UNIVERSITY OF ZAGREB
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY

Horvatovac 102a, Croatia, 10 000 Zagreb
Telephone: 385-1-460-6032
E-mail: doktorski_studij@chem.pmf.hr

Postgraduate University Programme: Chemistry

Area of Natural Sciences
Field of Chemistry

INSTRUCTIONS – REGULATIONS - PROGRAMME AND COURSE REQUIREMENTS
Academic year 2017/18

Zagreb, 2017

Chemistry

General information

Name of the study programme	Postgraduate University Programme: Chemistry
Study programme coordinator	Faculty of Science
Scientific or artistic field	Natural sciences
Scientific or artistic area	Chemistry

Requirements for admission to the doctoral study programme

The requirement for enrolment in doctoral study is completion of graduate studies with a master's degree in the field of chemistry or in some related study programs. Doctoral studies in chemistry can be taken by graduates in chemistry of the Department of Chemistry¸ Faculty of Science, or other related faculties of the University in Zagreb (Faculty of Chemical Engineering and Technology, Faculty of Food Technology and Biotechnology, Faculty of Chemistry and Biochemistry), graduates in molecular biology (Department of Biology, Faculty of Science), as well as graduates of two-subject educational studies if one of the subjects is chemistry. Graduates with equivalent degrees from other universities can also enrol as well as those with MSc degrees in chemistry. In principle, depending on the specialty and topic of the dissertation, additional courses can be assigned covering the differences in programmes.

Description of the doctoral study programme structure

The Doctoral Programme lasts for minimum 3 years with the average workload of 60 ECTS credits per year (180 credits in total). For obtaining the PhD title, the courses worth total 36 credits must be passed, while the research, valuated also with the methodologies outside the ECTS system, provides 110 credits. Obligatory activities comprise *Chemistry Seminar I* (8 ECTS-points), *Chemistry Seminar II* (8 ECTS-points), and participation in two generic/transferable skills workshops of eight-hour duration (8 ECTS-points) organised by Department of Chemistry (workshop author and trainer Zrinka Banić Tomišić, PhD):
1. *Knowledge and Intellectual Property Management, Technology Transfer and Innovation*, 4 ECTS-points
2. *Communication Skills*, 4 ECTS-points.

Participation in elective activities (attendance at public scientific lectures and colloquia in science, active participation in scientific conferences, attendance at scientific schools and workshops) provides the doctoral candidate with extra 10 ECTS credits. Elective activities are as follows:
• Participation at the scientific meetings (poster presentation: 2 ECTS-points, oral communication: 4 ECTS-points or 2 points for the co-author), scientific schools and workshops; total of 10 ECTS-points
• Attendance at public lectures and colloquia in the field of natural sciences.

The teaching is generally elective. The courses are classified in three categories: general, basic and specific courses. The compulsory courses for students of all specialties are: Chemistry Seminar I, Chemistry Seminar II, and Research activity. The basic courses cover the main disciplines within the specialties, and are supplemented with the specific courses. Each basic course provides 8 ECTS credits and each specific course provides 5 ECTS credits.

The total number of the taken basic courses may not be less than 2. The final (doctoral) thesis is the integral and the most significant element of the Programme.

Chemistry Seminar I is a presentation of a current scientific topic in or out of the field of the candidate's doctoral thesis and is defined in the 1st year of the Programme in agreement with the head of the specialty field. Chemistry Seminar II is a reasoned presentation of the thesis project and should be held in the 2nd year of the Programme. Presentation of the Chemistry Seminar I and Chemistry Seminar II earns 8 ECTS credits each. Also, the student's obligations in these courses include attendance at the seminars held by other doctoral candidates, as a requirement for obtaining the teacher's signature in witness of the completion.

Requirements for students' advancement to subsequent study years

First year enrolment: Two basic courses and one elected are taken in agreement with the specialty leader according to the Curriculum. At the very beginning of studies, before a supervisor is confirmed by the Department of Chemistry Council, Scientific Field Council and University of Zagreb, the supervisor's role is performed by a temporary study advisor appointed by the specialty leader. It is recommendable to sign up for doctoral courses also in other specialties and in related scientific fields (e.g., physics, biology, etc.) in interdisciplinary reserach. Specialty leader is entered as supervisor for *Chemistry Seminar I*, and after being appointed, supervisor for *Research Work* and *Chemistry Seminar II*. Changes of courses for which students have signed in are approved by the Doctoral Studies Council on an argumented request.

First year registration: Completion of courses and tutorials must be certified by the instructor's first and second signatures.

Second year enrolment: Doctoral students should write a small report on their previous work; the study advisor also submits a report on the student's achievement (special University forms). All reports are handed in to the specialty leader, who then gives guidelines for the subsequent course of studies and by his signature approves enrolment in the second year. In principle, three elected courses should be taken in the second year. It is mandatory to retake *Research Work* and *Chemistry Seminar II.* The condition for second year enrolment is a successful presentation within *Chemistry Seminar I* (8 points) and passed basic course examinations affording 16 points (24 ECTS points in all).

Second year registration: Courses completed for a total of 15 ECTS points and successfully done *Chemistry Seminar II*. *Chemistry Seminar II* involves oral defence of the announced doctoral dissertation topic, accompanied by its written argumentation.

Third year enrolment: Conditions: completed courses (first and second years) for a total of 36 ECTS points, and successfully done *Chemistry Seminars I* and *II* (8 points each, 52 in all). Students have to write a second report on their work and also the supervisor submits a report on the student's achievement (special University forms: dr.sc.04 and dr.sc.05.). All reports are handed in to the specialty leader, who then gives guidelines for the subsequent course of studies and by his signature approves enrolment. It is mandatory to retake *Research Work*.

Third year registration: All courses completed.

Enrolment in final doctoral study years: Doctoral students can enrol two final doctoral study years after the third year has been registered (but no more than 5 years in total). When enrolling into final years, students have to write a report on their work and also the supervisor submits a report on the student's achievement (special University forms: dr.sc.04 and dr.sc.05.).

Requirements for approval of the doctoral dissertation theme

By the end of the second study year, students should start the procedure of doctoral dissertation theme registration and supervisor appointment, and announce the date of *Chemistry Seminar* II. The Doctoral Study Council proposes a committee for theme acceptance to the Department of Chemistry Council. Students registering the dissertation theme must have passed examinations affording a total of at least 16 ECTS points as well as successfully done *Chemistry Seminar I* (additional 8 points, thus 24 points in all). After the committee for theme acceptance has been appointed, students have to present *Chemistry Seminar II*. Based on the Committee's opinion on the proposed theme and the held seminar, the Doctoral Studies Council proposes theme evaluation and supervisor appointment to the Department of Chemistry Council, which has to be approved by the Natural Science Council and the University Senate. It is the competence of the Theme Acceptance Committee to additionally evaluate the overall achievement of the doctoral candidate.

Conditions for study programme completion

The end of the study course begins with starting the procedure of the dissertation evaluation. Conditions for dissertation evaluation procedure include the passing of all examinations and fulfilling other curriculum requirements, elective activities and research work in a total amount of 180 ECTS points, as well as (co)authorship in a research paper in the field of dissertation theme, published or accepted for publication in a scientific journal registered within *Web of Science*.

Doctoral dissertation must contain an original scientific contribution, and should also prove the student's familiarity with current scientific literature in the field of the dissertation theme, his/her knowledge of theoretical tenets of the methods applied in the dissertation and, finally, his/her abilities to formulate his/her ideas, results and knowledge into a coherent and readable text. It is expected that the doctoral dissertation will give rise to at least three papers in scientific journals.

The submitted final thesis is evaluated by a committee of 3 or 5 members appointed by the Department of Chemistry Council on proposal of the Doctoral Study Council. Committee members can be university teachers and researchers in the ranks of assistant professor or research associates, or higher, working in the scientific field of the thesis. Upon acceptance of a favourable report on the submitted dissertation, the Faculty Council, on proposal of the Department of Chemistry Council, appoints a dissertation defence committee, applying the above criteria. For dissertation defence, at least one substitute member has to be appointed as well.

Since no comprehensive final examination is foreseen by the program of studies, during the dissertation defence examiners ask questions relating to the results and conclusions of the

thesis, as well as questions checking the student's knowledge of the wider field to which the thesis belongs.

The list of compulsory and optional courses with the number of teaching hours required for their fulfillment and the respective ETCS credit points (L – lectures; s/e – seminars/exercises; P – *ECTS* points)

A.General subjects (compulsory for all courses of lectures)			P
152786	(Field Coordinator)	Chemistry Seminar I	8
152787	(Field Coordinator)	Chemistry Seminar II	8
152986		Research Work*	110

* research work is mandatory in all three years of study

Major Field: INORGANIC AND STRUCTURAL CHEMISTRY (ASK)

B. Basic courses (2 are required)			L	s/e	P
152789	M. Cindrić, V. Vrdoljak	Synthesis, Identification and Application of Inorganic Compounds	20	10	8
152791	D. Matković-Čalogović, I. Đilović	X-Ray Structure Analysis	20	10	8
152792	E. Meštrović D. Cinčić	Solid State Chemistry of Drugs	20	10	8
152793	Ž. Skoko, I. Halasz	Diffraction in Polycrystalline Materials	20	10	8

C.Specific courses (elective)			L	s/e	P
152788	M. Cindrić	Kinetics and Reaction Mechanisms of Transition Metal Complexes	15	0	5
152790	M. Luić, V. Bermanec	Crystalography	20	0	5
152794	B. Prugovečki	Experimental Methods in Crystal Structure Analysis	15	5	5
152795	A. Moguš-Milanković	Investigation and Application of Inorganic Materials	15	0	5
152797	A. M. Tonejc, Ž. Skoko	Electronic Diffraction and Microscopy	15	5	5
152799	D. Matković-Čalogović	Selected Chapters of Bioinorganic Chemistry	15	5	5
152800	K. Molčanov, V. Stilinović	Selected Topics of Crystal Structure Analysis	20	0	5
152801	Z. Štefanić V. Stilinović	Group Theory in Crystalography	15	0	5
152802	D. Matković-Čalogović	Selected Topics in Inorganic and Structural Chemistry	15	0	5

Major Field: ORGANIC CHEMISTRY (OK)

B. Basic courses (2 are required))			**L**	**s/e**	**P**
152803	M. Žinić, L. Frkanec	Organic Stereochemistry	21	4	8
152804	S. Tomić-Pisarović, I. Primožič	Stereoselective Synthesis and Catalysis in Organic Chemistry	25	0	8
152805	K. Majerski, M. Šekutor	Methods in Organic Synthesis	25	0	8
152806	H. Vančik	Reaction Mechanisms in Organic Chemistry	25	0	8

