# 2017
# Febbraio

## Chim. Fisica CHIM02

**1**

**Prof. Riccardo Chelli** (4hr) riccardo.chelli@unifi.it
**Dr. Marco Pagliai** (4hr) marco.pagliai@unifi.it

### Computational methods in chemistry

**Course description:** The aim of the course is to provide basic knowledge of quantum chemistry calculations and molecular dynamics simulations for understanding articles of computational chemistry and performing simple calculations. The course is organized in lectures and a computer practice: Calculations based on density functional theory are presented discussing the results of structural and spectroscopic properties obtained for selected molecular systems; basic concepts of statistical-mechanics are reviewed. The fundamentals of molecular dynamics simulations are introduced focusing on the concept of force field. Some examples of chemical and physical properties computed through molecular dynamics simulations are shown. COMPUTER PRACTICE (2 hours): Ab initio calculations and molecular dynamics simulations will be carried out on simple molecules forming a ligand-receptor system.

**Period:** February
**Minimal number of students**: 1
**Final test:** review and discussion of a scientific paper on a topic covered by the course.

**2**

**Dr. Mariangela Di Donato** didonato@lens.unifi.it

### Applications of ultrafast spectroscopy

**Course description:** The course will illustrate the principal methodologies of ultrafast time resolved spectroscopy. Examples will be given concerning the study of photo-induced energy and electron transfer processes in complex molecular systems. The content of the four lectures will be:
-Introduction about ultrafast lasers and time resolved spectroscopic techniques
-Pump-probe spectroscopy to study energy and charge transfer in multicromophoric systems and proteins
-Infrared and Raman time resolved spectroscopies
-2D IR and visible techniques.

**Time period:** February 2017
**Minimal number of students:** 1
**Final test:** review and discussion of a scientific paper on a topic covered by the course.

## Chim. Fisica CHIM02/ Chimica dell'ambiente e dei beni culturali.CHIM12

**1**

**Dr. Becucci Maurizio** (4hr) maurizio.becucci@unifi.it
**Dr. Marilena Ricci** (4hr) marilena.ricci@unifi.it

### Optical Spectroscopies and their application to Studies in Conservation

**Course description:** We will present a survey of current applications of optical spectroscopy methods for the characterization of materials of interest for the conservation of the artistic materials.

We will cover both vibrational spectroscopy (including infrared, Raman and their enhanced versions in presence of metal nanoparticles; Ricci) and electronic emission spectroscopy (including LIBS, molecular fluorescence and related processes; Becucci).

**Time period:** February 2017
**Minimal number of students:** 3
**Final test:** critical discussion on a subject/paper to be agreed with the Docent.

## Chim. Inorganica CHIM03

**1**

**Prof. Luigi Messori** luigi.messori@unifi.it

### Anticancer metallodrugs and their molecular mechanisms: an update

**Course description:** Outline
1. General introduction on anticancer metallodrugs: the state of art
2. Proteomics as a tool to decipher the molecular mechanisms
3. Studies on some representative Gold Compounds
4. Cisplatin and its halido-replaced analogues (presented by Tiziano Marzo)

**Periodo**: February 2017
**Numero minimo di studenti per l'attivazione**: 5
**Metodo di valutazione**: review and discussion of a scientific paper on a topic covered by the course.

**2**

**Dr. Federico Totti** totti.federico@unifi.it

### Orbital Interactions in Chemistry

**Course description:** The course will cover the construction of molecular orbital interactions through a perturbative theoretical approach. In this framework, the operative applications will cover both organic and inorganic species. The aim of the course is to make the student able to sketch the electronic structure of the species under study in order to understand and predict their reactivity and electronic properties

