MASTER YEAR 1
COURSE DESCRIPTION

COURSE LIST

Course Title	Language	Duration	ECTS
Semester 1 - Mandatory Courses			**10**
Maths, Chemometrics, Physics and X-ray crystallography	eng	48 h	5
PSL-week		1 week	2
Project	eng	*c.a.* 30 h	2
Seminars	eng	*c.a.* 20 h	1
Semester 1 - Optional Courses			**20**
Choose 4 courses among 5*			
Molecular Design and Synthetic Tools	eng	48 h	5
Smart Materials Chemistry	eng	48 h	5
Theoretical Chemistry and Modelling	eng	48 h	5
Analytical and Physical Chemistry	eng	48 h	5
Chemistry and Life Sciences	eng	48 h	5
Semester 1 – Off Contract Course*			
French for foreigners	-		
Semester 2 - Optional Courses			**30**
Choose either full-time or part-time internship + course			**30**
Internship (full time ; 30 ECTS)	eng	Min. 110 days -Max. 132 days	30
Internship (≥ 24 ECTS) + extra courses (≤ 6 ECTS)***	eng		30
Semester 2 - Off Contract Course*			
French for foreigners	-		
TOTAL			**60**

* In exceptional case and upon approval by the M1 coordinator, 1 optional course during Semester 1 can be substituted by either one M2 course in PSL Master's Degree in Chemistry program (refer to https://www.psl.eu/formation/master-chimie) or one course offered by ENS (see appendix):
- Bioinorganic chemistry - 4 or 6 ECTS (incompatible with Chemistry and Life Science)
Note : This is not the same course 'Bioinorganic Chemistry (1 ECTS)' offered by ENSCP (see below)
- Cellular Biology II - 6 ECTS (incompatible with Smart Materials Chemistry)
- Epigenetics – 6 ECTS (incompatible with Theoretical Chemistry and Modelling)

** Off-contract course refers to course that does not yield any ECTS credits that contributes towards your master degree

***Upon approval by the M1 coordinator, extra courses in Semester 2 can be chosen from the list below, so that the total ECTS = 30 requirement is fulfilled.
- Advanced theoretical and computational chemistry – 2 ECTS (Master of Chemistry)
- Electronic Properties of Solids – 2 ECTS (ENSCP)
- Bioanalytical chemistry – 2 ECTS (ENSCP)
- Mastering Heteroelement and Catalysis for Applied Molecular Synthesis - 2 ECTS (ENSCP)
- Inorganic Assemblie : From Molecules to Materials – 1 ECTS (ENSCP)
- Bioinorganic Chemistry – 1 ECTS (ENSCP)
- Biointerfaces - 1 ECTS (ENSCP)
- Statistical Learning – 3 ECTS (ESPCI)
- Analytical chemistry – 3 ECTS (ESPCI)
- Soft Matter - 3 ECTS (ESPCI)
- Advanced Chemistry - 3 ECTS (ESPCI)
- Interface Physics Biology - 3 ECTS (ESPCI)
- Chemical Biology and Molecular Biotechnology - 3 ECTS (ESPCI)
- Synthetic Chemistry and Applications - 3 ECTS (ESPCI)

M1 schedule – Year 2025 - 2026

(Marginal changes in year 2026 - 2027 may occur)