C. Specific courses (elective)			**L**	**s/e**	**P**
152807	N. Basarić	Organic Photochemistry	15	0	5
152808	K. Majerski N. Basarić	Reactive Intermediates in Organic Chemistry	15	0	5
152809	S. Tomić-Pisarović	The Chemistry of Carbohydrates and Glycoproteins	15	0	5
152810	M. Žinić, L. Frkanec V. Tomišić	Supramolecular Chemistry	15	2	5
152812	Z. Mihalić	Computational Chemistry	15	0	5
152814	B. Žinić V. Petrović Peroković	Nucleosides and Nucleic Acids	15	0	5
152816	D. Vikić-Topić I. Biljan	Application of NMR Spectroscopy for Structure Determination of (Bio) organic Compounds	15	0	5
152818	S. Tomić-Pisarović	Biotransformations in Organic Chemistry	15	0	5
152819	I. Primožič	Modern Methods of Heterocyclic Synthesis	15	0	5
152820	I. Jerić V. Petrović Peroković	Structure, Function and Synthesis of Peptides/Proteins and their Conjugates	15	0	5
152821	I. Primožič, S. Raić-Malić	Development of the Most Effective Drugs	15	0	5
152822	V. Gabelica Marković	Analytical Methods in Organic Synthesis	15	0	5
152823	I. Primožič	Selected Topics in Organic Chemistry	15	0	5

Major Field: BIOCHEMISTRY (BK)

B. Basic courses (2 are required)			**L**	**s/e**	**P**
152828	B. Bertoša	Bioenergetics	20	0	8
152829	I. Gruić Sovulj, J. Rokov Plavec	Control Mechanisms of Protein Biosynthesis	20	5	8
152831	I. Gruić Sovulj, Z. Kovarik, Z. Radić	Enzymes: Kinetics and Reaction Mechanisms	20	0	8
152832	T. Žanić-Grubišić M. Dulić	Structure and Function of Plasma Membrane and Cell Wall	20	0	8

C. Specific Courses (elective)			**L**	**s/e**	**P**
152827	S. Barbarić, Đ. Ugarković J. Rokov Plavec	Regulation of Gene Expression, Post-translational Modifications and Protein Transport in the Cell	15	0	5
152833	M. Luić	Macromolecular Crystalography	10	5	5
152834	V. Mrša	Glycoproteins – Structure and Function	10	5	5
152835	R. Frkanec	Biotransformation of Drugs and Xenobiotics	15	0	5
152836	S. Frank	Biochemistry and Pathobiochemistry of Lipids and Lipoproteins	10	5	5
152837	R. Frkanec	Immunochemistry and Immunochemical methods	10	5	5
152838	S. Tomić	Modelling of Biomacromolecules: Structure, Complexes, Interactions	10	5	5
173225	M. Močibob	Methods of Protein Biochemistry	15	5	5
152839	M. Močibob	Selected Topics in Biochemistry	15	0	5

* The enrollment of courses in other fields is recommended, for example, the field of biology, module – molecular and cellular biology. In this case, the basic courses in other fields and departments are evaluated as basic courses in the Biochemistry department. The same applies for specific/optional courses

Major Field: PHYSICAL CHEMISTRY (FK)

B. Basic courses (2 are required)			**L**	**s/e**	**P**
152845	I. Ljubić T. Hrenar	Selected Topics in Quantum Chemistry	25	0	8
152846	T. Hrenar	Molecular Spectroscopy	25	0	8
152847	V. Tomišić G. Horvat, J. Požar	Statistical Thermodynamics and Irreversible Processes	20	5	8
152848		Chemical Kinetics	20	5	8

C. Specific courses (elective)			**L**	**s/e**	**P**
152844	V. Tomišić, T. Hrenar	Chemometrics	15	5	5
152849	M. Metikoš-Huković	Selected Topics in Electrochemistry	15	5	5
152850	T. Preočanin, S. Musić	Selected Topics in Interfacial and Colloid Chemistry	15	0	5
152851	B. Mihaljević	Radiation Chemistry	12	0	5
152852	D. Kralj	Equilibrium and Kinetics of Processes in Heterogeneous systems	10	2	5
152853	N. Trinajstić	Mathematical Chemistry	12	0	5
152855	M. Kralj	Nanotechnologies	15	0	5
152856	D. Kovačević	Physical Chemistry of Macromolecules	15	0	5
152857	T. Hrenar, N. Došlić	Theoretical Chemistry and Reaction Dynamics	15	0	5
152858	D. Kovačević	Selected Topics in Physical Chemistry	15	0	5

Major Field: ANALYTICAL CHEMISTRY (AK)

B Basic courses (2 are required)			**L**	**s/e**	**P**
152859	S. Rončević	Atomic Spectrometry in Analytics	20	10	8
152860	I. Ciglenečki Jušić	Electroanalytical Methods	20	10	8
152861	V. Drevenkar, M. Cindrić, N. Galić	Chromatographic Methods in Analytics	20	10	8
152863	P. Novak, K. Zangger, T. Hrenar, S. Kazazić	Modern Molecular Spectroscopy	25	5	8

C. Specific courses (elective)			**L**	**s/e**	**P**
152862	M. Ahel, S. Terzić	Analysis of Organic Contaminants	15	5	5
152864	P. Novak, N. Müller, V. Smrečki, J. Plavec, J. Parlov Vuković	Modern Methods of Structural NMR	20	0	5
152865	B. Gašparović, D. Omanović	Environmental Electrochemistry	10	5	5
152866	Z. Dragun I. Juranović Cindrić	Quality Control of Analytical Procedures	10	0	5
168988	S. Miljanić	Surface-Enhanced Vibrational Spectroscopy	10	0	5
152867	P. Novak	Selected Topics in Analytical Chemistry	20	0	5

Detailed list of courses

152788	Kinetics and reaction mechanisms of transition metal complexes
number of instruction hours	15
outline of course/module content	The determination of the rate law. The rate of a reaction and the rate law. Integrated forms of the rate expression. Monophasic unidirectional reactions. Monophasic reversible reactions. Multiphasic unidirectional reactions. Relaxation kinetics. Exchange kinetics. Inclusion of $[H^+]$ terms in the rate law. The deduction of mechanism. The rate law and mechanism. Activation parameters, thermodynamic functions and mechanism. Linear free-energy relationships. The relationship between the activation entalphy, entropy, and volume with mechanism. Medium effects on the rate. The experimental determination of the rate of reaction. Flow and relaxation methods. Large perturbation. Competition methods. Accessible rate constants using rapid reaction methods. Spectrophotometry. Non-spectrophotometric methods. Batch methods. The study of transients. The characteristics of substitution reactions. Substitution in octahedral complexes. Accelerated substitution of unidentate ligands. Replacement reactions involving multidentate ligands. Substitution in square-planar complexes. Substitution in tetrahedral complexes. Substitution in five-coordinate complexes. Substitution in organized surfactant systems. Substitution in metalloproteins. Oxidation-reduction reactions. Outer sphere reactions. Inner sphere redox reactions. Bridging ligand in inner-sphere redox reactions. Intramolecular electron transfer. Electron transfer in proteins. The modification of ligand reactivity by complex formation. The metal as a collecting point reactant. Promotion of reaction within the metal-bound ligand. Hydrolysis of coordinated ligands. Electrophilic substitution in metal complexes. Masking effects. Disturbance of reaction stoichiometry. Molecular strain alterations. Function of the ligand. Isomerism and stereochemical change. Conformational and configurational Isomerism. Spin equilibria in octahedral complexes. Linkage, geometrical, and optical isomerism. Octahedral, tetra-penta, hepta and octacoordinated complexes. Inversion and proton exchange at asymmetric nitrogen. Inorganic photochemistry. Kinetic factors affecting quantum yields. Photochemistry of Co^{III}, Rh^{III} and Cr^{III}. Polypiperidine complexes of Ru^{II}. Organometallic photochemistry. Photochemical generation of reaction intermediates. Organometallic substitution reactions. Ligand bonding. Metal carbonyl substitution reactions. Dissociation of other ligands. Ligand effects. Complexes with 17 electrons. Substitution on metal carbonyl complexes containing M−M bonds. Ligand substitution reactions on alkyl complexes. Hydride complexes. Nitrosyl, allyl, and other complexes. Homogeneous catalysis by transition metal complexes. Homogeneous hydrogenation of alkanes. Assymetric hydrogenation. Hydroformylation reaction. Wacker acetaldehyde synthesis. Hydrocyanation of 1,3-butadiene. Olephin methatesis. Polymerization of alkenes. Methanol carbonylation.
description of instruction methods	Lectures and seminars.
description of	Lectures, seminars, and consultations.

course/module requirements	
152789	**Synthesis, identification and application of inorganic compounds**
number of instruction hours	20 + 10
outline of course/module content	Introduction to synthetic methods and reactions in inorganic chemistry *e.g.* adition and substitution and oxido-reduction reactions, reactions of thermal disociation and in inert atmosphere, reactions of ligand substitution (*trans* effect) *etc.* Modern synthetic methods in synthesis of coordination compounds and polyoxometalates: reactions in solid state-grinding, in solution (organic solvents or water), hydrothermal synthesis; electrolytic oxidation. Isolation of inorganic compounds: chromatographic methods, vakuum sublimation, extraction and electrochemical crystalization. Methods of characterization: standard analytical and spectroscopic methods (IR, Raman, UV, NMR, EPR) X-ray diffraction methods etc. Applicationa of inorganic compounds: complexes as biological or industrial catalysts, clusters and polyoxometalates in catalytic reactions.
description of instruction methods	Lectures, seminars and consultations
description of course/module requirements	Presentation of current research in the field of synthesis and application or development of a new methods of identification inorganic compounds
152790	**Crystallography**
number of instruction hours	20
outline of course/module content	Basic characteristics of crystalline state - periodic crystals. Congruence and enantiomorphology. Symmetry elements: inversion centre, symmetry axes (axes of rotational symmetry, axes of rototranslation or screw axes, axes of inversion, axes of rotoreflection), reflection planes (glide planes). Crystal lattices - primitive and centred. Rational properties of lattices, crystallographic directions and planes (Miller indices), symmetry restrictions due to the lattice periodicity and vice versa. Point groups. The Neumann principle. The Laue classes. Crystal systems. The Bravais lattices (2D and 3D). Space groups (description and derivation of a few in accordance with the International tables for crystallography). Crystal morphology - crystal forms. The space group matrices. Crystal optics. The law of reflection and the law of refraction. Birefringence. Optically isotropic and anisotropic substances. Optical indicatrixes. Uniaxial and biaxial crystals. Polarizing microscope.
description of instruction methods	lectures, consultations, seminars,
description of course/module requirements	permanent evaluation, exams, seminars
152791	**X-ray structure analysis**
number of instruction hours	20 + 10
outline of course/module content	Diffraction intensities and new X-ray sources; symmetry of diffraction image and space group determination; calculation of structure factor amplitudes – data reduction: errors of intensity measurements,

