



MUNDUS CHEMOINFO+



European Master in  
Cheminformatics



# Erasmus Mundus Joint Master Chemo- informatics +



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UNIVERSITÀ  
DEGLI STUDI  
DI MILANO



University of Ljubljana



Bar-Ilan  
University  
ב"רן י"ל תל אביב









# About the master

Chemoinformatics+ is a two-year, 120 ECTS, multi-university Master programme opened since September 2022. It concerns the development, creation, organization, storage, dissemination, analysis, visualization and use of chemical information aimed at the discovery of molecules for therapeutic purposes, the validation and development of biological targets, and the anticipation of toxicity and ecotoxicity risks.

Within the last 20 years, Chemoinformatics has become a cornerstone for Chemical and Pharmaceutical industries. The Chemoinformatics+ consortium aims at training specialists with strong skills in chemistry, basic computer science and specific chemoinformatics methods. It seeks to improve the output expectations of the diploma in terms of excellence, employability and entrepreneurship.

## Who can apply?

- Holders of a Bachelor's Degree in Chemistry, Physical-Chemistry, Bio-Chemistry or equivalent,
- Students in the final year of their Bachelor's Degree graduated before the start of the Master,
- Holders of a Master in Chemistry, Physical-Chemistry, Bio-Chemistry or equivalent.

## Scholarships

The program offers **Erasmus Mundus scholarships**. The amount of these highly competitive student's grants is **1 400 euros** per month during the duration of the Master. The partners endeavour to propose regular Erasmus+ or third party financed scholarships to self-financed students.

## Scientific objectives

Chemoinformaticians are first and foremost chemists, with an experimental practice of chemistry. Therefore, this Master program combines high level training in chemistry, theoretical chemistry and chemoinformatics, computer sciences and data sciences and requires good skills in organic chemistry, physical chemistry, biochemistry, structural chemistry. The program includes lectures and tutorials in chemoinformatics, molecular modeling, quantum chemistry as well as software programming and database management. Recent developments in statistics and machine learning, specifically big data and artificial intelligence, are also addressed.

Students can choose one specialization between the following:

- In silico drug design of bioactive molecules,
- Chemoinformatics and physical chemistry,
- Chemoinformatics for biophysical & computational chemistry,
- Chemoinformatics for organic chemistry,
- Chemoinformatics and materials informatics.







## Professional objectives

Students who obtained the master are skilled in modelling, chemistry, physical chemistry, drug design and computing. They are trained as engineers and specialists with strong skills in the creation and management of databases, design of chemical and virtual screening databases, software programming, data mining and molecular modeling techniques.

## Professional competences targeted

- Creation, management and use of databases for chemistry subjects,
- Extraction, interpretation and analyse of chemical information,
- Development and validation of qualitative and quantitative chemical structure-activity relationships (QSAR/QSPR),
- Implementation of machine learning algorithms,

- Implementation and use of artificial intelligence technologies for solving chemical problems,
- Use of molecular modelling techniques and quantum chemistry to predict molecular and biological properties,
- Perform a virtual screening of chemical libraries,
- Implementation of chemical design strategies,
- Innovation, Research and Development in Chemoinformatics.

## Summer schools

The Chemoinformatics Summer School (CS3) is a central piece of the Erasmus Mundus master degree Chemoinformatics+. It offers advanced lectures from the best specialists worldwide in the field of Chemoinformatics.

The school proposes lectures in the morning and tutorials in the afternoon. It is a unique occasion to acquire new material

and get familiar with cutting-edge technologies from internationally recognized experts of the field. It is an agora of a very diverse community. As observed from past events, attendees population is typically composed of 50% students, 30% academics and 20% industrials; participants come from Japan, Switzerland, Check Republic, Hungary, England, US, Austria, Italy, Norway, Israel, Russia, Brazil, Croatia, Equator, India, the Nether-

lands, Poland, China. The participation is mandatory between the S2 and the S3.

Several specific events are satellites of the school: the molecular modelling project, a preparatory workshop dedicated to the industrial project and a hackathon dedicated to open science.

## Internship

A compulsory internship of 4 to 6 months in an industry or in a laboratory takes place in the fourth semester. It can be based in France or abroad. Nevertheless, students who stayed during the first year of the programme in their home country must do their internship abroad to fulfill mobility requirements.

Students must anticipate their research for an internship, especially as there are more administrative procedures if the student has to go abroad.

A professional from the host organisation supervises this internship. A teacher in charge is responsible for moni-



toring the internship, relations between the internship supervisor and the student and supervising the preparation of the report.

An agreement specifies all the conditions of the the internship, and must be validated by the coordinator.