Master in Chemistry PSL - YEAR 1 (2025-2026)																					
		MONDAY				TUESDAY				WEDNESDAY				THURSDAY				FRIDAY			
Weeks	Dates	8h30 - 10h30	10h45 - 12h45	13h45-15h45	16h00 - 18h00	8h30 - 10h30	10h45 - 12h45	13h45-15h45	16h00-18h00	8h30 - 10h30	10h45 - 12h45	13h45-15h45	16h00 - 18h00	8h30 - 10h30	10h45 - **12h15**	13h45 - 15h45	16h00-18h00	8h30 - 10h30	10h45 - 12h45	13h45 - 15h45	16h00-18h00
37	8-Sep-25	INTEGRATION WEEK				Bioionorganic chem. 1st class 10:30-12:15, room R @ ENS		INTEGRATION WEEK		Cell biology 1st class 9:15-12:00 - Room 306 @ENS - IBENS		INTEGRATION WEEK									
38	15-Sep-25		TCM	MDST		CLS	CLS					MCPX		MDST	MCPX			APC	APC	TCM	
39	22-Sep-25	TCM	Seminar	MDST		CLS	CLS				SMC	MCPX		MDST	MCPX			APC	APC	TCM	
40	29-Sep-25	TCM	Seminar	MDST		CLS	CLS			SMC	SMC	MCPX		MDST	MCPX			APC	APC	TCM	
41	6-Oct-25	TCM	Seminar	MDST		CLS	CLS			SMC	SMC	MCPX		MDST	MCPX			APC	APC	TCM	
42	13-Oct-25	TCM	Seminar	MDST		CLS	CLS			SMC	SMC	MCPX		MDST	MCPX			APC	APC	TCM	
43	20-Oct-25	TCM	Seminar	MDST		CLS	CLS			SMC	SMC			MDST	MCPX			APC	APC	TCM	
44	27-Oct-25	ALL SAINTS VACATION																			
45	3-Nov-25	TCM	Seminar	MDST		CLS	CLS (1h)			SMC	SMC	MCPX		MDST	MCPX			APC	APC	TCM	
46	10-Nov-25	Public holiday				Public holiday				SMC	SMC	MCPX		MDST	MCPX			APC	APC	TCM	
47	17-Nov-25	TCM	Seminar	MDST		CLS	CLS			SMC	SMC	Exam MCPX #1 13:45-14:45		MDST	MCPX			APC	APC	MCPX	
48	24-Nov-25	PSL WEEK																			
49	1-Dec-25	TCM	Seminar	MDST		CLS	CLS (1h)			SMC	SMC	SMC		MDST	MCPX			APC	APC	MCPX	
50	8-Dec-25	TCM	Seminar	MDST		CLS	CLS			SMC	SMC	MCPX		MDST	MCPX			APC	APC		
51	15-Dec-25	TCM	Seminar	MCPX		CLS	CLS (1h)			SMC	SMC	MCPX		MDST	MCPX			APC	APC	TCM	
52	22-Dec-25	CHRISTMAS VACATION																			
1	29-Dec-25																				
2	5-Jan-26	MDST	TCM	MCPX		CLS	CLS			TCM	MCPX	Project presentations		TCM	Project presentations			Project presentations			
3	12-Jan-26	MDST	TCM	MCPX		CLS	CLS (1h)			SMC	SMC	9:00-11:00 seminar presentations									
4	19-Jan-26	REVISIONS								Exam Cell biology 9:00-12:00		REVISIONS						Exam Epigenetics 9:30-12:00		REVISIONS	
5	26-Jan-26	MDST exam 9h-11h		TCM exam 13h30-15h30		CLS exam 9h-11h				SMC exam 9h-11h					MCPX exam #2 11:00-12:00			APC exam 9h-11h			
6	2-Feb-26	INTERNSHIP STARTING WEEK																			
		Internship min. 110 days - max. 132 days																			

Course label	Course title
MCPX	Maths, Chemometrics, Physics and X-ray crystallography
MDST	Molecular Design and Synthetic Tools
SMC	Smart Materials Chemistry
TCM	Theoretical Chemistry and Modelling
APC	Analytical and Physical Chemistry
CLS	Chemistry and Life Sciences

External courses at ENS		
Bioinorganic chemistry	Tuesday	10:30-12h15
Epigenetics	Friday	9:45-11:45
Cellular Biology II	Wednesday	9:00-12:10
Intro sciences du vivant	Friday	14:30-16:30

SEMESTER 1

M1	S1	MCPX - Maths, Chemometrics, Physics and X-ray crystallography
		Keywords: *mathematics, quantum physics, crystallography, Introduction to Chemometrics*

Course description and content

This module introduces the main concepts in mathematics, quantum physics, X-ray crystallography and chemometrics (introduction) necessary to follow the master program in chemistry .

The training is based on four main courses of 12 hrs each: mathematics, quantum physics, X-ray crystallography and chemometrics which are each presented with illustrating examples and exercises in class.

The main concepts covered are:

- in mathematics: linear algebra, Hilbert spaces, Fourier analysis, differential equations
- in quantum physics: the postulates and their application, the time-dependent Schrödinger equation, potential wells and barriers, the quantum harmonic oscillator, angular momenta
- in X-ray crystallography: crystal lattice, point symmetry, space groups, international tables for crystallography, reciprocal lattice, x-ray diffraction conditions, applications of XRD
- In chemometrics: descriptive statistics, statistical distributions, random variable, estimation, hypothesis testing, linear regression

Learning goals

The student should be able to:

- know the basic concepts of quantum physics and chemistry, such as linear algebra, Hilbert spaces, eigenfunctions, hermiticity, Fourier analysis as well as differential equations
- understand the main concepts of quantum physics and calculate the properties of simple quantum systems, including the use of algebra in Hilbert spaces
- describe the symmetries of crystals and their structures using the international tables for crystallography
- obtain structural information from powder X-ray diffraction patterns
- implement basic statistical tools to present and interpret their data

Prerequisite

- basics of linear algebra (matrices and operations on matrices, matrix diagonalization, vector spaces, scalar product), 1^{st} and 2^{nd} order differential equations, spherical coordinates, differentiation of multivariable functions, Laplacian and gradient operators
- basics of classical physics: momentum and angular momentum, kinetic and potential energies, conservation laws, elementary electrostatics and magnetostatics, plane waves, electromagnetic waves
- basics of Euclidian geometry: scalar and vector products, equation of plane and line

M1	S1	**Bibliographical project**
		Keywords: *chemistry, bibliography, state-of-the-art*

Course description and content

In this module, the students will select a research theme for a bibliographical study, within a list of topics proposed by PSL researchers in chemistry.

