



Course unit English denomination	Advanced NMR techniques
SSD	BIOS-07/A
Teacher in charge (if defined)	BELLANDA Massimo
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (70% minimum of presence) <input type="checkbox"/> No
Course unit contents	The course aims to strengthen the knowledge of students in NMR spectroscopy by covering subjects that are not commonly dealt with in undergraduate courses. In particular, a deeper insight is provided into the formalism of product operators, relaxation phenomena, multidimensional NMR techniques (homo- and hetero-nuclear correlation spectroscopy, NOE spectroscopy), NMR diffusometry and modern instrumentation (pulsed field gradients)
Learning goals	Knowledge: getting to know basis of advanced multidimensional NMR. Skills: acquire the knowledge of NMR as "tool-box" that can be used to solve scientific problems encountered in the research in chemistry. Competencies: gain an understanding on the usefulness of NMR in the different branch of chemistry
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	
Examination methods	The examination will be based on an oral presentation on a paper of interest related to the topics of the course. Evaluation will be based



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on the level of understanding of methodologies covered in the course and on the capabilities shown by the student to interpret them in the context of actual research problems.

Suggested readings

Slides/articles provided by the teacher

Additional information
(not mandatory)



Course unit English denomination	Electrocatalysis & Electrosynthesis
SSD	CHEM-02/A
Teacher in charge (if defined)	ISSE Abdirisak Ahmed (8h), DURANTE Christian (8h), FANTIN Marco (8h)
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	01-02/2026
Course delivery method	<input checked="" type="checkbox"/> In presence <input type="checkbox"/> Remotely <input type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input type="checkbox"/> Yes (% minimum of presence) <input checked="" type="checkbox"/> No
Course unit contents	<p>Introduction to electrochemical systems Conductors, interfacial potentials, double layer structure, electrode potentials, polarization, ideal polarized and non-polarizable electrodes.</p> <p>Electrosynthesis General cell designs, diaphragm materials, electrode materials, pretreatment and activation of electrode materials, reference electrodes, solvents and electrolytes, potentiostatic and galvanostic modes of electrolysis, figures of merit of electrolysis.</p> <p>Electrochemical kinetics kinetics of electron transfer at electrodes, Butler-Volmer equation; limiting cases of low and high overpotentials; effect of mass-transfer; Fick's laws of diffusion and their applications in electrochemistry; diffusion overpotential.</p> <p>Electrochemical techniques electrochemical methods in three- and four-electrode cell configurations; cyclic voltammetry: reversible, quasi-reversible and irreversible systems; effect of chemical reactions coupled with electron transfer(s); rotating disk and ring disk electrode; electrochemical impedance spectroscopy; electrochemical probe microscopy.</p> <p>Homogeneous electrocatalysis electrocatalysis by metal complexes, electrocatalysis by organic mediators; some homogeneous electrocatalytic reactions of relevance in electrosynthesis, and in energy conversion and storage; homogeneous photo-electrocatalysis.</p> <p>Heterogeneous electrocatalysis microscopical view of an electrocatalytic surface; a quantitative descriptor for catalysis: the Volcano plot; examples of important electrocatalytic processes: hydrogen evolution reaction; water splitting; O₂ reduction reaction, CO₂ reduction, activation of carbon-halogen bonds, etc.</p>



Learning goals	Knowledge: Fundamentals on thermodynamics and kinetics of electrode processes. Principal electrochemical techniques such as cyclic voltammetry and rotating disk and ring-disk electrode Skills: Designing electrochemical experiments Comprehension and interpretation of electrochemical data Competencies: Analysis of electrochemical reaction mechanisms Determination of kinetic parameters by electrochemical techniques
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	
Examination methods	At the end of the course, each student will be given one or more scientific papers dealing with the application of electrochemistry in important topics such as electrocatalysis, electrosynthesis, energy conversion, pollution remediation, etc. On the examination day, each student will be given 15-20 min to deliver an oral presentation on his/her assignment in the classroom, followed by a general discussion on the topic with the whole class.
Suggested readings	Slides/articles provided by the teacher
Additional information (not mandatory)	



