Second-cycle studies / Master's study

CHEMISTRY - specialisation with English as a medium of instruction - DIGITAL CHEMISTRY

Course of education 2022-2024

During each semester, the student should obtain a minimum of 30 ECTS points from obligatory and optional classes (elective).

Subject	Lecture	Auditorium classes	Laboratory classes	Total	E/P	ECTS
YEAR I - SEMESTER 1						
Repetitory in mathematics		30		30	P	3
Repetitory in general and inorganic chemistry		30		30	P	3
Repetitory in organic chemistry and biochemistry		30		30	P	3
Introduction to digital chemistry	15			15	P	1
Introduction to Python programming	15		45	60	E	5
Quantum chemistry in practice	30		45	75	E	6
Exploratory analysis of multidimensional chemical space	30		45	75	E	7
Foreign language II		30		30	P	2
Total semester 1	**90**	**120**	**135**	**345**	**3**	**30**
YEAR I - SEMESTER 2						
Introduction to R programming	15		45	60	E	5
Molecular mechanics & dynamics, coarse-grain modeling	30		45	75	E	6
Specialization lecture: ** Statistical mechanics in chemistry or Molecular descriptors	30			30	P	3
Graduate laboratory **			180	180	P	12
Facultative course I: Parallel programming in Python or Data bases & big data			*30*	*30*	*P*	*2*
Facultative course II: Microcontroller-based chemical diagnostics or Omics analysis in chemoinformatics		*30*		*30*	*P*	*2*
Total semester 2	**75**	**30**	**300**	**405**	**2**	**30**
Total year I	**165**	**150**	**435**	**750**	**5**	**60**

Subject	Lecture	Auditorium classes	Laboratory classes	Total	E/P	ECTS
YEAR II - SEMESTER 3						
Machine learning in chemistry	30		45	75	E	6
Interpersonal communication	15			15	P	1
The activities of the company in contemporary environment	30			30	P	2
MSc laboratory course **			180	180	P	10
MSc seminar **		30		30	P	4
Monographic lecture: ** Modern quantum chemistry in use or Machine learning algorithms for small datasets	30			30	P	3
Facultative course III: Insights into reaction mechanisms and kinetics via quantum chemistry methods or QSAR in toxicology			*30*	*30*	*P*	*2*
Facultative course IV: Statistical mechanics of biological macromolecules or Advanced nanoinformatics		*30*		*30*	*P*	*2*
Total semester 3	**105**	**60**	**255**	**420**	**1**	**30**
YEAR II - SEMESTER 4						
Economic activity law	30			30	P	2
MSc laboratory course **			190	190	P	10
MSc seminar **		30		30	P	4
Monographic lecture: ** Electronic structure of molecular anions or Computational nanomedicine and nanotoxicology	30			30	P	3
Facultative course V: Numerical methods with algorithms for physical sciences or Computationally Added Drug Design			*30*	*30*	*P*	*2*
Facultative course VI: Chemical bonding via quantum chemistry tools or Computational methods for designing advanced materials		*30*		*30*	*P*	*2*
MSc exam					E	*7*
Total semester 4	**60**	**60**	**220**	**340**	**1**	**30**
Total year II	**165**	**120**	**475**	**760**	**2**	**60**

Colours refer to two blocks of methods: (i) physics-based methods and (ii) data-based (chemoinformatics) methods

E – exam; P – pass with note; **classes conducted at the Department, where the student is doing his master's thesis

Second-cycle studies end with master's examination and obtaining the professional title of master's degree.