**Periodo**: Febbraio
**Numero minimo di studenti per l'attivazione**: 2
**Metodo di valutazione**: colloquio

## CHIMICA INDUSTRIALE CHIM/04

**Dr.ssa Camilla Parmeggiani** camilla.parmeggiani@unifi.it

### New materials for microrobotics and biology: the case of liquid crystalline polymers

**Course description:** Liquid crystal is a state of matter widely explored for different applications such as screens and displays. Combining liquid crystalline properties with those of elastomers results in a new class of material having interesting properties. Liquid crystalline elastomers (LCEs), materials well known as artificial muscles, are smart polymers able to respond to different external stimuli. When opportunely designed and prepared, such materials can be micro-patterned by the use of lithographic techniques and their deformation can be triggered by different stimuli, such as temperature, light, electric or magnetic fields. An excursion on this extraordinary class of materials, from its theorization to its design and synthesis will be addressed during the class together with some possible applications. From microrobotics to biology the course will describe how to properly modify the materials in order to approach different response and, later on, different targets demonstrating the versatility and innovativeness of LCEs.
**Periodo proposto**: febbraio 2017

**Numero minimo di studenti per l'attivazione**: 5
**Prova finale**: lettura critica di un articolo scientifico sugli argomenti del corso

## Chim. Organica CHIM06

**1**

**Prof. Mauro Adamo** madamo@rcsi.ie
Professor of Organic and Medicinal Chemistry, Royal College of Surgeons in Ireland

### Phase Transfer Catalysis

**Course description:** 1. Introduction to Phase Transfer Catalysis: mechanistic rationale, types of catalysts and notable reactions I;2. Introduction to Phase Transfer Catalysis: mechanistic rationale, types of catalysts and notable reactions II; 3. Phase Transfer Catalysis: industrial application and the manufacture of drugs ; 4. Phase Transfer Catalysis: industrial application and the manufacture of drugs II; 5. Enantioselective Phase Transfer Catalysis and synthetic applications I; 6. Enantioselective Phase Transfer Catalysis and synthetic applications II; 7. Enantioselective Phase Transfer Catalysis proceeding via bifunctional mode; 8. Phase transfer catalysis via metal salen catalysts

**Periodo:** 23 Gennaio – 13 Febbraio, 2017
**Numero minimo di studenti per l'attivazione**: 5
**Metodo di valutazione**: Discussion on a relevant paper published on the specific topic .

**PIA: Referente Prof. Stefano Menichetti**

**2**

**Dr. Alessandro Mordini,** alessandro.mordini@unifi.it

### Chemistry for energy: new generation photovoltaics

**Course description:** The course will illustrate the state of the art of the most important technologies for energy production in the field of photovoltaics and will focus on the chemical aspects of the emerging technologies with particular reference to the third generation one (DSSC= Dye Sensitized Solar Cells). The general principles of all avalilable technologies will be discussed emphasizing the key points of DSSCs. Concerning the latter, also the most important classes of molecules which have been used as photosensitizers will be discussed and complementary and alternative technologies will be illustrated.

**Periodo**: febbraio
**Numero minimo di studenti per l'attivazione**: 3
**Metodo di valutazione**: review and discussion of a scientific paper on a topic covered by the course.

**Interesse generale**

**Dr. Rob Van Daalen**

Rob van Daalen is Publisher at Elsevier responsible for 15 journals in the portfolio Physical and Theoretical Chemistry. He started at Elsevier as a Desk Editor working on Analytical Chemistry journals – which is also his background. Before joining Journal Publishing five years ago he was Product Manager for the Elsevier website, where he developed dedicated portals for Authors and Editors.

**Workshop on successfully writing, publishing and reviewing scientific articles**

**Course description**:
1: Author workshop.
Home assignment write abstract and title (A real article, without a title an abstract, will be given to the students who will be asked to write the abstract and title for the next lecture)
2: Homework discussion and short ethics lecture.
3: Reviewer workshop.
Home assignment: review a real article (a JCIS article will be selected).
4: the students will go through the article with the editor (Prof. D. Berti)

**Periodo**: Febbraio
**Numero minimo di studenti per l'attivazione**: 5
**Metodo di valutazione**: discussion of a scientific paper dealing with the topics developed in the course.

**Docente referente:** Prof. Debora Berti (debora.berti@unifi.it)

**Chim. Inorganica CHIM03**

# Dottorato internazionale in Structural Biology

## PhD course: Biophysical Applications of NMR Spectroscopy

Associate Professor Dr. Frans A.A. Mulder

CERM, University of Florence, February 2017

Goal of the course: To learn about the application of NMR spectroscopyf or the study of biophysical phenomena.