Course unit English denomination	Energy transport in molecular systems: description, characterization and modeling
SSD	CHEM-02/A
Teacher in charge (if defined)	COLLINI Elisabetta(16h), CORNI Stefano(8h)
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (80% minimum of presence) <input type="checkbox"/> No
Course unit contents	Aim of this course is to give a basic description of the energy transport phenomena between molecules in condensed phase. The course will: (i) provide a physical picture of these phenomena starting from molecular dimers an ending with molecular crystals and polymers; (ii) describe the techniques used to characterize these systems: absorption, fluorescence, and nonlinear optical spectroscopies experiments in the frequency and time domain; (iii) describe the main computational methodologies used to model energy and excitonic couplings.
Learning goals	Knowledge: physical picture of the energy transport between molecules, principles of the main spectroscopic and computational characterization techniques Skills: critically understand experimental and computational procedures used to investigate energy transport between molecules Competencies: inter
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	



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Examination methods	Presentation of a scientific article agreed upon with the lecturers
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Suggested readings	Slides/articles provided by the teacher
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Additional information (not mandatory)	
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Course unit English denomination	Information Literacy and Open Science
Teacher in charge (if defined)	Dr. Filippo Vomiero, Dr. Marina Zannoni, Dr. Michela Zorzi,
SSD	soft-skill course
Teaching Hours	12
Number of ECTS credits allocated	1.5
Course period	02/2026
Course delivery method	<input checked="" type="checkbox"/> In presence <input type="checkbox"/> Remotely <input type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (90% minimum of presence) <input type="checkbox"/> No
Course unit contents	Citation databases and bibliographic databases Search by topic: building a search string and filters Publishing a scientific article: <ul style="list-style-type: none">• Choosing the journal (STEM market, indexes)• The peer review process• Author facilitations Institutional repositories: PRA-Iris and Research Data Unipd Copyright Zotero <i>Optional: Reaxsys</i>
Learning goals	Autonomy in bibliographic research using the main scientific databases Knowledge of the publication process in a scientific journal Principles of Open Science, practices and tools in use at the university
Teaching methods	Lectures; exercises, innovative teaching tools for classroom interaction, with the aim of: <ul style="list-style-type: none">• teaching interactively• using the critical incident technique• promoting effective feedback• establishing authentic relationships in the classroom• developing collaborative and supportive peer relationships
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No The course is open only to PhD students of the following courses: Molecular Sciences, Material Science and Technology and Pharmacological Sciences



Prerequisites
(not mandatory)

Examination methods
(if applicable) Not applicable.

Suggested readings Course Moodle, module slides

Additional information



Course unit English denomination	Nucleic Acids: structures and emerging therapeutic applications
SSD	CHEM-07/A
Teacher in charge (if defined)	SISSI Claudia (12h), DALLA VIA Lisa (12h)
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input type="checkbox"/> In presence <input checked="" type="checkbox"/> Remotely <input type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (90 % minimum of presence) <input type="checkbox"/> No
Course unit contents	The nucleic acid world has been deeply revisited in the last years. Starting from the crystal structure solved by Watson and Crick this course will provide an overview of the variegate architecture that these fascinating molecules can assume. This journey will be then related to the huge potential it contains. Thus, the correlations between nucleic acid structures and biological functions as well as the application of nucleic acid as novel drugs and their potential in the field of medicinal chemistry will be discussed.
Learning goals	Knowledge: nucleic acids structures and complexes; nucleic acid-based drugs Skills: biophysical characterization, therapeutical applications Competencies: chemistry and medicinal chemistry
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	
Examination methods	Oral presentation and debate



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Suggested readings

Slides/articles provided by the teacher

Additional information
(not mandatory)



Course unit English denomination	An introduction to Python for chemical sciences: from fundamentals to data and HPC
SSD	CHEM-02/A
Teacher in charge (if defined)	
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input checked="" type="checkbox"/> In presence <input type="checkbox"/> Remotely <input type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (85% minimum of presence) <input type="checkbox"/> No
Course unit contents	The course, interspersed with practical exercises, is an introduction to using the non-assuming Python language previous programming skills. It will come to illustrate the use of some scientific Python libraries (e.g.numpy,matplotlib)
Learning goals	Knowledge: basics of Python languages and main scientific libraries Skills: Writing Python scripts/Jupyter notebooks useful for own research activity Competencies: Use and design of python to enhance research activity
Teaching methods	Frontal teaching intermixed with coding exercises
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers, provided the maximum number of allowed participants (30) has not been reached
Prerequisites (not mandatory)	
Examination methods	Software project assigned by the teacher
Suggested readings	Slides and Jupyter notebooks provided by the teacher