	polarisation and Lorentz factors, temperature parameters, intensity corrections due to sample deterioration, absorption; Fourier transformations in crystallography: theory, algorithms and application; structure factors and structure factor amplitudes; intensities and distribution functions for centrosymmetric and noncentrosymmetric crystals; Wilson statistics – calculation of temperature factor and absolute scale of intensities; the unitary and normalised structure factors, the reciprocal space in structure analysis; procedures for structure factor phase determination – direct methods based on algebraic methods and probability functions; vector methods for phasing – Patterson function: Harker lines and planes; isomorphous replacement – single (SIR) and multiple (MIR), Rossmann's method, translation and rotation functions; anomalous dispersion – phasing and absolute configuration and conformation determination; Fourier synthesis, electron-density maps and molecular structure determination; structure refinement: least-squares method – stereochemical constraints and molecular dynamics; Fourier analysis – modified electron-density maps: use of square function, nonlinear functions for improving resolution (solvent flattening, molecular averaging); numerical and graphical procedures for visualisation of molecular and crystal structures, calculation of molecular geometry, evaluation and interpretation of the structure, crystallographic databases, molecular graphics.
description of instruction methods	Lectures, seminars
description of course/module requirements	Written or oral examination or seminar work.
152792	**Solid state chemistry of drugs**
number of instruction hours	20 + 10
outline of course/module content	Introduction to solid state chemistry of drug. Importance of crystal structures in the research, development, production and application of active substances. Crystal growth and crystallization processes, the shape and size of the particles. Polymorphic form, solvates and hydrates and amorphous state. Hydrogen bonds and other no covalent interactions. Use of none no covalent interaction in the creation of new materials to improve the properties. Methods for the analysis of solids. Physical and chemical transformations. Phase diagrams of multicomponents systems. Interactions in multiphase systems. Compatibility and incompatibility of substances in mixtures. Intellectual property in the field of chemistry and pharmacy, and related fields
description of instruction methods	Lectures, seminars and exercises
description of course/module requirements	Oral and written exam, project-based work
152793	**Diffraction in polycrystalline material**
number of instruction hours	20 + 10
outline of course/module content	Scattering of X-rays by a free electron. Polarization. Scattering by several electrons and by atom. Crystal and reciprocal lattices. Diffraction by a small

	crystal. Laue equations. Structure factor for a Bragg diffraction maximum. Effect of temperature vibration on diffraction pattern. Integrated intensity for a small crystal and for a crystalline powder-polycrystal. Diffraction by a crystalline powder. Diffractometer recording of diffraction pattern and collecting of diffraction data. Instruments for high and low temperature, high pressure and controlled atmosphere. New trends in development of diffraction instruments. Synchrotron radiation. Diffraction of electrons and neutrons by a crystalline powder. Analysis of systematic and random errors in measurement of diffraction maximum position. Identification of a crystalline material, qualitative and quantitative phase analysis. Accurate measurement of unit-cell parameters. Study of order-disorder in a crystal lattice. Diffraction by a defect crystal. Broadening of diffraction maxima. Determination of pure diffraction profile. Selection of mathematical functions describing a diffraction profile. Crystallite size and lattice imperfections (strains). Faults in sequence of crystal-lattice plains. Study of solid solutions, phase transitions and phase diagrams. New methods in indexing of diffraction pattern of a polycrystal and solution of crystal structure. Strategies for structure solution from powder diffraction data. The original Rietveld method for structure refinement using the whole diffraction pattern of a polycrystal/powder and its further development. Scattering of X-rays in an amorphous material. Radial distribution function. Study of metallic glasses.
description of instruction methods	lectures, laboratory practice, consultations, seminars
description of course/module requirements	written or oral examination or seminar work
152794	**Experimental methods in crystal structure analysis**
number of instruction hours	15 + 5
outline of course/module content	Origins of X-rays; classical X-ray sources; synchrotron radiation. Effects of X-rays passing through solid material: X-ray diffraction, absorption, fluorescence, Compton effect; applications. Neutron diffraction, electron diffraction; comparison with X-ray diffraction. X-ray devices for examination of structural properties of materials. Geometry and construction of devices for X-ray diffraction; application of classical and modern X-ray devices in structural studies. Photographic techniques; types of cameras, crystal rotation and oscillation practice, identification of diffraction maxima. Diffractometer techniques. Detection and recording of X-rays. X-ray detectors and counters; classical and advanced detectors. Crystallization techniques. Selection of single-crystal sample for diffraction examination. Work with unstable materials. Analysis and interpretation of X-ray diffraction data from single crystal; precision and accuracy in determination of unit-cell parameters, symmetry and crystal structure. Strategies for structure solution from polycrystalline samples. Powder-pattern-fitting methods in crystal structure examination: individual profile fitting method, whole-powder-pattern decomposition method, Rietveld method; precision and accuracy. Structural analysis of amorphous materials; radial distribution function. X-ray scattering in amorphous material, EDXD method, EXAFS method. Radiation protection and security measures. Dosimetry.

description of instruction methods	lectures, laboratory practice, consultations, seminars
description of course/module requirements	written or oral examination or seminar work
152795	**Investigation and application of inorganic materials**
number of instruction hours	15
outline of course/module content	Ceramics: Preparation techniques, classes of ceramics, properties and applications. Dielectrics, pyroelectrics, piezoelectrics, ferroelectrics, electrical properties, electrical conductivity, dielectric properties, polarization of dielectrics and ferroelectrics, methods for investigation of phase transitions and electrical properties of ceramics. Electro-optical properties of ceramics and applications. Doping of ceramics, changes of structure and properties. Semiconductors: crystalline and amorphous semiconductors. Properties, electronic conduction, photoconduction. Hydrogenation and doping of semiconductors. Formation of defects in structure and changes of properties. Application of semiconductors in electronics and solar cells technology. Glasses: Principles of glass formation, nucleation/crystal growth. Composition–structure relationship. Glass microstructure, phase separation. Types of glasses, preparation techniques. Properties: optical, electrical, dielectric. Dependence of electrical conductivity on composition and temperature, electronic and ionic conductivity. Mechanical properties. Determination of size of crystals in glass matrix, changes of properties. Bioactive, radioactive glasses. Application in electronics, medicine, diagnostics and nuclear technology. Glass-ceramics: Preparation techniques. Glass-ceramics crystallization. Properties, thermal expansion, transparency, mechanical tension. Application in medicine and dental industry. Composites: Preparation techniques. Glass-polymer composites. Dependence of optical and mechanical properties on glass composition and types and concentration of polymers. Bioactive and biodegradable composites. Application in dentistry and medicine.
description of instruction methods	lectures, discussions, consultations, seminars
description of course/module requirements	Oral or written or seminar
152797	**Electron diffraction and microscopy**
number of instruction hours	15 + 5
outline of course/module content	Fundamentals of electron microscopy. Application of electron microscopy and electron diffraction in materials science, chemistry and geology. The modern methods of examination of materials in an electron microscope: Scanning electron microscope (SEM), SEM for enviromental examination (ESEM), of materials by energy dispersive X-ray analyses (X-ray mapping), Transmission electron microscopy and selected area electron diffraction (TEM and SAED), High resolution electron microscopy (HRTEM),

	Convergent beam electron diffraction (CBED). The interpretation of the TEM images and diffraction of the polycrystalline, monocrystalline and amorphous samples. The diffraction contrast. The defects characterisation in the material. Characterisation of stacking faults, tweens and antiphase boundaries using bright and dark field images. The phase contrast. The high resolution imaging. Observation of different type of defects in high resolution mode (HRTEM) and Z-contrast imaging with the resolution beyond 0.1 nm. The crystallographic image processing of high resolution images in order to determine the lattice deformation, dislocations, the lattice parameter , stacking faults, grain and phase boundaries. The structural resolution from 0.2 to 0.1 nm. The latest discoveries in electron microscopy will be given: observation of oxigen positions and bonds in cuprite; atomic–scale imaging of individual dopant atoms and clusters in silicon. The structure factor determination from HRTEM images and electron diffraction (ED). The application of Rietveld method to the images of nanocrystalline materials. The grain size, microstrain and unit cell parameters of nanocrystalline samples. The comparison of ED, X-ray and neutron diffraction. Exercises: Practical work in EM laboratory; the evaluation of TEM, HRTEM and ED images. The practical presentation of the methods working in the JEOL 200 kV EM. The HRTEM image processing analyses of some images and ED.
description of instruction methods	lectures, seminars
description of course/module requirements	Course attendance is controlled. The students receive the topics for written seminars and oral presentation. The results of the seminars will be included into the final note. The students will be given practical work in EM laboratory: the preparation of the samples for EM observation and practical review of the methods of high resolution microscopy will be given.
152799	**Selected chapters in bioinorganic chemistry**
number of instruction hours	15 + 5
outline of course/module content	Role of metal ions in biological systems. Metalloproteins. Analysis of structure and properties. Exchange of metal ions in insulin. Some methods of analysis of the coordination sphere environment: X-ray diffraction analysis, X-ray absorption spectroscopy (XAS, EXAFS). Data bases.
description of instruction methods	Lectures, seminars
description of course/module requirements	Written or oral examination or seminar work.
152800	**Selected topics of crystal structure analysis**
number of instruction hours	20
outline of course/module content	Interpretation of molecular and crystal structure using X-ray data-accuracy of the structure: analysis of experimental and systematic errors; the effect of atomic thermal vibrations and advantage of low temperature

	measurements of diffraction intensities; comparative advantages of X-ray, neutron and electronic diffractions in structure determination; chirality in crystallography and absolute configuration, application of stereochemical rules in molecular conformation and absolute configuration; significance of Ramachandran plots for determination conformations of peptides and proteins; molecular packing in the crystal- the analysis of intermolecular interactions-noncovalent interactions defining crystal packing, supramolecular assembling and nanomaterials: hydrogen bonds, C-H...pi, pi...pi interactions, van der Waals and Coulomb forces; correlation of molecular and crystal structures with chemical, physical and biological properties of the molecules; molecular modelling –the goal and methods; use of databases – access to data, selectivity and critical evaluation of information, the analysis of data, interpretation of data and correlation of experimental and theoretical values.
description of instruction methods	lectures, tutorials, and seminars
description of course/module requirements	permanent evaluation, exams, seminars
152801	**Group theory in crystallography**
number of instruction hours	15
outline of course/module content	Introduction to matrix algebra: operations with matrices, determinants, inversion and eigenvalues of a matrix; linear transformations, rotations; scalar and vector product. Fundamental group theory: group axioms, generators, subgroups; group decomposition, direct product of groups; irreducible representations, character tables; examples of symmetry groups. Crystallographic groups: point groups, plane groups, space groups; examples of the common groups and symmetry operations. Matrix representation of crystallographic transformations: coordinate transformations; keeping the right-handed coordinate system in transformations; conventions for standard and non-standard settings for space groups. Symmetry and physical properties of crystals: tensors of the second rank; elastic properties of crystals, piezoelectricity; group theory in connection with physical properties of crystals; Brillouin's zones, wave vectors, thermal properties of crystals. Thermal vibrations of crystals: vibrations of crystal lattice; molecular vibrations, normal modes of vibration; atomic thermal parameters; representation of anisotropic vibrations as thermal ellipsoids (ORTEP plots); symmetry constrains on thermal parameters. T,L,S matrices; correction of bond lengths due to thermal motion; Hirshfeld's model.
description of instruction methods	lectures, seminars, on-line lectures
description of course/module requirements	lectures, seminars, consultations
152802	**Selected topics in inorganic and structural chemistry**
number of instruction hours	15
outline of course/module content	Various topics of modern inorganic and structural chemistry, visiting scholar