Working in pairs and thanks to interactions with the research theme's proposers, they will produce:

- a written report providing state-of-the-art and perspectives
- an oral presentation followed by a questions session

Learning goals

The students should be able to:

- identify key literature, connections and development within a specific theme
- summarize and organize ideas and conclude about perspectives within a written document
- build a presentation based on these elements
- master the topic to convincingly answer questions from specialists and non-specialists

Prerequisite

- general knowledge in chemistry
- basic writing and presentation skills

M1	S1	Seminars

Learning goals

The objective of this seminar module is to introduce Master 1 chemistry students to the research activities carried out within PSL. The seminars are delivered by members of PSL research teams and present recent and ongoing research projects across the different fields of chemistry. By connecting the seminar topics to the various Semester 1 teaching modules, this course enables students to place the concepts learned in lectures into a broader research and scientific context.

By the end of the course, students will be able to critically analyze a scientific seminar, identify its key scientific questions, methodologies, and results, and communicate their understanding clearly and rigorously in an oral presentation and discussion.

Pre-requisites

Students are expected to have a solid background in fundamental concepts of chemistry, including physical chemistry, organic chemistry, inorganic chemistry, and analytical chemistry. A good understanding of basic chemical principles (thermodynamics, kinetics, structure–property relationships, and chemical reactivity) is required in order to follow the seminars, analyze the presented research work, and actively participate in discussions

<table>
<tr><td rowspan="2">M1</td><td rowspan="2">S1</td><td>MDST – Molecular Design and Synthetic Tools</td></tr>
<tr><td>Keywords: C-C bond formation, asymmetric synthesis, organometallic chemistry and catalysis, retrosynthesis, total synthesis, atom- and step-economy</td></tr>
</table>

Course description and content

This course will be divided into 3 units:

a) organic chemistry (KC)
Contents: Reactivity of carbonyl groups (asymmetric induction models…) and enolates (aldolisation, Zimmerman Traxler…); pericyclic reactions (Diels-Alder, sigmatropic rearrangements); chemistry of main group elements: boron, silicon (Peterson, Tamao…), sulfur (Julia, Swern…), phosphorus (Wittig, Mitsunobu…) andintroduction to ring forming reactions.

b) organometallic chemistry (RG)
Contents: structure and reactivity of transition-metal complexes, electron counting in complexes, elementary steps in organometallic chemistry, examples of catalytic reactions (carbonylation, metathesis, cross-coupling, etc.), extension to industrial synthesis of fine chemicals or to high-scale processes (eg: acetic acid in Cativa / Monsanto processes.

c) retrosynthetic analysis and total synthesis of bioactive compounds (K.C.)
This course will introduce the principles of retrosynthetic analysis and their applications for the design of synthetic routes, relying on the synthetic methods studied during the "Oranic Chemstry" course. Recent examples of syntheses of bioactive molecules (whether natural products or manufactured drugs) will serve as illustrations and a particular emphasis will be placed on atom- and step-economic synthetic strategies.
The course will be divided between classes and practical exercises that will take the form of team projects, which will be graded as part of the total grade for the course.

Learning goals *(Ce que les étudiants doivent être capables de faire à l'issue de l'enseignement)*
The student should be able to:
- Give the mechanism of multistep transformations of complex targets, interpret the diastereoselectivity of transformations based on simple models.
- Give a catalytic cycle for simple transformations in organometallic catalysis, and analyze the evolution of the oxidation state / electron number of the intermediates involved, as well as interpret the electronic effect of several ligands on the catalytic efficiency in some simple cases.
- do the retrosynthetic analysis of a given molecule, propose the key synthetic steps, devise an efficient synthetic strategy, solve a synthetic problem through teamwork.
- Extract the key data from a scientific publication.

Prerequisite
Good knowledge of reactivity of classic functional groups. Notions in atomistics and in (molecular) orbitals description for the organometallic courses.

M1	S1	SMC - Smart Materials Chemistry
		Keywords: soft matter, inorganic materials, hybrid systems, polymer, colloids, surfactants, synthesis, engineering, characterization

Course description and content

This course will provide the necessary skills to design smart materials based on inorganic and soft matter and hybrid systems. The general idea is to start from these concepts to develop smart materials and to show their richness and their applications in current areas such as health, energy, environment.
The course consists of three main parts:

"Soft Matter" encompasses very different materials that share in common weak cohesive forces and a great sensitivity to the environment: polymers, colloids, surfactants. Behind this apparent diversity, they exhibit common features that can be understood in terms of unifying concepts borrowed from thermodynamic and statistical physics: entropy, enthalpy, phase separation, molecular forces. This "Soft Matter" part will provide the student with a global approach connecting molecular design, synthetic chemistry, mesoscopic and macroscopic structure, material properties, and applications. Selected topics will include an introduction to polymers in bulk and solutions, colloids, and self-assembled systems. The concept of stimuli-responsiveness is also tackled: how to induce changes of molecular conformation (surfactants, polymers) and/or changes of assembling (gels, colloids, emulsions) and to control macroscopic properties (rheological, mechanical, interfacial as wetting, adhesion, friction) by triggering a stimulus such as temperature, pH, salt, light, electric and magnetic fields.