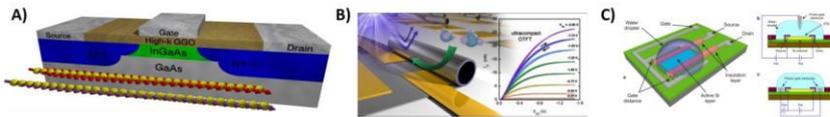
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Additional information
(not mandatory)

Max. number of participants: 30
Using of own laptop is strongly encouraged



Course unit English denomination	Semiconducting materials and their integration into transistors
SSD	CHEM-03/A
Teacher in charge (if defined)	CASALINI Stefano
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (70% minimum of presence) <input type="checkbox"/> No
Course unit contents	<p>Nowadays, the modern lifestyle is largely supported by hi-tech devices (laptops, e-watch, smart TVs, foldable devices, etc.), whose functionalities make either our personal and/or working place more comfortable or our actions more efficient.</p> <p>The field of electronics is extremely wide, hence these lectures are focused on different aspects of the working principles related to transistors based on both inorganic and organic materials. Metal oxide semiconductor field-effect transistors (MOSFETs) are one of the leading devices in modern technology. Special attention will be given to some types of organic transistors such as organic thin-film transistors (OTFTs), electrolyte-gated organic field-effect transistors (EGOFETs), organic electrochemical transistors (OECT) etc. (figure 1)</p> 
Learning goals	<p>Knowledge: the students will learn the principles of operation of MOSFET as benchmark, and they will learn the main discrepancies with electrolyte-gated organic transistors.</p>



Skills: the students will get the hands-on some standard protocols of photolithography and electrical measurement. As a consequence, the student will have the basic skills on manufacturing and measuring a transistor.
Competencies: the students will acquire a sufficient knowledge to identify and eventually solve specific issues related to a transistor.

Teaching
methods

Frontal teaching

Course on
transversal,
interdisciplinary,
transdisciplinary
skills

Yes
 No

Available for
PhD students
from other
courses

Yes
 No
Students external to the PhD Course admitted upon evaluation of the CV by the teachers

Prerequisites
(not mandatory)

Examination
methods

According to the research papers provided by the professor and the personal interest, the student will prepare an oral presentation (20-25 minutes maximum) on some basic aspects of electrolyte-gated transistors and their applications.

Suggested
readings

Slides/articles provided by the teacher

Additional
information
(not mandatory)



Course unit English denomination	Smart drug delivery systems
SSD	CHEM-08/A
Teacher in charge (if defined)	SALMASO Stefano (12h), MASTROTTO Francesca (12h)
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (75% minimum of presence) <input type="checkbox"/> No
Course unit contents	<p>Objectives. The course aims at introducing the features expected from advanced nanocarriers for drug delivery, their critical attributes and properties affecting the biopharmaceutical performances in vivo, the rational for design of “smart” multifunctional nanocarriers to exploit the phenotypic and microenvironmental features of peculiar tissues affected by diseases (e.g. tumor, inflammation) to increase site-selectivity. The concept behind remotely activated carriers will be discussed.</p> <p>Contents. Scope of nanomedicines in advanced therapies: advantages, expectations, risks. General concepts on the required properties to generate drug nanocarriers with suitable biopharmaceutical features: guidelines and rational. Peculiar microenvironments of disease sites that motivate the approach with “smart delivery systems”. The concept of “smart” nanocarriers: how nanocarriers can be endowed with active targeting capacity and responsiveness to microenvironment to improve their biopharmaceutical behaviour.</p> <p>Case studies with liposomes and metal based nanoparticles. Metal based nanoparticles: SPIONS and gold nanoparticles, characterization methods, approaches to confer responsiveness and targeting capacity, potential uses in diagnostics and drug delivery, remote activation of therapeutic activities. Liposomes: biophysics of lipid based carriers, loading strategies, microfluidics, interface ability with biological barriers.</p> <p>Polymer based nanoassemblies: novel copolymers design by using living radical polymerization techniques to obtain defined architecture, composition and molecular weight. Assembly of smart and functional nanocarriers (e.g. micelles, polyplexes, nanoparticles) for controlled release of drugs/therapeutic nucleic acids and specific targeting. Principles governing the assembly and drug loading.</p> <p>Nanotoxicity of drug nanocarriers: concept behind assessment of nanotoxicity and strategies to mitigate or remove nanotoxicity of drug carriers.</p>