description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and/or written exam
152803	**Organic Stereochemistry**
number of instruction hours	21 + 4
outline of course/module content	Historical introduction. Configuration and chirality, molecular geometry, molecular symmetry. Molecular models. Symmetry in organic chemistry. Stereoisomerism and chirality. Constitution, configuration, conformation. Molecular symmetry. Classification of molecules by their symmetry, the Schönfliess point group notation, symmetry elements, symmetry operations, point groups. Cahn-Ingold-Prelog conventions, types of chirality: chiral centre, chiral axe, chiral plane, helices. Molecules containing more than one centre of symmetry. Absolute and relative configuration, the experimental determination of the relative and absolute configuration. Principles relating to the separation of enantiomers. Optical activity, experimental methods for determination of configuration, chiro-optical methods: circular dichroism (CD) and optical rotatory dispersion (ORD). Octant rule. Determination of configuration by NMR: anisotropic effects, coupling constants, chiral shift reagents, NOE effects. Conformation of carbon compounds. Intramolecular symmetry: homotopicity, heterotopicity, enantiotopic and diasterotopic groups and faces. Stereoisomerism in cyclic molecules, cycloenantiomery and cyclodiastereomery. Applied stereochemistry. Chirality of supramolecular systems. Training on molecular models such as Dreiding and CPK (Corey, Pauling and Koltun) and on graphical workstation on computer generated models.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152804	**Stereoselective Synthesis and Catalysis in Organic Chemistry**
number of instruction hours	25
outline of course/module content	Introductory will be considered all basic stereochemical terms and concepts, as e.g. elements of conformational analysis and dynamic stereochemistry, indispensable for understanding stereoselective transformations in organic chemistry. Stereochemical terms (chirality, stereogenic center, prochirality, enantiotopy and diastereotopy of faces and ligands) will be explained and exemplified. Symmetry elements present in achiral, prochiral and chiral molecules will be indicated. The importance of kinetic control (diastereoselective transition states) of enantioselective and diastereoselective reactions vs. thermodynamic control will be emphesized. Diastereoselective reactions will be discussed on the classic examples of synthesis of enantiomerically enriched amino acids (Northrop, Vigneron), and on the Weinges synthesis of Me-DOPA. Mayers and Enders approach to the C-C bond-forming reactions using chiral auxiliaries (4,5-disubstituted 1,3-oxazolines; SAMP and RAMP)

	derived from the available building blocks will be elaborated. An example of chiral Mannich reaction based on L-proline-derived Mannich base will be given. Progress in the field of total syntheses of natural product, which usually consist of consecutive set of diastereoselective transformations starting from the «chiral pool», will be demonstrated by the classic Confalone synthesis of (+)-biotine, and recent process to the same product scaled-up by Novartis. Enantioselective catalytic reactions, formerly known as asymmetric syntheses, are devided according to the nature of the catalyst to organometallic, organocatalytic, and biocatalytic, i.e. enzyme catalyzed transformations. They represent unique set of synthetic methodologies to enantiomerically pure compounds (EPC). From a broad range of reactions catalyzed by the chiral organometallic complexes (D.1.) are selected hydrogenation of the C=C bond, cyclopropanation of C=C bond, and allylic alkylation. An overview of asymmetric organocatalysis will be supported by some recent examples. Some results of inspiring work of K.A. Jorgensen in this field (enantioselective Friedel-Crafts reaction, enantioselective Diels-Alder reaction with inverse electron demand) will be discussed as a separate chapter of oganocatalysis. Consideration of biocatalytic processes will include enzyme catalyzed kinetic and dinamic kinetic resolution, both catalyzed by lipases. Specific case of desymmetrization of meso-compounds will be exemplified by transformations cyclic anhydrides completed by chiral chemical auxiliaries. Separate chapter is devoted to analytical and preparative «chiral chromatography». Separation of enantiomers on the selected, brush-type chiral stationary phases (CSPs) and chromatographic control of optical purity will be discussed. Simulated moving bed (SMB) technology in the large-scale enantioseparation will be explained, and its advantages in development of chiral drugs underlined. Concluding chapter is devoted to the impact of stereoselective, in particular enantioselective, syntheses and chromatographic enantioseparation on development of new, enantiopure drug entities.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152805	**Methods in Organic Synthesis**
number of instruction hours	25
outline of course/module content	In the middle of the last century Woodward, Robinson and Eschenmoser described how synthesis of more complex molecules could be accomplished using a logical methodology which was named by Corey as retrosynthesis. Today most of synthetic problems are solved by such retrosynthetic analysis that breaks down the target molecule into simple, commercially available starting materials. In the framework of this class, different approaches to organic synthesis planning will be considered, including how to find a suitable starting substrate and applicable chemical

	reactions for the construction of target molecules as well as retrosynthetic transformations of the target molecule into synthetic precursors. The most common synthon types that are used to build up the carbon skeleton of more complex molecules will also be mentioned. Additionally, the class will focus on functional group transformations and reactions responsible for the construction of carbon-carbon bonds that are of special interest in organic synthesis. Topics that will be discussed include stereochemistry and conformations, control of stereochemistry during ring formation reactions, protecting groups, pericyclic, electrophile and radical reactions, oxidations and reductions, etc., as well as selected examples dealing with construction of bigger, more complex molecules.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152806	**Reaction Mechanisms in Organic Chemistry**
number of instruction hours	25
outline of course/module content	Quantitative relationships between molecular structure and chemical reactivity: Hammett equation, non-linear Hammett correlations, Yukawa-Tsuno equation and their applications to kinetics and to equilibria. Acid-base equilibria: brief overview of basic concepts, techniques of measuring acidity of organic compounds in the gas phase, properties and reactivity of carbanions (effect of substituents on stability, aromatic and antiaromatic anions, unimolecular rearrangements, carbanions in synthesis of organometallic compounds), effect of solvents on acidity, effect of electronic excitation on acidity of organic compounds, intra- and intermolecular hydrogen(proton) transfer in the ground state and the electronically excited states (experimental and theoretical approaches). Isolation and spectroscopy of reaction intermediates: matrix isolation (IR, UV, ESR, NMR), reaction intermediates in superacids ultrafast spectroscopies. VB-Model and its application to study of the reaction mechanisms: VB-model and aromaticity, SN1 and SN2 reactions, Marcus theory. Reactions in solid phase. Autocatalysis and selfreplication mechanisms.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152807	**Organic Photochemistry**
number of instruction hours	15
outline of course/module content	Principles of photochemistry. Primary processes in photophysics (absorption of electromagnetic radiation, electronic transitions, excited states, radiation and radiationless deactivation processes, Jablonski diagram, quantum yields, orbital symmetry, correlation diagrams, potential energy surfaces, conical intersections). Experimental methods in photochemistry and photophysics (absorption and emission spectroscopy, laser flash spectroscopy, lifetimes). Energy transfer (theory and

	applications, sensitization, quenching). Complexes in the excited state (excimers, exciplexes, electron transfer). Excited state proton transfer. Intramolecular photochemical reactions of alkenes and polyenes (isomerizations, cyclizations, rearrangements). Intra and intermolecular photochemical reactions of carbonyl chromophore. Intermolecular cycloadditions (cycloadditions of alkenes, polyenes, aromatic compounds, and carbonyl compounds with alkenes). Photosubstitutions and photoadditions (aromatic compounds and heterocycles). Photochemical reactions with oxygen. Applications of photochemistry in technology and medicine.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	written (essay) and oral (seminar to the students enroled in the programe)
152808	**Reactive Intermediates in Organic Chemistry**
number of instruction hours	15
outline of course/module content	This course comprises an overview of reactive intermediates chemistry with an emphasis on reactive radicals, radical-ions, diradicals, carbenes, nitrenes, strained molecules and other reactive intermediates such as quinone methides. The student will learn reaction mechanisms where the reactive intermediates are formed. In the study of reactive intermediates it is important to define reactive intermediates geometry and electronic structure. Student should acquire knowledge in the synthetic methods for the preparation of reactive intermediates, methods for the isolation in cryogenic conditions, as well as spectroscopic detection and characterization. Within the spectroscopic techniques the students should learn principles of electron-spin resonance and laser flash photolysis. The chemistry of reactive intermediates will be extended to the applications in the synthesis of complex molecules by use of modern catalytic methods of carbene organometalic complexes.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	essay (writen)
152809	**The Chemistry of Carbohydrates and Glycoproteins**
number of instruction hours	15
outline of course/module content	Introduction will deal with basic structures, nomenclature and stereochemistry of monosaccharides needed to understand complex phenomena in the chemistry of carbohydrates, such as mutarotation or anomeric effect. These will be further discussed from the aspects of energy, structure and kinetics. The structure vs biological activity of oligosaccharides and glycoproteins found in nature will be analyzed, as well as the significance of synthetic carbohydrates in biology and medicine. Recent synthetic approaches will be described in the synthesis of biologically active glycoconjugates, oligosaccharides and glycopeptides. Special topics will be the synthesis of glycosides using enzymes and the

	synthesis of glycopeptides on a solid phase. One more topic will cover complex interactions of reducing sugars with amino acids and peptides.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152810	**Supramolecular Chemistry**
number of instruction hours	15 + 2
outline of course/module content	Examples of natural supramolecular systems. Characteristics of biochemical processes - organic chemistry in vivo. Synthesis and properties of crown ethers and cryptands. Binding, extraction and transport of metal cations through natural and artificial membranes. Natural and synthetic ionophores. Concept of synthetic receptor and molecular recognition. Calixarenes, carcerands, spherands and polytopic receptors. Molecular recognition of aminoacids, peptides and nucleotides. Thermodynamics of supramolecular complexes. Non-covalent binding interactions in supramolecular chemistry: electrostatic, hydrogen bond, van der Waals and aromatic. Solvophobic effects. Supramolecular sysnthesis ans supramolecular chirality. Development of functional supramolecular systems. Self-assembly and self-organization. Chemosensors. Design of functional nano-dimensional assemblies. New supramolecular materials. Training: Design and Molecular modelling (SYBYL).
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152812	**Computational Chemistry**
number of instruction hours	15
outline of course/module content	Theoretical and practical introduction to modern computational chemistry, including applicability to real-world problems. Survey and comparison of molecular mechanical and quantum mechanical methods. Optimization techniques for detailed exploration of potential energy surfaces. Wavefunction analysis methods, stereoelectronic properties, intermolecular interactions, reactivity prediction. Excited states modeling. Solvent effects by continuum, discrete and combined approaches.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152814	**Nucleosides and Nucleic Acids**
number of instruction hours	15
outline of course/module content	DNA and RNA: biological information, chemical structure and properties, major conformations of natural nucleosides. SYNTHESIS OF NUCLEOSIDES: Vorbrüggen glycosylation (Silyl-Hilbert-Johnson Method), Fischer-Helferich: Silver and Mercury Salt Methods, fusion method, stereoselective synthesis