Where: aula seminari CERM.

Topics& Schedule:

- (Tue 14/02/17, 9:30 – 11:30)Protein electrostatics
- (Tue 21/02/17, 9:30 – 11:30) Hydrogen exchange and high pressure
- (Thu 23/02/17, 9:30 – 11:30) IDPs and chemical shifts
- (Tue 28/02/17, 9:30 – 11:30) Isotope labeling and relaxation dispersion

Learning outcomes and competences:

At the end of the course, the student **should be able to**:

- **Describe** how NMR is used to probe protein electrostatics
- **Describe** how protein hydrogen exchange NMR works
- **Describe** how pressure affects proteins
- **Describe** what NMR random coil chemical shifts and IDPs are
- **Describe** how protein methyl groups can be specifically labeled
- **Describe** how transverse relaxation dispersion NMR works
- **Understand** the information gathered from NMR titration experiments
- **Understand** how chemical shifts can be used to characterize protein disorder
- **Discuss** the advantages and limitations of NMR as a biophysicstechnique
- Be able to **rationalize** whether NMR is suitable for a given research question
- **Write and Present** about an advanced topic of NMR biophysics
- **Write and Present** in scientific English
- **Apply** NMR spectroscopy at a more advanced level to appropriate problems

Course contents: The course will consist of lectures and discussion.Students will study the material below ***before*** the corresponding lecture. After the lecture series, students are each handed a research article associated with the course subjects, about which they will write a report of max 8 pages. The course will close with 25 min presentations by each student about his/her subject.

| | |
|---|---|
| I: Protein electrostatics | Contemporary NMR Studies of Protein Electrostatics.<br>Hass MA, **Mulder FAA**.<br>Annu Rev Biophys. 2015;44:53-75. doi: 10.1146/annurev-biophys-083012-130351. Review. |
| II Hydrogen exchange and high pressure | Cavity as a source of conformational fluctuation and high-energy state: high-pressure NMR study of a cavity-enlarged mutant of T4 lysozyme.<br>Maeno A, Sindhikara D, Hirata F, Otten R, Dahlquist FW, Yokoyama S, Akasaka K, **Mulder FAA**, KitaharaR.<br>Biophys J. 2015 Jan 6;108(1):133-45. doi: 10.1016/j.bpj.2014.11.012.<br><br>Hydrogen exchange: the modern legacy of Linderstrøm-Lang.<br>**Englander SW**, Mayne L, **Bai Y**, Sosnick TR.<br>Protein Sci. 1997 May;6(5):1101-9. Review. |
| III IDPs and chemical shifts | Sequence-specific random coil chemical shifts of intrinsically disordered proteins.<br>Tamiola K, Acar B, **Mulder FAA**.<br>J Am Chem Soc. 2010 Dec 29;132(51):18000-3. doi: 10.1021/ja105656t.<br><br>Using NMR chemical shifts to calculate the propensity for structural order and disorder in proteins.<br>Tamiola K, **Mulder FAA**.<br>BiochemSoc Trans. 2012 Oct;40(5):1014-20. Review. |
| Isotope labeling and relaxation dispersion | Comprehensive and cost-effective NMR spectroscopy of methyl groups in large proteins.<br>Otten R, Chu B, Krewulak KD, Vogel HJ, **Mulder FAA**.<br>J Am Chem Soc. 2010 Mar 10;132(9):2952-60. doi: 10.1021/ja907706a.<br><br>Probing microsecond time scale dynamics in proteins by methyl (1)H Carr-Purcell-Meiboom-Gill relaxation dispersion NMR measurements. Application to activation of the signaling protein NtrC(r).<br>Otten R, Villali J, Kern D, **Mulder FAA**.<br>J Am Chem Soc. 2010 Dec 1;132(47):17004-14. doi: 10.1021/ja107410x. |