Learning goals	Knowledge: understand the need for novel delivery systems, understand the risks and applicability of nanomedicine, understand the issue of nanotoxicity Skills: rational design of targeted and smart nanomedicines; critical thinking concerning the potential use of nanomedicines. Competencies: multicultural approach to develop novel nanomedicines
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	Background information about chemistry and material sciences. Preferred basic level of biological knowledge.
Examination methods	Project proposal and defense based on knowledge/skills/competencies acquired along the course
Suggested readings	Slides/articles provided by the teacher
Additional information (not mandatory)	



Course unit English denomination	Transition metal catalysis for fine chemistry
SSD	CHEM-03/A
Teacher in charge (if defined)	BIFFIS Andrea (6h), TUBARO Cristina (6h), ZECCA Marco (6h), BARON Marco (6h)
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	09/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (75% minimum of presence) <input type="checkbox"/> No
Course unit contents	<p>The aim of this course is to introduce the students to the use of transition metal catalysts in homogeneous catalysis. In the first part of the course, the following general topics will be presented in detail:</p> <ul style="list-style-type: none">- introduction to chemical kinetics; kinetic nature of the catalytic action.- reaction mechanisms and kinetic laws for stoichiometric and catalytic reactions.- typical (pseudo)elementary reactions in homogeneous organometallic catalysis: oxidative addition, reductive elimination, migratory insertion, β-elimination.- carbene coordinated to transition metals: Schrock vs. Fischer type carbenes. <p>Subsequently, the concepts learned in the first part of the course will be applied to the rational understanding of the role played by transition metal centres as catalysts for selected chemical reactions, including but not limited to:</p> <ul style="list-style-type: none">- olefin metathesis.- C-C coupling reactions, with details on the Heck reaction.- aromatic C-H bond functionalization.- catalytic transformations of substrates containing multiple C-C bonds: alkenes, alkynes, allyls, dienes, dienyls, arenes.- catalytic transformations involving renewable feedstocks.
Learning goals	<p>Knowledge: knowledge of transition metal complexes and their reactivity in the presence of organic substrates.</p> <p>Skills: Understanding the factors affecting the reactivity of a metal complexes and its role as catalyst.</p>



	Competencies: Achieving know-how on the rational use of transition metal complexes as catalysts for selected reactions relevant to fine chemical synthesis
Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input type="checkbox"/> Yes <input checked="" type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	
Examination methods	Test with multiple choice questions on course topics. The test will be considered passed with at least half correct answers.
Suggested readings	Slides/articles provided by the teacher
Additional information (not mandatory)	



Course unit English denomination	Transmission Electron Microscopy: From Chemistry and Materials Science to Biology
SSD	CHEM-02/A
Teacher in charge (if defined)	AMENDOLA Vincenzo
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	06-07/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (80 % minimum of presence) <input type="checkbox"/> No
Course unit contents	<p>The course aims at providing an overview of the various characterization techniques relying on transmission electron microscopy (TEM) and their relevance in various fields of Chemistry, Materials Science and Biological Sciences.</p> <p>The contents will start with the fundamentals of electronic optics and TEM structure, with special emphasis on the two TEM instruments available at the University of Padova. Then the different imaging and analytical modalities (TEM, HRTEM, BF, DF, SAED, EDX, EELS, STEM, etc.) and the types of TEM equipment (standard, cryo, corrected, in situ, etc.) will be discussed with application examples. Practical sessions on software for TEM data analysis and a visit to the TEM facilities of UniPd will be also performed.</p> <p>At the end of the course, the PhD students will become aware of the technical possibilities made available by modern TEM equipment at UniPd and, in general, in the contemporary scientific panorama, and will develop individual skills for analysis and manipulation of data collected by direct access to the UniPd facilities.</p>
Learning goals	<p>Knowledge:</p> <ul style="list-style-type: none">- Fundamental principles of electron optics and the structural components of TEM.- Understanding of TEM imaging and analytical techniques (e.g., TEM, HRTEM, BF, DF, SAED, EDX, EELS, STEM).- Types and functionalities of advanced TEM instruments (e.g., cryo-TEM, aberration-corrected TEM, in situ TEM).- Practical applications of TEM in Chemistry, Materials Science, and Biological Sciences.- Capabilities and specific features of the TEM facilities at the University of Padova. <p>Skills:</p>