	of nucleosides: from a glycal, or by construction of the heterocycle in the presence of the sugar moiety, etc. SUGARS. Ribose and 2-deoxyribose-reactions of anomeric centre and other OH-group (protection, activation). CHEMICAL TRANSFORMATIONS OF NUCLEOSIDES: structural modifications of natural nucleobases (electrophilic substitution and addition in the heterocyclic moiety of nucleosides, etc) C-nucleoside analogues (pseudouridine, stability of N- and C-glycosidic bond,), intramolecular transformations of nucleosides (the reaction in nucleosides where both the heterocyle and the sugar moieties have participated in cyclonucleoside formation), reactions of nucleosides in sugar moiety (acyclic nucleoside analogues, cyclic analogue, biological effects, antiviral derivatives) NUCLEOTIDES AND OLIGONUCLEOTIDES synthesis of nucleotides (protection groups for nucleobases, sugar hydroxyl groups and phosphates; phosphorylating reagents, modified nucleotides), synthesis of oligonucleotides (phosphotriester method, phosphate method; in solution, on polymer supports; modified oligonucleotides, purification and identification techniques).
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152816	**Application of NMR Spectroscopy for Structure Determination of (Bio)organic Compounds**
number of instruction hours	15
outline of course/module content	Basic principles. Important NMR nuclei (1H, 13C, 15N, 17O, 19F, 31P, etc.). Application of two-dimenzional NMR techniques in organic and bioorganic chemistry. Correlation spectroscopy trough spin-spin interactions (COSY, RELAYH, HETCOR etc.) and through dipole-dipole interactions (NOESY, ROESY etc.). 2DJ-resolved spectroscopy. Multiple-quantum correlation spectroscopy (DQCOSY, INADEQUATE, etc.). Long-range effects in NMR spectroscopy: substituent and isotope effects on chemical shifts, spin-spin coupling and dipole-dipole interactions. Nuclear Overhauser effect (NOE) in structure detemination. New multi-dimensional techniques (inverse techniques: HSQC, HMBC; gradient spectroscopy: GRASP; 3D techniques, etc). Dynamic NMR. NMR spectra of organic and bioorganic molecules including metals (51V, 59Co, 113Cd, 183W, 195Pt, 199Hg).
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152818	**Biotransformations in Organic Chemistry**
number of instruction hours	15
outline of course/module content	Enzymes as biocatalysts in organic chemistry: isolation and purification of enzymes, design of functional enzymes, immobilization procedures, enzyme´s bioinformatics, the use of enzymes in organic solvents, enzymic kinetic resolutions. The use of enzymes as catalysts in the synthesis/hydroysis of C-O bonds, C-N bonds, formation/cleavage of P-O

	bonds, formation of C-C bonds. Enzymes in the reduction/oxidation reactions, isomerizations, introduction/cleavage of protecting groups. The use of biocatalysts in industrial processes. The use of modified enzymes, hemisynthetic enzymes and catalytic antibodies in organic synthesis.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152819	**Modern Methods of Heterocyclic Synthesis**
number of instruction hours	15
outline of course/module content	The modern methods for the synthesis of heterocycles will be presented. In the introduction, the basic concepts and reactions related to heterocyclic chemistry will be scrutinized. Furthermore, a detailed analysis of following reactions types will be performed: Pd-catalyzed reactions asymmetric synthesis of heterocyclic compounds; synthesis of heterocycles using microwave irradiation. Heterocycle synthesis via radical reaction.Total synthesis of complex heterocyclic natural products; New processes for the synthesis of biologically relevant heterocycles.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152820	**Structure, Function and Synthesis of Peptides/Proteins and their Conjugates**
number of instruction hours	15
outline of course/module content	Introduction - peptides, proteins and their conjugates - structure and role in biological processes - model for the study of biological processes Synthesis of peptides and proteins - chemical vs enzymatic methods, chemo-enzymatic approach - protecting groups, activation, deprotection, solution-phase vs solid-phase peptide synthesis - modified peptides and peptidomimetics Chemical methods for the synthesis of peptides and proteins - stepwise synthesis - fragment assembly - directed assembly - examples, advantages and disadvantages of certain methods Glycoproteins, Lipoproteins, Phosphoproteins, Nucleopeptides - structure and function - synthetic methods - application in research
description of instruction methods	Lectures, seminars, and consultations
description of	oral and written exam

course/module requirements	
152821	**Development of the Most Effective Drugs**
number of instruction hours	15
outline of course/module content	Principles of medicinal chemistry. Receptors and drug action:drug-receptor interactions, ion channels, G-protein-coupled receptors, nuclear receptors, protein kinases, intracellular receptors for gene transcription regulation, antibacterial inhibitors of protein synthesis, enzymes as drug targets. Strategies in drug discovery: natural product as a source for new drugs, existing drugs as a basis for new drugs, disease models as screens for new drugs, rational approach in drug design, bioisosterism, prodrugs. Development of the most effective drugs. Inhibitors of prostaglandin synthetase: analgetics and antiinflamatorics, inhibitors of angiotensin converting enzyme (ACE): antihipertensive agents, calcium chanel blockers, drugs for the treatment of angina and hypertension, antagonists of histamine receptors (H2) as anti-ulcer drugs, proton pump inhibitors and gastric acid secretion inhibitors, antidepressants based on serotonine modifications, ligands for benzodiazepine receptors: hypnotic, anxiolytic, anticonvulsant and muscle relaxant agents, antagonists of histamine receptors (H1): drugs for the treatment of allergic rhinitis, nucleoside analogues inhibitors of HIV reverse transcriptase as drugs for the treatment of AIDS, fluoroquinolones as antibacterial DNA gyrase inhibitors
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152822	**Analytical methods in organic synthesis**
number of instruction hours	15
outline of course/module content	Identification of organic compounds by spectral methods (IR, UV, NMR and Mass Spectrometry) Chemical analysis by other instrumental techniques. General techniques for separation and purification including Gas Chromatography and HPLC Preparation of organic compounds.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152823	**Selected Topics in Organic Chemistry**
number of instruction hours	15
outline of course/module content	Various topics of modern organic chemistry, visiting scholar
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152827	**Regulation of gene expression, postsynthetic modifications and protein**

	transport in the cell
number of instruction hours	15
outline of course/module content	*Control of gene expression*: molecular mechanisms of transcriptional regulation in prokaryotes. Regulation of transcription - initiation in eukaryotes (*cis*-regulatory elements, general and specific transcription factors). Mechanisms of transcription factor activity regulation. Role of chromatin structure in transcription regulation (covalent modifications in histone tails and chromatin structure remodelling). Methods for analyzing protein-DNA and protein-protein interactions and chromatin structure analysis. *Post-transcriptional modification and processing of pre-mRNA* (alternative splicing). *Transport of proteins through secretory and cell organelles*. Co-translational translocation of secretory proteins across the ER membrane. Secretory pathway and vesicular transport. Signal sequences and molecular mechanisms of protein transport in mitochondria and nucleus. *Post-translational modifications of proteins*. Protein folding, glycosylation, phosphorylation, proteolysis.
description of instruction methods	lectures, individual consultations
description of course/module requirements	oral exam and seminar presentation of recent publication/s on the chosen specific subject covered by the course program
152828	**Bioenergetics**
number of instruction hours	20
outline of course/module content	Introduction: thermodynamics in biochemistry. Molecular interpretation of thermodynamical principles. Thermodynamical properties of macromolecular solutions. Thermodynamics of equilibrium and nonequilibrium states. Reversible and irreversible processes. Mechanisms of endergonic processes in biological and biochemical systems. Metastability, chemical potential of functional groups in biochemical systems. Enzymatic complexes. Energetic potential in living cells. Thermodynamics of membrane transport. Stabilisation of protein structure. Stabilisation forces and interactions in process of protein folding. Structural and functional domains. Uncovalent interactions: strength, energy and distance dependence. Models for studding uncovalent interactions in biochemical systems, importance of solvation. Dynamics of protein's structure. Protein-ligand interactions and their thermodynamical properties. Analysis of experimental data. Equilibrium processes, equilibrium constants – measurements and interpretation. Energetics of enzyme catalysis, transition state theory, energy of activation. Influence of steric factors on enzyme catalysis. Conformational changes: molecular mechanisms, cooperativity, allosteric effects. Mechanisms of cooperativity. Negative cooperativity. Physiological importance of cooperativity. Examples.
description of instruction methods	Lectures, seminars, consultations.
description of course/module	Oral exam

requirements	
152829	**Control mechanisms in protein biosynthesis**
number of instruction hours	20 + 5
outline of course/module content	The accuracy and the fidelity of transmission of genetic information with special emphasis on translation: the error frequency, structural bases of accuracy, optimising the speed and the accuracy, comparing the accuracy of three polymerases (DNA-polymerase, RNA-polymerase; peptidyl-transferase), synthetic and editing mechanisms of aminoacyl-tRNA synthetases, substrate channeling, the active role of the ribosome in protein biosynthesis, proofreading, consequences of mistranslation, adaptive translation, the accuracy of organellar protein synthesis, incorporation of nonstandard amino acids into proteins.
description of instruction methods	lectures and seminars
description of course/module requirements	seminars, oral presentations
152831	**Enzymes: kinetics and reaction mechanism**
number of instruction hours	20
outline of course/module content	Chemical catalysis (transition state theory, principles of catalysis, covalent catalysis, kinetic isotope effect); Enzyme catalysis; The basic equations of enzyme kinetics (steady-state kinetics, Michaelis-Menten model, inhibition, multisubstrate systems); Measurements and magnitude of individual rate constants (conventional methods, rapid methods-stopped flow, relaxation, quenching, analysis of pre-steady state and relaxation kinetics); The pH dependence of enzyme catalysis; Practical methods for kinetics and equilibria; Detection of intermediates in enzymatic reactions; Irreversible inhibition; Allosteric interactions (positive and negative cooperativity, Hill equation); Stereochemistry of enzymatic reactions; Enzyme-substrate complementarity and the use of binding energy in catalysis; Specificity of enzyme catalysis (limits on specificity; editing or proofreading mechanisms); Catalytic RNA; Selected examples of enzymatic reactions.
description of instruction methods	Lecturing would be performed through lectures, discussions of problems and selected literature examples.
description of course/module requirements	Course attendance, written and oral exams
152832	**Structure and function of membranes and cell walls**
number of instruction hours	20
outline of course/module content	Dynamics and structure of biological membranes: General principles, composition, dynamics, structure and organisation of biological membranes. Structural composition of membrane lipids and proteins. Integral and peripheral membrane proteins, interactions with the membrane lipids. Asymmetrical lipid composition in the outer and inner part of membrane bilayer: synthesis, organisation and transport of membrane lipids. Carbohydrates of the cell membrane: lectins, selectins, modification of carbohydrates in the Golgi apparatus, glycosylation of