In the "Inorganic Materials" part, basics of the solidification and material stability will be firstly presented. Materials concerned are ionic solids, ionocovalent and ionometallic solids. Basic concepts on the electronic band structures and structure-properties relationships will be envisioned. We will present the fundamental aspects in the synthesis of inorganic materials, including phase diagrams, concepts of growth of inorganic materials from nanocrystals to large size materials including glass, ceramics and vitroceramics as well as single crystals elaboration. Their respective properties and characterization methods will be studied. Intrinsic and extrinsic defects in solids with formation and stabilization mechanisms will be presented as well as the remarkable properties associated with these defects. Overview of the optical, electrical and magnetic properties in the inorganic materials will be presented.
The diffusion properties in solids and a quick recapitulative about electrochemistry and its application to solids and solid/liquid interfaces will also be presented and applied to the development of battery materials, focusing on the tradeoff between energy/power density and scalability.

The third part will be devoted to "Hybrid Materials" and will focus on the concepts to develop smart materials.
The basic concepts of coordination chemistry including geometry/reactivity/stability of coordination complexes will be evoked, followed by ligand field theory and the electronic properties of solids. These concepts will be applied to the synthesis, properties and applications of crystalline porous solids (Metal-Organic Frameworks).

Learning goals
The student should be able to:
- mobilize a multidisciplinary background in chemistry and physics to rationalize important material behaviors in Soft Matter (*i.e.* solubility *versus* phase separation).
- draw analogies between different soft materials
- address the description of the main structural types characterizing solids
- understand the different existing synthesis routes for the development of inorganic materials

Prerequisite
Basic knowledge of inorganic and organic chemistry
Basic knowledge of solid state and coordination chemistry, chemical bonding, group theory.
Basic knowledge of thermodynamics: entropy, enthalpy, free energy, phase separation, molecular forces

M1	S1	**TCM - Theoretical Chemistry and Modelling**
		Keywords: electronic structure, statistical mechanics, quantum chemistry, density functional theory, thermodynamics

Course description and content

Part 1: Electronic Structure Theory (24h)

The knowledge of the electronic structure of molecules and extended systems allows for the understanding of their reactivity and properties. Here we will first provide a general introduction to the methods and concepts encountered when aiming at describing the electronic structure of single to multi electronic atoms and molecules. After the introduction of Schrödinger equation and of the common approximations applied to solve it, we will detail the Hartree-Fock method and define the concept of electronic correlation.

Next, advanced electronic structure methods enabling the treatment of electron correlation will be introduced focusing on Density Functional Theory. The coupling and extension of ab-initio approaches to describe condensed phases (solution, solids) will be detailed. Multi-layer methods combining Quantum and Classical approaches will be introduced for the simulation of complex environments.

Part 2: Fundamentals of Statistical Mechanics and molecular Dynamics (24h)

Statistical mechanics is one of the pillars of modern physics, linking the laws of physics at the microscopic scale, at the quantum (Schrödinger's equation) or classical level (Newton's laws), with the properties of matter and its macroscopic behavior (the laws of thermodynamics). We introduce the fundamentals of statistical mechanics, and introduce the concepts of temperature, work, heat, and entropy, the postulates of statistical mechanics, the notion of statistical ensembles and their use in the calculation of average quantities. We will cover simple models that are widely found throughout physics and chemistry: harmonic oscillator, ideal and nonideal gases, phase transitions, mean field approximations. Next, we will introduce the students to two main classes of molecular modelling methods, molecular dynamics and Monte Carlo simulations. We will contrast the approaches of quantum chemical and classical methods, and provide an introduction into mesoscale modeling methods, such as lattice-based simulations and kinetic Monte Carlo. Finally, we will provide theory and application of molecular dynamics for biological systems, covering classical molecular dynamics, enhanced sampling techniques, and hybrid quantum/classical methods.