# Maggio-Giugno

## CHIM02

**Prof. Thomas Beck** thomas.beck@uc.edu
**Dept. Chemistry, U. Cincinnati**

### Ion Solvation

**Course description:** The proposed lectures will first provide an overview of ion solvation, focusing on its basic physical aspects. We will go all the way back to the initial continuum solvent model of Born, see how that physically motivated model has guided future thinking, and discuss recent advances in more complex continuum models. We will test how far these models can go in explaining ion specificity, and then proceed to discuss the importance of discrete molecular models, at least for the first solvation shell. We will give a background discussion that shows how modern quantum chemistry methods can be used to include that first solvation shell and then show that, in fact, continuum models can be quite accurate for ion-solvent interactions outside the first solvation shell. A tutorial overview of modern theories of solvation will be given that shows the utility of spatial partitioning of the free energies (and enthalpies and entropies) for gaining helpful insights into solvation.
After establishing these basic methods for studying ions in solvents, we will proceed to give many examples from our own and other research that illustrate the uses of the theory. The applications will include: ions near water interfaces, ions in protein channels, surfactants and soap harshness/mildness, and ions in organic solvents used in batteries and supercapacitors. A conclusion of our work is that, while approximations can be made for long-ranged interactions between ions and solvents, the nearby interactions of ions with water or organic solvent molecules are very intense and involve the full range of quantum mechanical effects such as exchange-correlation, electrostatics, induction, and dispersion.
The main goal of the lectures will be to introduce the students to clear physical insights from theory that can help to understand some chemical phenomena. We will conclude with a couple of lectures on the importance of ion solvation in the renewable energy sciences, especially for energy storage.

**Periodo:** May-June
**Numero minimo di studenti per l'attivazione**: 2
**Metodo di valutazione**: Review and discussion of a scientific paper on a topic covered by the course.

**PIA: Referente Prof. Pierandrea Lo Nostro**

## Chim. Organica CHIM06

**Prof. Michael Chorev** michael_chorev@hms.harvard.edu
Harvard Catalyst : The Harvard Clinical and Translational Science Center

### Peptide-based drug development

**Course description:** The expanding role of peptides and their mimics as diagnostic and therapeutic agents is drawing a great attention in today's basic, translational and clinical research activities. Prominent examples include oxytocin, insulin, cyclosporine, salmon calcitonin, and parathyroid hormone that are widely used in childbirth, diabetes, immunosuppression, and osteoporosis, respectively. At present, >40 peptides are marketed worldwide, ~ 270 peptides are in clinical phase testing, and ~400 are in advanced preclinical phases. Effective introduction and application of peptides to the numerous potential indications need to overcome the Inherent limitations presented by the chemical nature, physical properties and biological susceptibilities of peptide structures. To overcome these deficiencies there is an urgent need for developing feasible and novel approaches to come up with peptidic and peptidomimetic materials that will turn them

into potent, safe, and effective therapeutic agents. For example, the peptide-based drug Zoladex for treating prostate and breast cancers, and endometriosis was made more resistant to metabolism by incorporating a non-coded aza-amino acid residue at the C-terminus. Peptide-based vaccines offer new and promising therapeutic approaches to treat cancer and malaria. Novel antimicrobial peptidic agents are tested in the fight drug-resistant infections. All the above requires an integrative inter- and multidisciplinary approach to identify the macromolecular targets and analyze their structures, understand the mode and details of peptide-target interactions, and the mechanisms involved in bioavailability, distribution, and clearance, that effect efficacy and toxicity. Our proposal offers to invite Professor Michael Chorev a renowned outstanding peptide scientist, who has contributed extensively to the advancement of bioactive peptides as promising drug-like molecules to come as a visitor to share with us his experience and insight.

**Periodo**: 15 May 2017-15 June 2017
**Numero minimo di studenti per l'attivazione**: 5
**Metodo di valutazione**: Reading and discussion of scientific papers on "Peptide-based drug development

**PIA: Referente Prof. Anna Maria Papini**

# Settembre

## C. Analitica CHIM01

**1**

**Dr. Prof. Dr. Stephan Pflugmacher Lima** stephanpflugmacher@icloud.com
Technische Universitaet Berlin - Institute of Biotechnology