	lysosomal enzymes, diseases related to impaired glycosylation, erythrocyte cell membrane, spectrin, cytoskeleton, anion channel-protein band 3, ABO antigens, structure of A, B, and H antigens. Transport of small molecules across cell membrane: driving forces and gradients, protein carriers, ion channels, gap junctions, control of opening and closing, acetylcholine receptor, structure and function of voltage gated Na+ channel, K+ channel, specificity and selactivity of ion transporters, carrier transport, symport, antiport, transport ATPases, MDR-multidrug resistance transporters of drugs. Families of transport proteins, ABC transporters, CFTR, peptide transporters, Ca2+ pumps, glucose transporters, kinetics of Na+/glucose co-transport, asymmetrical distribution of protein transporters. Specific proteins of the intracellular organelles: mechanism of the intracellular membrane synthesis, cytosol derived proteins, protein and peptides specific for nucleus, mitochondria, peroxisomes, and endoplasmic reticulum. Transport of water across the cell membrane, osmotic pressure, epithelial renal cells, aquaporin. Bacterial cell walls-structure and biological activity: Gram positive and Gram negative bacteria. Endotoxins-structure and biological activity. Peptidoglycans-structure, enzymatic degradation, biological characteristics and influence on immunological system. Artificial membranes: liposomes as a model system of lipid bilayer. Preparation, characterisation and application in biology and medicine.
description of instruction methods	lectures or tutorials, depending on number os students
description of course/module requirements	oral examination and presentation of seminar on the selected topics
152833	**Macromolecular crystallography**
number of instruction hours	10 + 5
outline of course/module content	Crystallization-sample preparation for X-ray diffraction experiments, determination of crystal symmetry. Data collection. Evaluation of X-ray diffraction intensities. Phase problem solution. Fourier synthesis. Interpretation of electron density maps, rough model. Refinement of the rough model and adjustment with measured intensities. Primary, secondary, tertiary structure of the macromolecule. Structural evaluation of the model and recognition of the protein biological function by using databases and structural bioinformatics (Cambridge Structural Database, Protein Data Bank, SwissProt, Phyre, etc.).
description of instruction methods	lectures, consultations, seminars
description of course/module requirements	permanent evaluation, exams, seminars
152834	**Glycoproteins – Structure and Function**
number of instruction hours	10 + 5
outline of course/module content	Glycoprotein structure. O- and N-glycosidic linkage to proteins. Structure of O-glycosidically linked carbohydrate chains. Structure of N-glycosidically linked carbohydrate chains. Biosynthesis of O-glycosidically linked carbohydrate chains. Biosynthesis of N-glycosidically linked carbohydrate chains. Control of protein glycosylation. Role and importance of protein

	glycosylation. Reversibile glycosylation.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152835	**Biotransformation of Drugs and Xenobiotics**
number of instruction hours	15
outline of course/module content	Biotransformation of drugs and endogenous compounds catalyzed by specific enzymes. Oxidations and reductions (dehydrogenases, aminooxidases, xantin oxidases, cytochrome P-450). Hydrolysis (esterases, amidases, lipases, penicillinases). Acetylation and acylation (N-acetyltransferases, N-acyltransferases). Glucuronidation (UDP-glucuronyltransferases). Sulfoconjugation (sulfotransferases). Conjugation with glutathione (glutathiontransferases). Examples of biotransformation of drugs for each group of reactions. Structure-activity relationship. Genetic polymorphism. Inhibition and induction of enzymes involved in biotransformation of drugs. Mechanism of toxic metabolites formation.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152836	**Biochemistry and Pathobiochemistry of Lipids and Lipoproteins**
number of instruction hours	10 + 5
outline of course/module content	1. Biochemical and biophysical characteristics of lipid molecules: triglycerides, fatty acids, cholesterol, cholesterol ester, phospholipids 2. Lipoproteins: composition, classification, biochemical/biophysical properties 3. Biogenesis and metabolism of triglyceride rich lipoproteins:Chilomikrons, VLDL,; the role of lipoprotein lipase (LPL), LPL-knock out mice-a model for human LPL-deficiency; why LPL-deficiency is lethal in mice but not in humans? How experimental gene therapy using recombinant LPL-adenovirus facilitates survival of LPL-deficient mice? 4. Biogenesis and metabolism of low density lipoprotein: Generation of LDL, LDL receptor, molecular mechanisms of regulation of LDL receptor synthesis; LDL-receptor deficiency in humans, mutations in LDL receptor and in PCSK9; drugs and approaches used for treatment of hypercholesterolemia: statins, LDL apheresis, gene therapy; new drugs in clinical trials: limitapide and mipomersen 5. HDL-its role in reverse cholesterol transport (RCT): the role of ABCA1 and ABCG1 in the first step of RCT; the role of SR-BI, LCAT and CETP in HDL maturation; the role of hepatic SR-BI for delivery of HDL associated cholesterol ester into liver 6. Pathogenesis of atherosclerosis-the role of LDL, HDL and macrophages; application of synthetic HDL (reconstituted HDL), apoAI mimetics and mutant apoAI in the treatment of atherosclerosis; experimental atherosclerosis 7. Endothelial lipase-modulator of abundance, structure and function of

	HDL.
description of instruction methods	Lectures, seminars, problem based learning,
description of course/module requirements	oral and written exam
152837	**Immunochemistry and Immunochemical Methods**
number of instruction hours	10 + 5
outline of course/module content	Purpose and characteristics of laboratory testing Chemical and physicochemical methods (chromatography, filtration, electrophoresis) Basic interactions Ag-Ab (structure, binding, affinity, avidity) Immunization (immunogens, haptens) Immunoanalytical methods (agglutination and precipitation, radial and double diffusion, immunoelectrophoresis, immunoblotting) Immunoassays-competitive and non-competitive (radioimmunoassay, enzyme-immunoassay, fluorometric immunoassay)
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152838	**Modelling of biomacromolecules: structures, complexes, interactions**
number of instruction hours	10 + 5
outline of course/module content	Experimental techniques used to determine 3D molecular structure. Protein data base. Servers for homology modelling. Empirical *vs* quantum mechanical molecular modelling. Hierarchy of molecular modelling methods. All atom and Coarse grained molecular modelling. Concept of force field and parametrization. Computation of energy, properties and reactivity of molecules Energy optimization, conformational analysis, molecular dynamics, Monte Carlo analysis. Importance of solvent in molecular modelling. Molecular ensembles and their thermodynamical properties. Molecular docking - concept, type and computational programs. Hybrid molecular mechanical- quantum mechanical models. Computational programs for molecular modelling – basic characteristics and algorithms.
description of instruction methods	Lectures, exercises and seminars
description of course/module requirements	Direct contacts with students, Pp presentations, WEB, and blackboard,
152839	**Selected Topics in Biochemistry**
number of instruction hours	15
outline of course/module content	Various topics of modern biochemistry, visiting scholar
description of instruction methods	Lectures, seminars, and consultations

description of course/module requirements	oral and/or written exam
152844	**Chemometrics**
number of instruction hours	15 + 5
outline of course/module content	Elementary statistics: basic probability theory, most frequent univariate and multivariate distributions, hypothesis testing (location, dispersion and distribution tests). Analysis of variance: one-way, two-way and multi-way ANOVA (fixed effect models, with and without interaction). Regression analysis (least-squares method): linear models (straight line, multiple and polynomial regression, tests of significance of regression parameters, confidence intervals, weighted regression, goodness-of-fit test), non-linear regression (basic concepts and methods). Optimization: the Simplex method. Data smoothing and filtering. Cluster analysis. Principal components analysis, principal components regression, partial least squares, factor analysis. Non-parametric statistics: location, correlation and distribution tests, analysis of variance.
description of instruction methods	Lectures, consultations and seminars
description of course/module requirements	Seminar and oral exam
152845	**Selected Topics in Quantum Chemistry**
number of instruction hours	25
outline of course/module content	Overview of modern quantum-chemical methods; Hartree-Fock (HF) self-consistent field theory (SCF) for closed and open shells; Description of dynamic and nondynamic electron correlation; Single-determinant reference (post-HF) methods; Multiconfigurational methods in quantum chemistry (CASSCF, CASPT2); Density functional theory (DFT); Time-dependent DFT formalism (TD-DFT); Variational Transition State Theory; Comparison of single reference, multireference and DFT treatments.
description of instruction methods	lectures (presentations), consultations
description of course/module requirements	seminar (brief presentation), oral exam
152846	**Molecular Spectroscopy**
number of instruction hours	25
outline of course/module content	Interactions between electromagnetic radiation and molecules, line shape. Experimental methods in spectroscopy. Rotational spectroscopy: rigid rotor model and deviations from a rigid rotor model, Stark effect, hyperfine splittings; determination of molecular structure; study of van der Waals complexes. Vibrational spectroscopy: normal modes of vibrations,

	rotational structure of bands, large amplitude motions. Electronic spectroscopy: coupling of angular momenta in atoms and molecules; states of polyatomic molecules; vibrational structure of bands; Renner-Teller effect, Jahn-Teller effect, rotational structure of bands; photoelectronic spectroscopy. Lasers and laser spectroscopy: general features and properties, resonant Raman spectroscopy, coherent Raman scattering, laser magnetic resonance, saturation spectroscopy, laser induced fluorescence, multiphoton absorption.
description of instruction methods	Lectures, consultations and seminars.
description of course/module requirements	Oral and written exam.
152847	**Statistical Thermodynamics and Irreversible Processes**
number of instruction hours	20 + 5
outline of course/module content	*Theoretical Phenomenological Thermodynamics:* Mathematical and physical background (Pfaff forms, homogeneous functions, Jacobians, characteristic functions). Axiomatics (principle of Carathéodory). Relativistic generalisation. *Theoretical Statistical Thermodynamics:* Theory of probability. Principles of quantum mechanics. Stationary model (the method of ensembles). Classical approximation, the partition function method. The evaluation of the stationary model, density matrix. Fluctuations. The method of molecular partition function. Models based on canonical ensemble: Debye model of crystal, real gases and electrolyte solutions (P. Debye i E. Hückel, J. E. Mayer, Monte Carlo methods and molecular dynamics). *Irreversible processes:* Generalised fluxes and forces, linear phenomenological relations (Onsager). Nonlinear phenomena (dissipative structures, oscillating chemical reactions). *Thermochemistry:* Thermometry. Calorimetry. Standard thermodynamic properties. Tables of thermodynamic properties.
description of instruction methods	Consultations and seminars
description of course/module requirements	Seminar
152848	**Chemical kinetics**
number of instruction hours	20 + 5
outline of course/module content	Chemical reaction. Chemical kinetics. Rate of chemical reactions and the differential form of the law of rate of chemical reactions. Experimental determination of the rate of chemical reaction. Integrated form of the law of rate of chemical reactions. Determination of rate of chemical reactions. Chemical reaction rate constant, reaction order and molecularity of chemical reactions. Experimental determination of rate constants of chemical reactions. The single-phase unidirectional and reversible reactions. Polyphasic unidirectional and reversible reactions. The relaxation kinetics. Dependence of the chemical reaction on temperature. Kinetic theories of reaction rates – definition and postulation of the chemical reaction mechanism and its verification - the activation parameters (activation enthalpy, entropy and volume). The linear