Learning goals

The student should be able to:
- understand the meaning of the Schrödinger equation
- know the common approximations used to solve the Schrödinger equation
- describe a multi-electronic atomic or molecular system using the Hartree-Fock method
- define the concept of electron correlation
- know the difference between classical and quantum models
- understand the fundamentals of Density Functional Theory
- understand how one can simulate periodic systems
- calculate the partition function of a given system
- determine the thermodynamic properties from the partition functions
- apply a mean field approximation
- use equations of state and phase diagrams
- understand the fundamentals of molecular simulation in chemistry, and their ties to statistical mechanics
- know differences between molecular simulation techniques
- choose an appropriate simulation technique for a given complex question
- read a computational chemistry article and understand the methodology and its limitations

Pre-requisites

BSc level in physical chemistry, quantum chemistry, thermodynamics

M1	S1	**APC - Analytical and Physical Chemistry**
		Keywords: solution chemistry, separation sciences, electrochemistry, molecular spectroscopy, Spectroscopy, Imaging, Optics, Magnetic Resonance, X-ray, scattering, diffraction, molecular and nanoparticular structure, analytical methods, biomedical.

Course description and content

The course aims at arming the student with fundamental concepts in solution chemistry, separation sciences, electrochemistry, and molecular spectroscopies enabling to understand and address experimental questions on how to characterize, analyze, separate molecular components in solutions or complex mixtures towards the building up of an efficient analytical method.

(i) **Solution chemistry**: Basic principles of solution chemistry: aqueous solutions (from diluted to concentrated), activity coefficient, acid/base, complexation equilibria, complexation coefficient. Control of the chemical separations (solubilization, precipitation, liquid/liquid extraction, liquid/solid extraction) through the understanding of the reactions involved in solution. Introduction to non-aqueous solutions (micelles, molecular solvents, ionic liquids, supercritical fluids) (Anne Varenne; 6h)

(ii) ***Separation Sciences****: basic concepts in analytical separations (chromatographic or electrophoretic): classifications, objectives, interactions controlling the separation selectivity, operating conditions affecting separation efficiency, fundamental parameters quantifying the performance of analytical separations, case studies towards the development of analytical strategies (Fanny d'Orlyé; 6h).*

(iii) **Electrochemistry**: fundamental principles of electrochemistry, in particular microelectrolysis and the current-potential characteristics i=f(E) to elaborate a basis for the approach in analysis. An overview of the effect of the size of the electrode and the chemical medium on i=f(E) curves will also presented (Dimitri Mercier; 9h).

(iv) **Molecular spectroscopy**: General introduction to spectroscopy across the electromagnetic spectrum (NMR, IR, ro-vibrational spectroscopy, UV–Vis, etc.), spins, and selection rules. Optical spectroscopies: basics of absorption and emission; effects of molecular structure and environment; lifetimes of excited electronic states; quantum yield and non radiative transitions; fluorescence quenching; Jablonski diagram. NMR: structure of 1D NMR spectra (energy levels; time independent Schrödinger equation; angular momentum operators; NMR interactions — Zeeman, chemical shifts, J coupling); principles of a 1D NMR experiment (vector model; nuclear magnetization; Bloch equations; radiofrequency pulses; Fourier transform). (Kong Ooi Tan; 6 h)

(v) **Building up analytical methods**: The strategies and techniques used for the construction of the whole analytical process (sampling, sample treatment, separation techniques and coupling with performant detection methods) adapted for the analysis of complex samples will be presented. Concepts such as biomarker, interferents, standard, sample matrix effects, speciation, bioassays formats, screening test and/or quantitative analysis (internal and external calibrations) will be illustrated. Finally, the concept of method/test validation and analytical quality parameters (sensitivity, LOD, LOQ, precision, trueness, etc.) will be afforded in the view of the development of new analytical strategies. (Laura Trapiella, Anne Varenne, Fanny d'Orlyé, Dimitri Mercier,Kong Ooi Tan; 9h)

(vi) **Radiation-based analysis: from spectroscopy to imaging :** The objective of the course is to provide advanced knowledges from Optical and Magnetic Resonance spectroscopy to Imagings in order to probe the structure of chemical objects developed in the latest innovations and technological developments in chemistry and in biology. The course prepares chemists or physicochemists students to the applications of basics concepts of spectroscopies for the understanding and work in cutting edge spectroscopic to imagings techniques in advanced theoretical, experimental and applied research performed in academic and industrial laboratories.

This course covers a range of experimental methods, and spectroscopy. Optical, Magnetic Resonance and scattering-based approaches, used to characterize structures at the nm to micrometer length scales, from molecules, nanoparticles to microsize organic objects

Part 1: Radiation-based analysis, from spectroscopy to imaging (part I): basics of the chemical probes and probing methods at the molecular level will be presented in MR, optical (NIR, UV-Vis) fluorescence methods to characterize the structure and understand the properties of probes for biology. Advanced applications in cellular diagnosis or for novel therapies will be detailed (including photoactivable biomolecules, NIR probes for image guided therapy, biphotonic methods, MRS/MRI basics applications) (Bich Thuy Doan; 6h).