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- Operate TEM-related software for data analysis and image processing in normal TEM, diffraction, STEM and EDX modes.
 - Interpret and analyze TEM data across various imaging and spectroscopic techniques.
 - Identify the appropriate TEM method for specific scientific investigations.
 - Navigate and utilize the TEM facilities at the University of Padova effectively.
- Competencies:
- Critically evaluate TEM data and derive meaningful scientific conclusions.
 - Design experimental strategies using TEM for multidisciplinary research.
 - Collaborate effectively with facility experts and interdisciplinary teams.
 - Adapt and apply TEM methodologies to address complex research questions.
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Teaching methods	Frontal teaching
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	Background in at least one of the disciplines or topics related to the course (Chemistry, Pharmaceutical Sciences, Biology, Materials Science, Electron Microscopy)
Examination methods	Written reports on the practical activities carried out during the course
Suggested readings	Slides/articles provided by the teacher
Additional information (not mandatory)	The course will be divided in three 8-hours modules spread over the teaching sessions, each made of a passive lesson part and a practical part. Whenever possible, international guest speakers will be invited to cover specialized topics.



Course unit English denomination	Advanced Strategies applied to the discovery and production of active ingredients in the pharmaceutical industry
SSD	CHEM-05/A
Teacher in charge (if defined)	MARTA DE ZOTTI
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	09/2026
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input type="checkbox"/> Yes (% minimum of presence) <input checked="" type="checkbox"/> No
Course unit contents	<p>This course provides a comprehensive overview of the pharmaceutical industry, beginning with an examination of the Industrial Production of active pharmaceutical ingredients, detailing industrial-scale strategies with a focus on the generic market. It then transitions to state-of-the-art Computational Drug Design, covering structure-based and ligand-based approaches, and the integration of AI/ML throughout the drug discovery pipeline. Students will learn about the Generation of crucial data for drug discovery, including Biological and Drug Metabolism and Pharmacokinetics (DMPK) evaluation, involving the analysis of drug-target interactions and a drug's absorption, distribution, metabolism, and excretion through relevant in vitro and in vivo studies. Finally, the course offers a clear and thorough understanding of Regulatory Affairs in Pharma and Intellectual Property Aspects, equipping students with the knowledge to protect their innovations and navigate global market access.</p>
Learning goals	<p>Knowledge: computational drug design (structure/ligand-based, AI/ML), data generation (biological/DMPK, drug-target analysis, ADME), and pharmaceutical regulatory/IP aspects for global market access. They will understand industrial-scale API production, particularly in the generic market.</p> <p>Competences: comprehending the entire drug development process, integrating computational and experimental approaches, evaluating drug properties, navigating regulatory landscapes, and understanding industrial production complexities, enhanced by insights from experienced industrial scientists.</p> <p>Skills: applying drug design principles, interpreting drug data, analyzing regulatory requirements, and understanding IP protection.</p>
Teaching methods	Frontal teaching



Course on transversal,
interdisciplinary,
transdisciplinary skills

Yes
 No

Available for PhD
students from other
courses

Yes
 No

Students external to the PhD Course admitted upon evaluation of the CV by the teachers

Prerequisites
(not mandatory)

Examination methods

Oral presentation or a written essay on a literature article or a topic related to the Course contents.

Study material

Slides/articles provided by the teachers

Additional information
(not mandatory)

The course will greatly benefit from the insights and expertise of industrial scientists Antonio Ricci*, Luca Ferrari*, Marco Macis*, Alfonso Pozzan#, Iuni Trist#, Elisabetta Perdoni#, Erika Torchio#, Laura Castelletti#, Stefano Fontana#, Chiara Pignaffo#, Cristina Piazza*, Roberta Sulcis*