### Ecotoxicology meets Organic Chemistry

**Course description:**
**1) Structural Organic Chemistry in Ecotoxicology**: Methods of structural chemistry in assessment of ecotoxicological effects of organic xenobiotics are described. Fate modelling on structural properties, the use of model substances and structure-specific methods are discussed.
**2) Chemistry of organic pollutants in ecotoxicology with special focus on agrochemicals:** Persistant organochlorines, PCB dioxins and pesticides such as carbamates, pyrethroids and pyrethrins are discussed. Their behaviours in the environment and effects on biota.
**3) Principles in Ecotoxicology:**Uptake and distribution of xenobiotics in organisms, Biotransformation phases and enzyme systems, reactive oxidative species, where do they come from?, Oxidative stress the damages (lipidperoxidation, proteinoxidation, DNA damage), antioxidative defense, non- enzymatic based (tocopherols, ascorbate, glutathione, liponic acid), enzymatic based (superoxid dismutase, catalase, peroxidase).
**4) Water – a highly necessary resource and how we treat or should treat this resource:** What is „water“, the chemical point of view, water crisis in a global perspective, political water programs, facts about safe water, drinking water, climate change effects, how we use water, sustainable water use, water from an extraterrestrial point of view.
**5) Green Liver Systems – Ecofriendly Way of Water Purification:** Using aquatic macrophytes for water purification, examples from Brasil, South Korea, PR China, Africa will be presented.

**Periodo**: September
**Numero minimo di studenti per l'attivazione**: 2
**Metodo di valutazione**: review and discussion of a scientific paper on a topic covered by the course.

**PIA: Referente Dr Alessandra Cincinelli**

**2**

**Dr. Simona Scarano** simona.scarano@unifi.it

### Optical methods based on Surface Plasmon Resonance (SPR): from propagating to localized plasmons. Fundamentals and applications in analytical and bioanalytical chemistry

**Course description:** Fundamentals of Surface Plasmon Resonance (SPR) and applications to optical (bio)sensors (2 hrs). The emerging field of Localized SPR (LSPR), a brief overview on nanomaterials (metallic, semi-metallic, alloys) and their features for LSPR applications (2 hrs). Classic vs. localized SPR: advantages, features and perspectives of plasmonic nanomaterials applied to analytical applications. State of art on the main application fields (2 hrs). Metallic nanoparticles for a new generation of colorimetric assays. New applications towards smart, cheap and versatile analytical platforms (2 hrs).

**Periodo**: September
**Numero minimo di studenti per l'attivazione**: 5
**Metodo di valutazione**: review and discussion of a scientific paper on a topic covered by the course.

## Chim. Inorganica CHIM03

**1**
**CHIM03**

**Prof. Jurgen GAILER** jgailer@ucalgary.ca
University of Calgary, Department of Chemistry

**A perspective on the application of metallomics tools in drug discovery".**

**Course description:** Prof Gailer, on sabbatical leave from the University of Calgary, will describe some potent investigation tools, based on chromatography, that are suitable for the study of the metabolism of metal containing substances. These processes are relevant both in environmental chemistry and in medicine, in particular when considering the metabolism of metal based drugs.

**Periodo**: September 2017
**Numero minimo di studenti per l'attivazione**: 3
**Metodo di valutazione**: Review and discussion of a scientific paper on a topic covered by the course.

**PIA: Referente Prof Luigi Messori**

**2**

**Dr. Marta Ferraroni** marta.ferraroni@unifi.it

**Biocrystallography: principles and applications**

The course is designed to provide students with some of the fundamental principles of the three-dimensional structure determination of biological macromolecules by X-ray crystallography and its application in multiple areas of research and for different technological applications. The course will cover some fundamental aspects of crystallography and protein structure. The techniques of crystallization, the methods and strategies for data collection and for the structural characterization of proteins by X-ray diffraction will be also discussed.

**Proposed period:** September
**Minimum number of students:** 2
**Metodo di valutazione**: The final exam will consist of the discussion by the student of a recently published article and relevant to the course content.