Part 2: Radiation-based analysis, from spectroscopy to imaging (part II): The course cover a range of optical and scattering-based methods, used to characterize structures at the nanometer to micrometer length scales. The theory of scattering (light, small angle X-ray) will be established. Models of scattering patterns will be presented to determine molecular weight, radii, shape, and inter-molecular attraction/repulsion forces involved in molecular assemblies, macromolecules, colloids, up to spatial organization of biological matter. (Christophe Tribet; 6h).

Learning goals

The student should be able to:

- Predict acid-base, complexation or precipitation reactions in a system knowing its composition,

-Control the reactions involved in solution to develop efficient chemical separations in complex mixtures

-Understand the fundamental aspects of electrochemistry, how to integrate the effect of the chemical medium (acidity, complexation, precipitation) and the size and shape of the electrode in the establishment and plot of i = f (E) curves,
- Understand the principal forces and identify interactions that control the performances of analytical separations, evaluate the relative performance of these separations across different modes, understand and use analysis results.
- Understand the physical principles of NMR (spectroscopy and imaging) and optical spectroscopies. Discover the main imaging probes. Understand cutting edge techniques in MR and optical spectroscopy to imaging in advanced experimental and theoretical research.
- Know the more common methods used for the environmental and biological analysis
- Built up an adapted and efficient analytical method regarding the sampling, sample treatment and analytical determination of a given molecule/compound
- to understand the general principles of optical methods used to characterize the size and shapes of nanoparticles, molecular or macromolecular assemblies by i) elastic static scattering, ii) high resolution microscopies, iii) dynamic light scattering and tracking of single particle/molecules.

Pre-requisites

Basics in thermochemistry, inorganic chemistry, organic chemistry, optics, molecule interactions, complexations, physical chemistry in solution.
Mathematical basics applied to thermodynamics (integration, derivatives, exact total differentials, cross derivatives, differential equations). Basics of quantum physics and chemistry (Schrödinger equation, energy levels). Descriptive 1D spectroscopy (1D proton) NMR, absorption spectra in optical spectroscopies).

M1	S1	Course Title: Chemistry and Life Sciences
		Keywords: cellular biology, molecular biology, proteins, nucleic acids, lipids, carbohydrates

Content
The course includes two parts that will be taught in parallel, in a synchronized manner.

Part 1: Biomolecules
Here are explicitly described the mechanisms of biosynthesis, degradation and role of biomolecules, biological small molecules and metals.

1.1 Nucleic acids
What is a nucleic acid? Classes of nucleic acids, chemical composition; structure (description);
DNA and RNA modifications,
mRNA, rRNA, tRNA, LncRNA, RNA interference and microRNAs, RNA degradation
Synthesis of nucleic acids in the cell: replication, transcription, telomere elongation, DNA repair; telomerase, shelterin transcription, splicing
Experimental synthesis of nucleic acids: solid-state synthesis, PCR.

1.2 Proteins
What is a protein? chemical composition; structure (description, brief review of methods, structure prediction); post-translational modifications; classes of functions.
Synthesis of proteins in the cell, ribosomal translation,
Experimental synthesis of proteins: recombinant protein expression, solid-state synthesis, control of stereochemistry

1.3 Glycans
Where are these biomolecules biosynthesized and degraded, what is their function (structure vs signaling), membrane damage, ferroptosis
- Introduction into glycan structures
- Functions of glycans
- Fundamental notions of glycochemistry applied to biological questions

1.4 Lipids
Where are these biomolecules biosynthesized and degraded, what is their function (structure vs signaling), membrane damage, ferroptosis (see part 1)
- Introduction into lipid structures
- Functions of lipids with a focus on structure, compartmentalization of the cell require to separate specific chemical reactions, intracellular trafficking and signaling

1.5 Methods to characterize biomolecules and their interactions
- Determining the sequence (mass spectrometry-based proteomics/lipidomics/glycomics, methods for sequencing nucleic acids including illumina and nanopore)
- Determining the size and shape (SDS-PAGE, SEC-MALS, NMR diffusion)
- Methods to predict and characterize structures (X-ray, cryoEM, NMR, CD, alphaFold)
- Methods to quantify interactions (SPR, ITC, thermophoresis, FRET, NMR titrations)

1.5 Designing the elements of life
-Introduction to protein design
-Introduction to synthetic biology

Part 2: Biological mechanisms for the chemist

The mammalian cell: structure, function and dynamics of organelles, contact and communication
Here are described the structure and function of cell organelles making life possible.