*Fresenius Kabi
Evotec



Course unit English denomination	Structural analysis of small- and macro-molecules by X-ray crystallography
SSD	CHEM-03A; CHEM-05/A
Teacher in charge (if defined)	Prof. Marco Baron Dr. Marzio Rancan Prof. Alessandro Dolmella Prof. Roberto Battistutta
Teaching Hours	24
Number of ECTS credits allocated	3
Course period	<u>09/2026</u>
Course delivery method	<input type="checkbox"/> In presence <input type="checkbox"/> Remotely <input checked="" type="checkbox"/> Blended
Language of instruction	English
Mandatory attendance	<input checked="" type="checkbox"/> Yes (75% minimum of presence) <input type="checkbox"/> No
Course unit contents	<p>The course will be organized in four different units. All the teaching units present theoretical and hands-on sessions:</p> <ol style="list-style-type: none">1) <u>Data collection and data reduction</u> After a brief introduction on what is a single crystal and what is X-ray diffraction, the first unit of the course focuses on the single crystal X-ray diffraction experiment. Details will be provided about the set-up of the diffractometer and on the different steps of the diffraction experiments:<ul style="list-style-type: none">- Selecting, mounting and centering the crystal;- Unit cell determination;- Data collection strategy;- Integration and corrections of the collected frames;- Space group determination.2) <u>Small molecules crystal structure solution and refinement</u> After a brief overview of the main structure solution methods for small molecules, this section will focus on the structure refinement process using state-of-the-art and widely adopted software (e.g., SHELXL). Particular emphasis will be placed on:<ul style="list-style-type: none">- Criteria to guide a good structure refinement;- The use of restraints, constraints and free variables;- Disorder and refinement of disorder;- The “squeeze” algorithm: why and when use it;- Placing hydrogen atoms in the model;- Twinning;- Absolute configuration determination.



3) Data validation and presentation

This unit of the course regards crystallographic data validation and presentation.

The parameters that indicate the goodness of the refined molecular model will be presented and discussed with focuses on the generation of the CIF file (crystallographic information file) and on the CIF validation process (the checkCIF process) according to the IUCr ([International Union of Crystallography](#)) recommendations.

Furthermore, the up-to-date software to analyze and present crystallography data (PLATON, ORTEP, Mercury) will be illustrated with hands-on examples.

4) Introduction to protein crystallography

An overview of the differences between small molecules and protein crystallography will be presented, in particular for:

- crystallization methods, properties of crystals, automated data collection at synchrotrons
- solving the phase problem: the advent of the AI in protein crystallography

In the second part, we will focus on model refinement and validation:

- from the first electron density to the final “validated” model; examples and practical demonstrations (with software “Phenix” and “Coot”)
- The PDB and the correct interpretation of the protein structures.

Learning goals

Knowledge:

Upon completion of this course, doctoral students will have acquired the following key knowledge objectives:

- A comprehensive understanding of fundamental concepts in crystallography, including the principles of diffraction and the instrumentation used in this analytical technique. This foundational knowledge will enable students to grasp the theoretical basis of crystallographic analysis.
 - Proficiency in applying X-ray diffraction techniques to single crystals. Students will gain expertise in analyzing structures ranging from small molecules to biological macromolecules (proteins). This knowledge will be crucial for characterizing and understanding the structural properties of these molecular and supramolecular materials.
 - A critical awareness of the current state-of-the-art in X-ray diffraction techniques, including recent advancements and limitations. Students will explore potential future developments in structural characterization methods that go beyond single-crystal X-ray diffraction. This forward-looking perspective will prepare them to adapt to and potentially contribute to emerging technologies in the field.
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Through these objectives, students will develop a robust skill set in crystallographic analysis, enabling them to conduct advanced research in molecular and material sciences fields.

Skills:

The skills that a student will acquire through the course are:

- Crystal structure solution and refinement using different state-of-the-art software (Olex2, ShelXle, Phenix, Coot)
- Data integration and correction using different state-of-the-art software (Apex6, Crysalis Pro)
- Integration and refinement of twinned data
- Data validation and presentation

Competencies:

The determination of the molecular structure of small molecules and macromolecules is fundamental to studying their properties. Single-crystal X-ray diffraction is the leading technique for studying the structural properties of complex and advanced materials. The course aims to provide students with advanced competences in structural determination and analysis of the final models using single crystal X-ray diffraction.

By the end of the course, the students will be able to:

- Critically analyze the results obtained in a structural determination using single crystal X-ray diffraction.
- Fully exploit the potential of this technique to apply it to their own research projects.

Teaching methods	Frontal teaching and hands on sessions
Course on transversal, interdisciplinary, transdisciplinary skills	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No
Available for PhD students from other courses	<input checked="" type="checkbox"/> Yes <input type="checkbox"/> No Students external to the PhD Course admitted upon evaluation of the CV by the teachers
Prerequisites (not mandatory)	
Examination methods	Practical exam: refinement of a provided crystal structure.
Suggested readings	Slides/articles/books provided by the teachers
Additional information (not mandatory)	
