enamines.
- Synthesis and evaluation of biologically active compounds: isosters of dipeptides, inhibitors of proteases, apoptosis inducers.
- Selective recognition and catalysis with artificial peptides and proteins.
- Liquid-phases synthesis: modification of soluble carriers and preparation of bio-conjugates.

9. *Biocatalysis in Non-conventional Media*

- Hydrolases in non-conventional media.
- Kinetic and computational investigations of the enzymatic selectivity.
- Environmental-friendly enzymatic syntheses of pharmaceutical products.
- Applications of whole cells in organic solvents.

10. *Pharmaceutical Chemistry*

- Research and development of ligands for the receptors of the peptidergic system.
- Design, synthesis and biological evaluation of nitrogen heterocycles as potent and selective antagonists for the several subtypes of adenosinic receptors.
- Research and development of ligands for sigma-receptors.

11. *Mitochondrial-Targeting Drugs*

- Inhibitors of cyclooxygenases and of lipoxygenases.
- Synthesis and pharmacological investigation of imidazobenzodiazepinic compounds with high selectivity towards peripheral benzodiazepine receptors.
- Synthesis of quinone derivatives as modulators of the permeability through the mitochondrial transition channel.

12. *Chemotherapics*

- Design, synthesis and biological assessment of compounds possessing antimycotic and antimycobacterial activity.
- Design, synthesis and biological assessment of pharmacologically relevant porphyrin derivatives.

13. *Extractive Chemistry*

- Extraction from basidiomycetous fungi and structural determination of active principles behaving as inhibitors of thrombin.
- Extraction from legumes and structural determination of active principles having hypoglycemic activity.

14. *Innovative Pharmaceutical Technologies*

- Hybrid metal-organic polymer nanoparticles (in particular microspheres of poly-epsilon-caprolactone coated with copper nanospheres).

- Technological-pharmaceutical applications of super-critical fluids.
 - Design and development of controlled-release pharmaceutical formulations for oral administration.
15. *Pharmacokinetic*
- Design, synthesis and evaluation of the pharmacokinetic properties of polymer-drug conjugates.
 - Immobilization of enzymes on insoluble solid phases for increasing their catalytic activity.
16. *Analytical and Environmental Chemistry*
- Studies of environmentally-relevant analytical issues and of advanced methods for the treatment of experimental data. Development of models for the spatial-temporal distribution of chemical species in eco-systems, in urban and industrial environments.
 - Analytical investigations on the toxicity deriving from the exposure to chemical species, through physical models and the determination of quantitative relationships between chemical structure and experimental properties.
 - Assessment of skin permeation of industrial pollutants.
17. *Food Chemistry and Phytochemistry*
- Determination of the qualitative and quantitative composition of foods and dietary-supplements.
 - Qualitative and quantitative chemical analysis of medicinal plants and of their derivatives.
 - Development of analytical procedures for the determination of additives and pollutants in foods, food-supplements, medicinal plants and their derivatives.
 - Qualitative and quantitative determination of algal toxins in seafood, in phytoplankton and in water nearby fish and shellfish farms.
18. *Quality, Efficacy and Safety of Foods, Dietary-supplements and Medicinal Plants*
- Evaluation of the problems related to the use of medicinal plants and herbal drugs as food supplements and as phytotherapeutic agents.
 - Studies of the biological properties and evaluation of the efficacy of medicinal plant preparations.
 - Safety assessments for substances found in foods and herbal drugs.
 - Physiological-nutritional assessments for traditional foods and for innovative nutrients, in particular "functional foods".
 - In vitro and in vivo evaluation of the biological effects of toxins contaminating seafood.
19. *Quality Assurance and Certification*
- Procedures in experimental research for quality assurance
 - Determination of food composition through chemometric methodologies for quality control.
 - Methodologies for the certification of system and product quality.
20. *Chemical Engineering Science and Technology*
- Characterization of high molecular weight organic compounds and of ionic liquids.
 - Applications of supercritical fluids: solubility and impregnation of carotenoids.
 - Experimental determination and modelling of high pressure phase equilibria.
 - Technological applications of supercritical fluids: precipitation processes through antisolvent.
 - High pressure absorption processes.
 - Simulation of complex systems through multiscale techniques.
 - Up-grade of polymeric materials from industrial waste.
 - Simulations of fuel cells.
 - Design of multi-functional materials through molecular modelling techniques.
 - Rheological investigation of complex systems.
 - Investigations on systems for the controlled release of drugs.
 - Rheological investigation and optimization of industrial formulations.
 - Molecular simulation techniques applied to the calculation of physical-chemical properties of industrially relevant compounds.
 - Molecular simulation of systems of bio-medical relevance.
 - Extraction processes from natural matrices.
 - Environmental and process simulations for an eco-compatible industrial development.

- Modelling of biological processes and of related plants for the abatement of VOCs (volatile organic compounds).
- Membrane separation processes.
- Treatment of industrial waste in anaerobic reactors.
- Modelling and control of processes for the treatment of industrial waste water.
- Modelling of drug release and absorption processes