## Job prospects

Jobs for the holders of the Master's degree in Chemoinformatics are mainly in the Chemical, Biotechnology and Pharmaceutical industries, including biotechnology start-ups. The outlets concern also the industrial software sector (creation and distribution of softwares for chemistry, for the management or control of processes, for scientific equipment, ect). The combination of skills that students acquire during the Master's programme ensures professional integration and

careers developments. This flexibility offers a wide and diversified spectrum of opportunities in several professional sectors. More specifically, the professions targeted in Chemoinformatics are:

- Researchers,
- Teachers,
- Application scientists,
- Software developers,
- Data scientists,
- Software quality control,
- Project manager,
- Consultant,
- Sales representatives

## Our partners

Due to actual circumstances, the track between Kiyv and Strasbourg (Ultra large chemical library design and virtual screening) is not open for application.





# Mobility scheme

The Erasmus Mundus Chemoinformatics+ Masters Course involves a minimum of two mobility periods during the two years of the programme. In total, the student must have visited at least three countries for a minimum stay of one se-

mester in each and receive a joint Master degree upon graduation.

A student may start at his/her home university; in this case, he/she will be obliged to do a mobility for his/her internship.

Each track includes summer schools and training in an academic laboratory or in the industry in the last semester.

Track	Year 1		Year 2		
	S1	S2	S3	S4	
<i>In silico drug design</i>	University Paris Cité	University degli studi di Milano	University Paris Cité	Internship	Mandatory Summer School
<i>Chemoinformatics for physical chemistry</i>	University degli studi di Milano	University degli studi di Milano	University of Strasbourg	Internship	
<i>Chemoinformatics for biophysical and computational chemistry</i>	University of Ljubljana	University of Ljubljana	University of Strasbourg	Internship	
<i>Chemoinformatics for organic chemistry</i>	University Nova de Lisboa	University Nova de Lisboa	University of Strasbourg	Internship	
<i>Chemoinformatics and material informatics</i>	Bar-Ilan University	Bar-Ilan University	University of Strasbourg	Internship	
					Optional Summer School



# In Silico Drug Design

## University of degli studi di Milano, University Paris Cité

The University of degli studi di Milano and Paris Cité provide a course in silico drug design : bioactive molecules. This 2-year Master consists of 4 semesters, one in each university with an internship during the last semester. Students obtain a French-Italian double degree with the Erasmus Mundus label upon graduation.

In Strasbourg, Milan and Paris, students will obtain strong knowledge on therapeutic targets (biological macromolecules), biochemistry and acquire advanced skills on computer modelling of target interactions with molecules. For example, in silico approaches such as biostatistics and data analysis, Python programming, structural bioinformatics, molecular dynamics, modelling, docking methods, and virtual screening are addressed.

This course trains professionals from the private and public sectors, both in France and in Europe, who are involved in research using in silico approaches in the field of therapeutic innovation and/or oriented towards the development of pharmacological molecules. It offers all the complementary skills required for the research and design process of new therapeutic molecules and the computational modelling of macromolecules and their drug partners.

## Learning outcomes

- Design new therapeutic molecules, assisted by computer,
- Solid knowledge of chemical compounds and their toxicity and of therapeutic targets (biological macromolecules), in biochemistry and physics-chemistry as well as notions of medicinal chemistry and molecular medicine,
- Advanced skills in computer modelling of chemical target-molecule interactions, modelling, in silico approaches such as biostatistics and data analysis (QSAR), programming, chemoinformatics, structural bioinformatics, molecular modelling and dynamics, molecular docking methods and virtual screening.

## Organisation of the studies

1 <sup>st</sup> Year		2 <sup>nd</sup> Year	
Semester 1	Semester 2	Semester 3	Semester 4
University of Paris Cité	University of degli studi di Milano	University Paris Cité	Internship

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# Chemoinformatics and Physical Chemistry

## University of degli studi di Milano, University of Strasbourg

The Universities of degli studi di Milano and Strasbourg provide a course in chemoinformatics and physical chemistry in English and Italian. The first year in the University of degli studi di Milano is taught in Italian (50%) and English (50%). Bibliographic references and documents are available in English. It is also possible for the students to make all exams in English. Students obtain a French-Italian double degree with the Erasmus Mundus label upon graduation.

In Milan, students will learn methods for the modelling and simulation of biomolecules, the fundamentals of chemoinformatics and databases, and the basics of physical chemistry and NMR spectroscopy. They also acquire the capacity to apply computer-aided approaches and develop software to solve complex chemical problems.

## Learning outcomes

- Understand, build and analyze quantum chemistry and molecular mechanics models,
- Use of databases in Chemistry,
- Implementation of programming workflows and computer simulation of biomolecules,
- Modelling physico-chemical processes,
- Theoretical and practical knowledge of methods for the structural characterization of compounds,
- Critically assess the experimental results of physical chemistry experiments.