2.1 The central dogma of molecular biology
- DNA, support of genetic information: Chromatin: structure and dynamics, nucleosome et epigenome (structure vs transcriptional repression role)
- Genetic vs. epigenetic mechanisms of cell adaptation, cell types and differentiation, stem cells...
- Epitranscriptomic

2.2 Cell trafficking
Structure of the plasma membrane
Endocytosis, lysosome, Endolysosome, autophagosome, exocytosis (EVs), Peroxisome
Endoplasmic Reticulum and Golgi
Protein organelle targeting (post-translational modifications), protein degradation (lysosome vs proteasome), folding with chaperones, translocation, unfolded protein response and diseases,

2.3 the cell and its environment

Contact and communication: Small molecules and metals in the cell
Biosynthesis and role of hormones and growth factors…, cell signaling

2.4 Cell metabolism

Krebs cycle, ATP production, production of (epigenetic) metabolites and lipid degradation
Mitochondria

2.5 Dynamic of the cell : cell cycle and cell death

Dynamics of the cell
Cell cycle/ senescence / quiescence; genetic vs. epigenetic mechanisms of cell adaptation, cell types and differentiation, stem cells…
Cell death
Programmed cell death and other vulnerabilities
Apoptosis / Necroptosis/ Pyroptosis / Autophagy/ Ferroptosis
epigenome targeting drugs
DNA damage and repair
Homologous recombination, non-homologous end joining, base/nucleotide-excision repair, mismatch repair, DDR drugs, PARP inhibitors (proliferation) and concept of synthetic lethality

Learning goals
The student should be able to:
- Understand the overall organization and the basic functions of a cell
- Know the classes of biomolecules, how they are synthetized in the cell and by the chemist
- Have enough background knowledge to understand how to target cellular processes with synthetic molecules

Prerequisites
The class is an introduction to biology for chemists. Some basic knowledge on cells and their organelles, proteins and nucleic acids will be useful but not necessary.
Some undergraduate organic chemistry is required to understand the synthesis of biomolecules.

SEMESTER 2

<table>
<tr><td>M1</td><td>S2</td><td colspan="2">Course Title: Research Internship
Keywords:</td></tr>
<tr><td colspan="2">ECTS : 24 to 30</td><td>Total duration : minimum 100 worked days – maximum 132 worked days</td><td>grading: Report and oral presentation</td></tr>
<tr><td colspan="4">Description
The research intership can be performed either in an academic laboratory or in the private sector. It must be research oriented.</td></tr>
<tr><td colspan="4">Learning goals
The student shoulb be able to conduct a small research project, to plan and carry out experiments, to understand the theoretical bases of his/her project, to interact with other researchers and staff members, to make written and oral reports of his/her results.</td></tr>
<tr><td colspan="4">Pre-requisites
None</td></tr>
</table>

Optional course

M1	S2	**Course Title: Advanced theoretical and computational chemistry** *Keywords:*

Description

The course will provide an advanced perspective both on theoretical models and simulation techniques treating several among the topics detailed below. Regarding numerical simulations, building on the introduction given in the advanced class, this course will address a range of modern techniques, including first-principle methods, extended statistical ensembles, description of nuclear quantum effects via path-integral simulations, multi-scale strategies, and the combination with machine learning approaches. Various applications of these techniques to condensed phase chemistry will be studied. This course will also present advanced theoretical models to describe chemical reactivity; starting from Transition State Theory, the course will introduce the concept of friction on barrier-crossing, its formal description via stochastic approaches and will finally address the complex case of non-adiabatic chemical reactions.

Concerning electronic structure methods, the course will explicitly address state of the art methods enabling the first-principle simulation of spectroscopic properties of molecules and extended systems. Perturbative and variational methods allowing to obtain accurate vibrational spectra will be introduced and compared to approaches based on dynamical approaches. Linear response –in the framework of the Time Dependent DFT approach- will be introduced and the simulation of the photophysical properties of molecular and extended (3D, 2D, 1D) systems will be discussed.

The accuracy and the limit of these methods (coupled with embedding techniques and/or multi-layer approaches to simulate the environment) will be illustrated through selected examples.

Learning goals

The student should be able to:

- understand the main concepts related to the modeling of spectroscopic properties of molecules and extended systems
- list the tradeoffs involved in different molecular simulation techniques
- write up a work plan for a multi-scale simulation strategy
- compare experimental data, computational results, and theoretical models of reactivity
- understand articles on machine learning techniques applied to chemistry

Pre-requisites

BSc level in statistical physics, quantum chemistry, physical chemistry

Appendix

Here includes the course description of the three optional courses (only 1 can be chosen ; see the course list in the beginning in the document) offered at ENS for semester 1 at M1 level.

M1	**S1**	**Course Title** <u>**Bioinorganic chemistry: metal ions from biology to environment**</u> *Keywords: metal ions, metalloproteins, bio-metallic complexes, environmental pollution, metal detection*

Description

This lecture presents recent advances in applied inorganic chemistry, focusing on its connection with biology and the environment. It delves into the fundamental thermodynamics and reactivity principles of inorganic chemistry through examples from biological systems and the environment. The course explores how living systems use the specific physicochemical properties of metal cations and how these ions impact pollution. Topics include endogenous metallic systems like metalloproteins, metal ions in the environment, and methods for their detection and imaging within cells. The course also examines the accumulation of metal ions as a valuable resource in biological systems. Using mercury as a case study, it will address issues of metallic environmental pollution. The tentative program covers the role of metal cations in biology, fundamental inorganic chemistry from a biological perspective, metal ions at the origin of life, metals as a resource, bio-accumulation, and metal detection, with case studies on mercury and copper.