**3**

**Dr. M. Mannini** matteo.mannini@unifi.it

**Characterization of nanomaterials by scanning probe microscopies**

**Description:** The course will explore the working concepts and characterization capabilities of the main scanning probe microscopy (SPM) techniques available for the morphological characterization of nanomaterials focusing on thoseassembled on solid surfaces. Starting from an overview of the working principles of Scanning Tunneling Spectroscopy (STM), Atomic Force Microscopy AFM and Scanning Near-field Optical Microscopy (SNOM) a detailed description of capabilities andlimitations of the different techniques will be providedin order to assimilate the criteria adopted to select the most suited ones for a specific characterization. If possible during the course an experimental session of measurements using a Scanning Probe Microscopy system will be carried out by the students.

**Periodo**: Settembre2017
**Numero minimo di studenti per l'attivazione**: 3
**Metodo di valutazione**: discussione su un caso di studio pubblicato su riviste internazionali inerente una delle tecniche di indagine descritte nel corso.

## CHIM03/CHIM06

**Dr. Alessandro Pratesi** e.mail: alessandro.pratesi@unifi.it

### Mass spectrometry fundamentals : an overview of available techniques and their applications in bioinorganic chemistry

**Course description:** Outline

1. Introduction to Mass Spectrometry
2. Brief description of ion separation methods
3. Description of the available ion sources and mass analyzers
4. Interpretation of a mass spectrum
5. MS/MS and MSn
6. Mass spectrometry analysis of peptides and proteins
7. Evaluation of the reactivity of some metallodrugs against model proteins

**Periodo**: September
**Numero minimo di studenti per l'attivazione**: 3
**Metodo di valutazione**: review and discussion of a scientific paper on a topic covered by the course.

## Chim. Organica CHIM06

**1**

**Prof.ssa Francesca Cardona** (4hrs) francesca.cardona@unifi.it
**Dr.ssa Camilla Parmeggiani** (4hrs) camilla.parmeggiani@unifi.it
CNR and LENS

### Approaching metabolic disorders: small molecules versus multivalent architectures

**Course description:** The course will briefly describe Lysosomal Storage Disorders (LSDs), a class of rare metabolic diseases, and the current treatment possibilities. Then the Pharmacological Chaperone Therapy (PCT), an emerging and promising alternative, will be introduced. This approach is based on the use of reversible inhibitors of the deficient enzymes carrying missense mutation, capable of enhancing their residual hydrolytic activity at sub-inhibitory concentration. Iminosugars are among the most promising pharmacological chaperones. Their synthetic approaches and biological assessment will be briefly summarized and some relevant examples presented.
The second part of the course will move from monovalent iminosugars to multivalent ones. The concept of multivalency (multivalent receptors and/or multivalent inhibitors) will be addressed. Some interesting synthetic procedures and biological data regarding multivalent iminosugars for the treatment of LSD will be described.

**Periodo proposto**: settembre
**Numero minimo di studenti per l'attivazione**: 5
**Prova finale**: review and discussion of a scientific paper on a topic covered by the course.

# Corsi non attivati 2017

**Chim. Inorganica CHIM03 / Fis01**

**Dr.ssa M. Fittipaldi** maria.fittipaldi@unifi.it

**Electron Paramagnetic Resonance: Fudamentals and applications.**

**Course description:** This group of lectures is aimed at providing the basic concepts needed to use and analyze the information which can be obtained by Electron Paramagnetic Resonance spectroscopy, while presenting some case studies of application of the different variants of this technique in Chemistry, Physic, Biology and Material Science.

The course is subdivided in two different modules, to be taught in September 2014 and September 2015. The two modules are independent on each other, but anybody interested in the second one -devoted to pulsed techniques- is strongly advised to follow also the first one, which is devoted to more general subjects.

The course will focus on the following topics:

*2^ module (September 2017)*

Introduction to pulsed EPR spectroscopy; The Density Matrix; The magnetization in the sequences of pulses: spin echoes. Application of ENDOR, ESEEM, HYSCORE e ELDOR-detected NMR spectroscopy to measure hyperfine interactions. Structural determination by using pulsed EPR and spin labels.

**Periodo**: September 2017

**Numero minimo di studenti per l'attivazione**: 3

**Metodo di valutazione**: lettura critica e discussione di un articolo scientifico sugli argomenti del corso; Critical reading and discussion of a scientific paper on EPR subject.