Jagiellonian University in Krakow

Semester 3 syllabus

Course catalog	ECTS
Internship and Transferrable Skills	10
Forensic Chemistry - Laboratory	5
Forensic Chemistry	5
Multivariate Analysis in Chemistry	5
Quantum-Chemical Molecular Modelling	5
Spectroscopic Methods for Characterization and Imaging of Biomaterials	5

Mandatory

Elective courses: 20 ECTS to choose

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Course title	FORENSIC CHEMISTRY - LABORATORY		
Information	Number of credits: 3 ECTS	Number of taught hours 40 h	Number of hours expected of student personal work: 35 h (total 75 h)
Synopsis	The aims of this unit are: • To highlight the most important issues of forensic chemistry and to develop the competence of the students in this field. • To introduce the analytical problems in forensic toxicology and criminalistics • To train students in selected analytical techniques used in forensic chemistry Identification of unknown substances (microscopic techniques, presumptive tests, gas chromatography with mass spectrometry). Comparative analysis of DNA fragments (isolating genetic material from biological material, gel electrophoresis and NanoDrop spectrophotometry. Examination of documents - ink discrimination: microscopic techniques, capillary electrophoresis. Analysis of biological material for judicial purposes (high-performance liquid chromatography). Crime scene investigation. Identification of traces, e.g. fingerprints, bloodstains, footprints, ground serial numbers on metal surfaces (microscopic techniques and presumptive tests).		
Learning outcomes / skills and competencies	Knowledge – Student knows and understands: • Student can apply chemistry and technical science to describe properties of material/substances of forensic trace • Student can utilize calculation methods in the exploration of data derived from analysis forensic • Student can use the methods of analytical and physical chemistry, suitable for identification and differentiation of substances of forensic trace as well as Student knows the limitations of these methods • Student possesses the knowledge about safe work in toxicological and criminalistics laboratories, following the rules of law. Skills – Student can: • Student can minutely plan identification and comparative investigation of a selected trace. • Student can describe a used analytical method as well as interpret the results of identification analysis of selected traces. • Student can explain the interdisciplinary character of analysis of forensic traces. • The student knows English to the extent enabling the use of English-language literature in the field of forensic chemistry. • Student can present the application of modern microanalytical techniques for determination of organic and elemental composition and he/she can describe possible source of errors. Social competences – Student is ready to: • Student can assess its responsibility (also legal) for acquired results and their interpretation.		
Teaching staff and contact email	Dr. Małgorzata Król, Dr. Habil. Katarzyna Madej, Dr. Aneta Woźniakiewicz, Dr. Habil. Katarzyna Kurpiewska, Dr. Joanna Loch		
Examination			

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Course title	FORENSIC CHEMISTRY		
Information	Number of credits: 2 ECTS	Number of taught hours 20 h	Number of hours expected of student personal work: 30 h (total 50 h)
Synopsis	1. Introduction to areas of criminalistics and analytical problems (parts I and II - the application of analytical chemistry methods in forensic examinations). 2. Crime scene investigation. 3. Drugs profiling and mass spectrometry in forensic analysis 4. Forensic alcohology and toxicology. 5. Problems of forensic toxicological analysis. Characteristics of biological and non-biological materials in forensic toxicological analysis. Methods of isolating xenobiotics (e.g. alcohols, addictive substances and substances used in human and animal doping) from biological material. Screening methods in forensic toxicology. Analytical methods for the determination of xenobiotics in toxicological expertise. Interpretation of results and forensic toxicologist test. Toxicologist as an expert witness in court.		
Learning outcomes / skills and competencies	After completing this unit the student should be able to understand/can: • main problems related to the forensic chemistry, • different methods and techniques used for analysis of biological tissues and criminalistic traces, • description of the role and tasks of a chemist as a forensic expert. • knowledge of chemistry and technical sciences to describe the properties of materials forming a forensic trail. He can use the knowledge of analytical chemistry to identify and mark xenobiotics in the material collected during the autopsy. familiarization with the procedures for testing drivers for the presence of alcohol and alcohol-like substances. Can define the purpose and tasks of different areas of toxicology • computational methods to analyze the results of forensic traces analysis, prospective and retrospective in forensic alcohology. • methods of analytical and physical chemistry, useful in the identification of materials forming a forensic trail and knows their limitations. • action of selected xenobiotics which are the cause of fatal poisoning. • use scientific literature in order to select an analytical method and interpret research results • explain the interdisciplinary nature of research on forensic trace materials. He can use the knowledge of general toxicology in the interpretation of markings for the purposes of prosecution, courts and police. • use professional literature on research in the field of forensic chemistry. • assess responsibility - including legal responsibility for the obtained results and their evaluation		
Teaching staff and contact email	Prof. Dr. Habil. Wojciech Piekoszewski, Dr. Habil. Katarzyna Madej, Dr. Habil. Renata Wietecha Posłuszny (Professor JU), Dr. Habil. Michał Woźniakiewicz (Professor JU) (michal.wozniakiewicz@uj.edu.pl), Dr. Małgorzta Król, Prof. Michael Cole (guest lecturer, Anglia Ruskin University, Cambridge, England)		
Examination			