Tentative program:
Introduction: role of metal cations in biology; bio-metallic complexes and biomolecules; fundamental of inorganic chemistry with the prism of biological systems
Metal ions at the origin of life
Metal: a precious resource
Metal and bio-accumulation
Metal detection in biological systems
Two cases studies: Hg and Cu, toxicity and essentiality

Learning goals

To understand how specific physio-chemical properties of metal cations are used by living systems and impact environmental pollution

Pre-requisites

This course requires basic notions in inorganic chemistry

M1	S1	**Course Title: <u>Cell biology II : traffic, motility, biophysics</u>** *Keywords: cytoskeleton, membrane traffic, adhesion, biophysics, nucleocytoplasmic transport, cell cycle, cell migration, cancer biology*

Please refer to the course website for the most up-to-date information:
https://www.edu.bio.ens.psl.eu/spip.php?article59&lang=fr

Description

This course covers major topics in cell biology, including membrane trafficking, cytoskeleton organization, the establishment of cell polarity, cell cycle control and division, and cell adhesion and migration. These cellular functions are examined in the context of both normal and cancer cells. The curriculum also includes innovative biophysical approaches to cell biology, such as cellular bio-mechanics and micro-rheology. The course is structured as a series of 2-hour research seminars taught by leading cell biologists from various research institutions

Suggested readings in relationship with the module content (textbook chapters, reviews, articles) :
– Molecular Biology of the Cell, Alberts (Garland Science Ed) ; Cell Biology, Pollard § Earnshaw (Saunders Ed) – The Cell Cycle. Principles of control, D. Morgan (NSP Ed) – Physical Biology of the Cell ; Phillips, Kondev & Theriot (Garland Science Ed) – Optional : The biology of cancer, Weinberg (Garland Science Ed)

Course material:
PowerPoint presentations of lectures will be available. Suggested readings include "Molecular Biology of the Cell" by Alberts, "Cell Biology" by Pollard & Earnshaw, "The Cell Cycle" by D. Morgan, "Physical Biology of the Cell" by Phillips, Kondev & Theriot, and optionally "The biology of cancer" by Weinberg

Learning goals

To understand key aspects of cell biology and innovative biophysical approaches, taught through research seminars by leading experts.

Pre-requisites

Cell biology I (L3/BSc) or basic notions in cell biology

M1	S1	**Course Title: <u>Epigenetics: from biological phenomena to molecular mechanism</u>** *Keywords: gene, genome, mendelian and non-mendelian inheritance, DNA and histones modifications, heterochromatin, euchromatin, transposons, RNA interference, epimutations, ChIP-seq, DNA bisulfite treatment, sRNA-profiling, Chromosome conformation capture*

Please refer to the course website for the most up-to-date information:
https://www.edu.bio.ens.psl.eu/spip.php?article48&lang=fr

Description

This course aims to uncover the paradigms of epigenetics, from observed phenomena to their molecular underpinnings. It is organized through seminars and article analysis. Topics covered include the maintenance of chromatin states, the role of small and long non-coding RNAs in epigenetic regulation, parental imprinting, X-inactivation in mammals, paramutation, transgenerational epigenetic inheritance in plants, and prions as an epigenetic phenomenon

Course material:
PDFs of presentations are available online. Suggested readings include "Epigenetics" (2nd ed.) by Allis et al., and several key review articles on the subject

Suggested readings in relationship with the module content (textbook chapters, reviews, articles) :
– Epigenetics (2nd edition), Allis CD, Caparros M-L, Jenuwein T, Reinberg D, Cold Spring Harbor Laboratory Press.(2015) **–** Epigenetics, cellular memory and gene regulation. Henikoff S, Greally JM. Curr Biol. 26(14):R644-8 (2016) **–** Transgenerational epigenetic inheritance : myths and mechanisms. Heard E, Martienssen R. Cell 157(1):95-109 (2014) **–** Regulation of X-chromosome dosage compensation in human : mechanisms and model systems. Sahakyan A, Plath K, Rougeulle C. Philos Trans R Soc Lond B Biol Sci. 372(1733) (2017) **–** Different yet similar : evolution of imprinting in flowering plants and mammals. Pires ND, Grossniklaus U. F1000Prime Rep, 6:63 (2014) **–** Paramutation and related phenomena in diverse species. Hollick JB. Nat Rev Genet. 18(1):5-23 (2017).

Learning goals

To discover the paradigms of epigenetics, from epigenetic phenomena to the underlying molecular mechanisms.

Pre-requisites

Genetics/epigenetics course and molecular biology.