	relationships between the free energy of the reaction and the activation free energy. Dependence of the reaction rate on the properties of the media.
description of instruction methods	Lectures, tutorials and seminars
description of course/module requirements	Seminar work, oral exam
152849	**Selected topics in Electrochemistry**
number of instruction hours	15
outline of course/module content	*The Interfacial Structure:* Thermodynamics of the electrified interphases, Work function, Fermi level, Electrode Potentials, metal/electrolyte and semiconductor/electrolyte interfaces. *Electrode Kinetics:* Rate - potential relationships, Kinetics of linear sweep voltammetry, Irreversible and reversible reactions, Reaction orders, Electrode kinetics as a function of the interphasial structure, Electrochemical reaction mechanism determining. *Quantum-Oriented Electrochemistry*: Quantum-mechanical formulation of the exchange current (Electrochemical reaction rates), Quantum-mechanical model of the electrochemical reaction of hydrogen evolution, A stochastic theory of electron transfer. *Stability of Materials and Electrocrystallization*: Electrochemical kinetics as the bases for corrosion reactions, Mechanisms of corrosion reactions, Experimental investigation of corrosion, Methodology of corrosion protection, Surface modification with organic additives, organic films (self-assembled monolayers), oxide passive layers of nano-thickness, Kinetics of self-assembling processes, Progress in theory of electrocrystallization, Electrodeposition, Electrochemical approach to nanotechnology. *Electrocatalysis*: Functional materials, Electrocatalysis at a molecular level. *Electrochemical energy storage and electrochemistry of clean environments*: hydrogen energy, Fuel cells, Efficiency of light to electrical energy conversion, Electrochemical wastewater treatments. *Experimental techniques:* Stationary and nonstationary electrochemical techniques, Electrochemical impedance spectroscopy. Laboratory work: Electrochemical processes under activation control: Kinetics of hydrogen evolution reaction on the Ni electrode; Linear Voltammetry; Electrochemical impedance spectroscopy (EIS). Electrochemical processes under diffusion control: Redox reaction on the Pt electrode; cyclic voltammetry (stationary Pt electrode); Linear Voltammetry (Pt rotating disc electrode, Pt-RDE). Electrochemical quartz crystal nanobalance (EQCN): electrodeposition of metals (Cu, Ni) and organic molecules on the solid substrate.
description of instruction methods	Lectures, Seminars, Laboratory work.
description of course/module requirements	Seminar, Oral exam.
152850	**Selected topics in interfacial and colloid chemistry**
number of instruction	15

hours	
outline of course/module content	Equilibrium of surface reaction (1pK, 2pK and MUSIC model). Association of counterions. Specific adsorption. Experimental methods for surface characterization (potentiometric, electrokinetic, calorimetric, light scattering, etc.) and interpretation of the experimental data. Micro emulsions: formation. Electrical conductivity. Aggregation and adhesion of colloid particles. Kinetics. The precipitation processes from electrolyte solutions. Examples for the precipitation of metal oxides and their structural, nano/microstructural, magnetic and other properties. Applications of Mossbauer, FT-IR, UV/Vis/NIR and other spectroscopies in the investigation of precipitation processes. Application of high resolution scanning electron microscopy in the investigation of colloid particles.
description of instruction methods	lectures (presentations), consultations
description of course/module requirements	seminar (brief presentation), oral exam
152851	**Radiation Chemistry**
number of instruction hours	12
outline of course/module content	INTRODUCTION Types of ionizing radiation. The significance of the effects of ionizing radiation in the basic and applied science. Historical overview of the development of radiation chemistry. THE INTERACTIONS OF IONIZING RADIATION WITH MATTER Radiation energy loss in matter. Particle radiations: neutrons, electrical charged particles: electrons and ions. Electromagnetic radiations. Gradient energy loss (LET). The absorption of radiation energy in the matter. DETECTION AND MEASUREMENT OF RADIATION EFFECTS Detection and measurement of the amount of absorbed energy (radiation dosimetry). Time-resolved techniques for reactive short-lived species detection. PHYSICO-CHEMICAL EFFECTS OF IONIZING RADIATION Spatial and temporal distribution of events in the irradiated material. Structure of traces of ionizing radiation. Formation and chemical reactions of reactive short-lived species: electrons, ions, excited molecules and free radicals. RADIATION EFFECTS ON WATER AND WATER SOLUTION Primary yields of reactive species in radiolysis of water. The effects of pH and LET. Kinetics in radiation chemistry. RADIATION EFFECTS ON BIOLOGICAL MOLECULES Biological macromolecules and DNA. Influence of dose, dose rate, the environment, the concentration of oxygen, temperature, LET. Radiation sensitivity. Oxidative stress. RADIATION EFFECTS ON CELLS AND UNICELLULAR ORGANISMS Direct and indirect effects. Targets theory. Molecular theory. APPLIED RADIATION CHEMISTRY Radiation processing and sterilization of medical products, food irradiation, polymer modifications. Industrial radiation sources and facilities. Potential applications of radiation processing currently under research and development. RADIATION EFFECTS ON BIOLOGICAL SYSTEMS Dose-effect relationships. Redox processes in Biology and parallels in radiation chemistry. Radical/oxidative stress.

description of instruction methods	Lectures, problem solving, consultations, visit gamma 60Co irradiation facility and radiation laboratory
description of course/module requirements	Examinations and consultations are being held at the request of students at any time.
152852	**Equilibrium and kinetics of processes in heterogeneous systems**
number of instruction hours	10 + 2
outline of course/module content	Equilibria in the solid/liquid systems and supersaturation: solubility product, concentrations and activities in supersaturated solutions, some critical values. Kinetics and mechanisms: foramtion of solid phase from supersaturated solutions (nucleation and crystal growth); dissolution. Properties of the solid phase: crystal shapes and their size distribution, hydrodinamic factors, chemical properties, taložni dijagrami, utjecaj primjesa. Secundary changes of the solid phase: transformation, coagulation, agglomeration. Application.
description of instruction methods	Lectures, consultations and seminars.
description of course/module requirements	Oral exam.
152853	**Mathematical chemistry**
number of instruction hours	12
outline of course/module content	Presentation of data. Data sets and partialy ordered data sets. Data mapping and grouping. Data clustering. Neural networks. Orthogonal polynomials. Fourier, Walsh, Hadamard and other transformations. Representation of chemical structures. Adjacency matrix. Distance matrix. Discrete mathematics in chemistry. Graphs. Algorithms on graphs. Complexity. Information theory in chemistry. Topology in chemistry. Chirality of molecules. Symmetry of molecules. Rigid and flexible molecules. Permutationally inverse groups. Molecular similarity. Molecular diversity. Combinatorial chemistry. Mathematical planning of chemical synthesis. Combinatorial counting. Isomers. Matching. Conjugated rings. Recurent counting. Molecular properties and their modeling by topological and other descriptors. QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship). Distributions. Statistics. Correlations. Factorial analysis.
description of instruction methods	Lectures, consultations
description of course/module requirements	Oral exam
152855	**Nanotechnologies**
number of instruction hours	15
outline of course/module	Physical basics of nanoscience and nanotechnology. Selected examples of

content	research in physics, chemistry and biology and interdisciplinary research.
description of instruction methods	Lectures and e-learning.
description of course/module requirements	A 20-minutes seminar and final test.
152856	**Physical Chemistry of Macromolecules**
number of instruction hours	15
outline of course/module content	Macromolecules: polymers, polyelectrolytes, polysaccharides, proteins; structural models, chain configuration; effect of structure and molar mass on physico-chemical properties of macromolecules. Electrostatic interactions in macromolecule solutions; problem of excluded volume, application of numerical simulation methods. Methods for determination of molar mass; osmotic pressure, sedimentation, viscosity. Methods for particle size determination; light scattering, x-ray scattering, neutron scattering, microscopic methods. Polymers in solution; solubility, conformation, formation of polyelectrolyte complexes. Polymers on surface; polymer adsorption, kinetics of adsorption, polyelectrolyte multilayers, polyelectrolyte brushes.
description of instruction methods	lectures (presentations), consultations
description of course/module requirements	seminar (brief presentation), oral exam
152857	**Theoretical Chemistry and Reaction Dynamics**
number of instruction hours	15
outline of course/module content	Mathematical introduction: operator algebra, Fourier transformation, numerical and statistical methods, Schrödinger equation, Born-Oppenheimer approximation. Classical dynamics: classical trajectories, force fields, distribution of velocities, constraint and restraints, ab initio molecular dynamics, time dependent properties. Quantum dynamics: time independent wavefunction, model potentials: scattering and bound states, solution of Schrödinger equation, time development of wavefunction, operator of time development, time development of wavepackets, multiconfigurational time dependent Hartree method. Reaction dynamics: molecular reaction dynamics, activation energy, potential energy surfaces and chemical reactions, time resolved spectroscopy, nonadiabatic dynamics.
description of instruction methods	Lectures, consultations and seminars.
description of course/module requirements	Oral and written exam.
152858	**Selected Topics in Physical Chemistry**
number of instruction hours	15
outline of course/module	Various topics of modern physical chemistry, visiting scholar

content	
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
152859	**Atomic spectrometry in analytics**
number of instruction hours	20 + 10
outline of course/module content	Atomic spectrometry methods in analysis of elements, historical development, present state, application to individual elements. Preparation of samples: sampling, storage, mineralization, extraction and concentration of elements before analysis. Sources of contamination. Theory of atomic spectrometry: absorption, emission and fluorescence. Atomic absorption spectrometry (AAS): basic principle (instrumentation, techniques, automation, sources of energy), calibration, atomization in flame, electrothermal atomization, interference effects, background correction, special techniques (cold vapor, hydride generation). Atomic emission spectrometry (AES): flame, plasma, glow discharge as excitation sources; spectrometer constructions; detection of emission signal. Advanced instrumental techniques based on hyphenated systems: gas and liquid chromatography, capillary electrophoresis, glow discharges coupled with plasma and/or mass spectrometer. Comparison of methods: detection limits, concentration range, efficiency in analytical demands. Environmental risk assessment (chemical species and adaptation, estimation of bioavailability, variations, representative species and deficiency, extrapolation laboratory-enviro152859nment); analytical monitoring of environmental impacts; modern instrumental methods in quality control; essential and toxic materials, additives; present scope and challenges in forming of new regulative procedures.
description of instruction methods	Lectures, seminars, laboratory demonstrations, consultations
description of course/module requirements	Written and/or oral exam
152860	**Electroanalytical methods**
number of instruction hours	20 + 10
outline of course/module content	Basic definitions and concepts of electroanalysis: ions, electrolytes, charge. Galvanic article and electrolysis. Electrochemical cells, thermodynamic properties and electrode potentials. Electric double layers. Basics of kinetics and mechanisms of electrochemical reactions (velocity, voltage dependence, transport processes - diffusion, migration and convection). Faraday and non-faraday processes. Diffusion and kinetics controlled processes. Reversibility, quasi reversibility, irreversibility of the reactions. Electrochemical experiment: different electrode types, "green electrochemistry", electrochemical cell, basic electrolytes, instrumentation (analogue - potentiostat, galvanostat and digital), electrochemical sensors, nanoparticle based sensors. Overview of electroanalytical methods with their backgrounds: trigger and response signals (Potentiometry, Voltammetry, Amperometry, Electrogravimetry, Kulometry, Spectroscopy,