## Organisation of the studies

1 <sup>st</sup> Year		2 <sup>nd</sup> Year	
Semester 1	Semester 2	Semester 3	Semester 4
University of degli studi di Milano	University of degli studi di Milano	University of Strasbourg	Internship

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## More details :





# Chemoinformatics for biophysical and computational chemistry

## University of Ljubljana, University of Strasbourg

The Universities of Ljubljana and Strasbourg offer a course in chemoinformatics for biophysical and computational chemistry. This 2-year Master consists of 4 semesters: the first year in Ljubljana and the second year in Strasbourg with an internship during the last semester. Students obtain a French-Slovenian double degree with the Erasmus Mundus label upon graduation.

In this module, students will learn about the latest developments and best practices in decision making using data and models for drug and material design. They will also learn the basics of modelling biophysical events using real-life examples. Through practice, students will learn the algorithms needed for scientific programming.

This master's degree program combines high-level training in chemistry, biophysical chemistry, and chemoinformatics. At the end of the program, students will also improve their knowledge in the field of computer science and will be able to work with big data.

## Learning outcomes

- Ability to apply knowledge, understanding, and problem-solving skills to new and unusual circumstances within broader (or multidisciplinary) areas associated with chemical sciences,
- Ability to integrate knowledge and deal with complex situations, form judgements despite incomplete information while being firmly aware of the ethical responsibilities of applying one's knowledge and judgement,
- Ability to understand and write computer software using procedural, object and programming workflow paradigms.

## Organisation of studies

1 <sup>st</sup> Year		2 <sup>nd</sup> Year	
Semester 1	Semester 2	Semester 3	Semester 4
University of Ljubljana	University of Ljubljana	University of Strasbourg	Internship

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# Chemoinformatics for organic chemistry

## University Nova of Lisbon, University of Strasbourg

The University Nova of Lisbon and the University of Strasbourg provide a course in chemoinformatics for organic chemistry. This 2-year Master consists of 4 semesters: the first year in Lisbon and the second year in Strasbourg with an internship during the last semester. Students obtain a French-Portuguese double degree with the Erasmus Mundus label upon graduation.

Organic chemistry provides essential concepts for Chemoinformatics such as molecular structure and design, reactivity, mechanisms and spectroscopy. In addition to Chemoinformatics and IT courses, Lisbon offers a program with courses in organic synthesis, bioorganic analytical chemistry, medicinal chemistry, physical organic chemistry and entrepreneurship.

It aims to train qualified professionals with specific skills in chemical analysis, characterisation and intelligent development of new drugs, rationalisation of the interaction of drugs with biological systems, design of new materials, more efficient and sustainable synthetic methodologies as well as software programming.

## Learning outcomes

- Create, manage and use databases on chemistry subjects,
- Analyse and interpret chemical information,
- Design innovative organic chemical structures,
- Design of asymmetric chemical libraries.

## Organisation of studies

1 <sup>st</sup> Year		2 <sup>nd</sup> Year	
Semester 1	Semester 2	Semester 3	Semester 4
University Nova de Lisboa	University Nova de Lisboa	University of Strasbourg	Internship

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# Chemoinformatics and material informatics

## Bar-Ilan University, University of Strasbourg

The University of Bar-Ilan and the University of Strasbourg provide a course in chemoinformatics and material informatics fully taught in English. This 2-year Master consists of 4 semesters: the first year in the University of Bar-Ilan and the second year in the University of Strasbourg with an internship during the last semester. Students obtain a French-Israeli double degree with the Erasmus Mundus label upon graduation.

At Bar-Ilan University, students will apply chemoinformatics methodologies to chemistry and materials sciences, with emphasis on renewable / green energy (e.g., solar cells). Specific attention is put on the 3D structures of molecular systems (e.g., materials) using different levels of theory (e.g., DFT calculations, force fields) and on relevant descriptors for these systems. The course expands on construction of and navigation in compounds / materials spaces, through predictive models for key properties.

## Learning outcomes

- Present clearly and unambiguously research results, conclusions and rationale underpinning these; orally or by poster presentation to specialist and non-specialist audiences,
- Design innovative new nanomaterials,
- Design innovative new materials for energy production and storage.

## Organisation of studies

1 <sup>st</sup> Year		2 <sup>nd</sup> Year	
Semester 1	Semester 2	Semester 3	Semester 4
Bar-Ilan University	Bar-Ilan University	University of Strasbourg	Internship

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## Find us

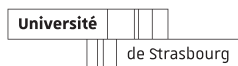
 ChemoinformaticsPlus

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## Our partners



UNIVERSITÀ  
DEGLI STUDI  
DI MILANO



University of Ljubljana



Bar-Ilan  
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## Our associate partners



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