	Electrochemical Impedance Spectroscopy). Examples of the use of electroanalytical methods in analytical chemistry related to professional and scientific-research work.
description of instruction methods	Lectures, seminars, laboratory demonstrations, consultations
description of course/module requirements	Written and oral exam + seminar paper
152861	**Chromatographic methods in analytics**
number of instruction hours	20 + 10
outline of course/module content	The types of chromatography analytical techniques: relative to aggregate states of stationary and mobile phase, performance, and physicochemical processes. Theory of chromatographic processes. Factors that influence chromatographic processes. Separation efficiency and selectivity. Generating of chromatographic analytical data and data processing. Analyte characterization and quantitative analysis of specific mixture components. Selection of chromatographic method relative to analyte chemical properties. Sample preparation prior to chromatographic analysis. Liquid Chromatography (LC): Stationary and mobile phase properties. Adequate instrumental and detection techniques for specific analyte analysis. High Performance Liquid Chromatography: liquid adsorption chromatography, partition liquid chromatography. Normal- and reversed-phase chromatography. Ion-pair chromatography. Chiral chromatography. Ion-exchange chromatography. Size exclusion chromatography. Multidimensional chromatography and hyphenated instrumental techniques. Chromatographic separation and protein mixture analysis. Applications. Gas Chromatography (GC): Selection of suitable mobile and stationary phases. Gas-liquid chromatography. Adsorption chromatography. Design of gas chromatography system. Multidimensional chromatography and hyphenated instrumental techniques. Applications. Supercritical fluid chromatography. Properties of mobile and stationary phases. Design of chromatography system. Capillary electrophoresis. Principle. Adequate instrumental and detection techniques. Capillary electrochromatography. Micellar electrokinetic chromatography. Applications.
description of instruction methods	Lectures, seminars, laboratory demonstrations, consultations
description of course/module requirements	Written and oral exam
152862	**Analysis of organic contaminants**
number of instruction hours	15 + 10
outline of course/module content	Introduction to analytical chemistry of organic contaminants; inventory of contaminants - priority pollutants; physico-chemical characteristics of organic contaminants; sampling, sample processing and sample storage; sample enrichment and clean-up; qualitative and quantitative analysis; chromatographic methods; spectroscopic methods; electrochemical

	methods; immunochemical methods; hyphenated analytical techniques (GC-MS, LC-MS, GC-ICP-MS); analysis of selected groups of specific organic contaminants - hydrocarbons, volatile halogenated hydrocarbons, chlorinated pesticides, polychlorinated biphenyls, herbicides, brominated flame retardants, phenols, surfactants, pharmaceuticals, organometallic compounds; statistical analysis of experimental data - application in environmental studies.
description of instruction methods	Lectures, seminars, laboratory demonstrations, consultations
description of course/module requirements	Written and/or oral exam
152863	**Modern molecular spectroscopy**
number of instruction hours	25 + 5
outline of course/module content	The signal and noise. Spectroscopy in time and frequency domain. Fourier transformation (FT) and spectroscopy. Interferometry and FT in infrared spectroscopy (IR). Dispersive and FT Raman spectroscopy. Near IR spectroscopy (NIR). Two-dimensional IR spectroscopy. Time-resolved vibrational spectroscopy (rapid scan and step scan). Pulse nuclear magnetic resonance (NMR) techniques. FT in NMR; two- and multidimensional techniques. NMR parameters (chemical shifts, couplings, relaxation times) and molecular structure. NMR and conformational analysis. Molecular interactions studied by NMR and drug design. Mass spectrometry (MS). Mass analysers; sector, quadrupol, ion cyclotron resonance and FT (FT ICR), time of flight (TOF). Ionization methods; electron impact (EI), chemical ionization (CI), fast atom bombardment (FAB), laser desorption ionization (LDI), matrix assisted laser desorption ionization (MALDI), electrospray ionization (ESI). Tandem MS (MS/MS, MSn). Spectra interpretation. Mechanisms of fragmentation. Analysis of complex mixtures by using hyphenated techniques GC-MS, LC-MS, LC-NMR etc.
description of instruction methods	Lectures, seminars, demonstrations, consultations
description of course/module requirements	Written and/or oral exam
152864	**Modern methods of structural NMR**
number of instruction hours	20
outline of course/module content	Solid state NMR, CP MAS NMR techniques, quadrupolar nuclei, correlation between solid state NMR spectra and macroscopic properties, cross-relaxation and cross-correlation, modern multipulse techniques. Computational methods for determination of chemical shifts and spin-spin couplings, molecular dynamics and solvent models, visualisation of nuclear shielding and couplings. Calculation of NMR chemical shifts in proteins and nucleic acids, characterisation of NMR tensors and couplings in hydrogen bonded systems. Structure determination of nucleic acids by using one- and multi-dimensional NMR techniques and molecular modelling, base pairs and hydrogen bonding, interactions of cations and nucleic acids, binding

	kinetics studies. Interactions of small molecules and biological receptors by NMR, transferred NOE techniques, saturation transfer difference techniques (STD), diffusion editing techniques, NMR screening (SAR by NMR and others).
description of instruction methods	Lectures, seminars, demonstrations, consultations
description of course/module requirements	Written and/or oral exam
152865	**Environmental electrochemistry**
number of instruction hours	10 + 5
outline of course/module content	Fundamentals of electrochemical measurements: current, charge, potential, charge and mass transfer, electrochemical cell, phase boundary electrode/electrolyte, oxido-reduction and adsorption processes; electrochemical methods and techniques (potentiometry, amperometry, voltammetry, polarography, conductometry, stripping methods, etc.); electrochemical instrumentation and equipment. Application: Electroanalysis of inorganic and organic substances of natural and anthropogenic origin in water, air, sediments and soil - Environmental monitoring. *In-situ* electrochemical sensors (ion selective electrodes, pH, oxygen, redox potential, H2S, etc.) Electrochemical techniques for removal of wastes from waters. Electrochemistry for healthy environment (CO2 fixation, photo-electrochemistry, etc.)
description of instruction methods	Lectures, seminars, laboratory demonstrations, consultations
description of course/module requirements	Written and/or oral exam and/or seminar paper
152866	**Quality control of analytical procedures**
number of instruction hours	10
outline of course/module content	Quality control is the essential component of the quality assurance of analytical procedures. It has the purpose to reduce the analytical errors, while the results that should fit the purpose, have the required accuracy and precision. The components of the quality control are the following: equipment adequate to the purpose and the scope of the analysis; competent and qualified personnel; good laboratory praxis; good metrology praxis; standard operation procedures that include validated analytical methods; special purpose protocols; internal audit; the use of certified reference materials and samples; data storage and data availability; laboratory records; reports; education and training of the laboratory personnel. Proficiency testing of the laboratory and the accreditation.
description of instruction methods	Lectures, seminars
description of course/module requirements	Written (seminar paper)and oral exam

152867	**Selected Topics in Analytical Chemistry**
number of instruction hours	20
outline of course/module content	Various topics of modern analytical chemistry, visiting scholar
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
168988	**Surface-Enhanced Vibrational Spectroscopy**
number of instruction hours	10
outline of course/module content	Surface-enhanced vibrational spectroscopy (SEVS) - methods of qualitative and quantitative analysis of molecules close to or bound to the metallic nanostructured surface. Structural sensitivity - vibrational spectrum as molecular fingerprint. Analytical sensitivity - signal enhancement with respect to the normal vibrational methods: up to 10E3 for the techniques of the surface-enhanced infrared spectroscopy, up to 10E12 for the techniques of the surface-enhanced Raman spectroscopy. Selectivity - determined by the analyte structure and properties of the metallic surface. Mechanisms of the vibrational signal enhancement: electromagnetic mechanism and chemical mechanism. Surface selection rules. Types, preparation and properties of the metallic nanostructured substrates essential for observation of the surface-enhanced vibrational signal. Analysis and interpretation of the spectra. Application: structural characterization of ultra-thin films and assembled molecular layers, in-situ monitoring of photochemical, catalytic and electrochemical reactions, study of biomolecules, e.g. specific DNA sequences, nucleic acids, phospholipids and proteins, as well as complex biological structures, such as cells and microorganisms., design and development of sensors and biosensors, detection of pollutants, analysis of pharmaceutical substances and detection of analyte when coupled with the separation techniques (capillary electrophoresis, chromatography). Principle and application of the following techniques of the linear and non-linear surface-enhanced vibrational spectroscopy: surface-enhanced infrared absorption (SEIRA), surface-enhanced Raman scattering (SERS), surface-enhanced resonance Raman scattering (SERRS), surface-enhanced Raman optical activity (SEROA), surface-enhanced hyper-Raman scattering (SEHRS), surface-enhanced coherent anti-Stokes Raman scattering (SECARS).
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam
173225	**Methods of Protein Biochemistry**
number of instruction hours	15 + 5
outline of course/module	Setting up a laboratory and basic equipment for biochemical research.

content	Buffers and reagents necessary for working with proteins and protein purification. Protein isolation from raw biological material, methods of lysis and disruption of various cell and tissue types. Maintaining protein stability during isolation, handling and purification. Buffer and solvent exchange using semipermeable membranes: dialysis and ultrafiltration. Protein purification and concentration by precipitation using ammonium sulphate, polyethylene glycol, organic solvents and trichloroacetic acid. Chromatographic techniques of protein separation and purification: ion-exchange chromatography, hydrophobic interaction chromatography, size-exclusion chromatography. Affinity chromatography: conventional methods of affinity chromatography and affinity chromatography of tagged recombinant proteins. Affinity chromatography of glycoproteins and immunoglobulins. Use of protein tags in biochemistry, in vivo and in vitro protein tagging and labelling. Fluorescent labelling, covalent modification and protein immobilization. High pressure and high performance liquid chromatography, properties of chromatography resins and instrumentation for high performance protein purification. Theoretical fundaments of electrophoresis and electrophoretic protein separations. Native and denaturing electrophoresis. SDS-PAGE, isoelectric focusing and 2D-PAGE. Detection of macromolecules after electrophoretic separation. Western blot. Capillary electrophoresis. Protein analysis: determination of protein concentration and enzymatic activity. Detection and quantification of impurities in protein samples. Analysis of structural heterogeneity. Analysis of posttranslational modifications. Target enrichment. Special considerations for handling of membrane proteins, macromolecular and ribonucleoprotein complexes, supramolecular structures.
description of instruction methods	Lectures, seminars, and consultations
description of course/module requirements	oral and written exam