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Course title	MULTIVARIATE ANALYSIS IN CHEMISTRY		
Information	Number of credits: 5 ECTS	Number of taught hours 45 h	Number of hours expected of student personal work: 80 h (total 125 h)
Synopsis	Statistical treatment of experimental data. Introduction to mathematical modelling of processes. Empirical modelling. Linear models: determination of the model parameters and the corresponding variance-covariance matrix, model adequacy testing. Nonlinear models. Design of experiments. Optimization methods: single factor, gradient, simplex, Monte Carlo, Genetic Algorithm. Statistical treatment of multidimensional data. Introduction to the Principal Component Analysis (PCA) and Factor Analysis (FA), Cluster Analysis (CA), Pattern Recognition methods, Artificial Neural Networks (ANN), and other chemometric methods. .Regression models for two-way two-block data analysis: Multiple Linear Regression (MLR), Principal Component Regression (PCR) and Partial Least Squares (PLS) regression, non-quantitative and Quantitative Structure-Activity Relationships (SAR and QSAR), Alternating Least Squares Multiple Component Resolution (ALS-MCR), Learning machine, Classification reporting.		
Learning outcomes / skills and competencies	After completing this course the student should be in a position to propose and apply different data processing methods in order to retrieve the valuable information from the experimental data.		
Teaching staff and contact email	Dr. Habil. Michał Woźniakiewicz (Professor JU): michal.wozniakiewicz@uj.edu.pl), Dr. Habil. Kamilla Małek (Professor JU): kamilla.malek@uj.edu.pl		
Examination			

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Course title	QUANTUM-CHEMICAL MOLECULAR MODELLING		
Information	Number of credits: 10 ECTS	Number of taught hours 90 h	Number of hours expected of student personal work: 45 h (total 135 h)
Synopsis	The course covers practical aspects of molecular modelling with quantum-chemical methods. The lectures and computer lab cover: using quantum chemical software – general rules; input data for quantum chemical calculations; available software; Born-Oppenheimer approximation; potential energy surface (PES), stationary points on PES; practical aspects of geometry optimization of molecular systems; optimization of minima (reactants, products) and saddle points (transition states); reaction paths on PES; commonly used computational methods; variational and perturbational methods; Hartree-Fock method (HF); restricted and unrestricted HF (RHF and UHF); ab initio and semiempirical methods; basis sets in ab initio calculations; molecular orbitals, electron density, population and bond-order analysis; visualisation methods; chemical bond; differential density (deformation density); delocalized and localized orbitals; localization methods; vibrational analysis; normal modes; electron correlation; post-HF methods; Density functional theory (DFT) and Kohn-Sham (KS) method; practical aspects of DFT calculations; exchange-correlation functional choice; chemical reactivity; single- and two reactant reactivity indices; interaction energy partitioning methods; modelling elementary reactions of complex processes; thermodynamic properties; free-energy of chemical reactions other topics: modeling of large systems, hybrid methods (QMMM), solvent effects.		
Learning outcomes / skills and competencies	After completing this unit the student should be able to: • To build upon and extend the theoretical concepts introduced during the bachelor degree programme. • To develop the competence and confidence of the students in performing quantum-chemical calculations and interpreting their results. • To highlight modern methods of computational chemistry • To identify appropriate method for particular applications. • Choose and apply the appropriate computational method to a given problem; • Discuss in a comprehensive way the basic theoretical background of various computational methods and their applicability to various problems; • Estimate the degree of reliability of the results; • Explain to a non-specialists how computational quantum chemistry can be expected to provide valuable information in different areas of chemistry and related disciplines.		
Teaching staff and contact email	Prof. Dr. Habil. Artur Michalak: michalak@chemia.uj.edu.pl		
Examination			

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Course title	SPECTROSCOPIC METHODS FOR CHARACTERIZATION AND IMAGING OF BIOMATERIALS		
Information	Number of credits: 5 ECTS	Number of taught hours 65 h	Number of hours expected of student personal work: 60 h (total 125 h)
Synopsis	The course provides the basics of modern spectroscopic methods to study biological materials (in particular cells and tissues) and overview of their applications: basics of microscopy; confocal microscopy; basics of imaging methods currently used in medical diagnostics: MRI, CT, PET and ultrasonography and their limitations/drawbacks; principles of FT-IR spectroscopy and microscopy including description of IR modes; principles of Raman spectroscopy and microscopy; high resolution Raman imaging (TERS) and multiphoton methods (CARS, SRS, TPEF), super-resolution spectroscopic imaging methods (e.g. STORM, PALM, STED), multimodal imaging; high-resolution surface imaging methods (AFM, SNOM, SEM, TEM, STM); basics of chiroptical spectroscopy; examples of applications as well as pros and cons of discussed techniques; instrumentation: features of objectives and light sources (e.g. brightness, stability, spectral characteristics, coherence); types of light sources, including thermal, laser, synchrotron radiation; comparison of spectroscopic and electron microscopes, combination of near field and spectroscopic microscopes; operation, construction and function of dispersive elements; operation and construction of detectors.		
Learning outcomes / skills and competencies	Seven lab classes cover practical aspects regarding Raman, infrared, AFM and fluorescence spectroscopy and microscopy, as well as chemometric analysis and prepare students to obtain three-dimensional images of studied biological materials; determine distribution of biocomponents in biological samples; determine topography and physicochemical properties of surfaces of biological materials; record Raman, IR and fluorescence and AFM images of biological materials; analyze the spectra: preprocessing of spectra, uni- and multivariate analysis; document obtained results and reach conclusions. After completing this unit the student should be able to: • Explain the physicochemical basics of discussed spectroscopic methods; • Understand and critically evaluate scientific articles regarding the subject; • Critically compare spectroscopic methods to other techniques introduced previously during the learning program; • Select appropriate spectroscopic techniques and data analysis methods to solve specific research problems regarding biological samples; • Based on up-to-date scientific articles prepare a multimedia presentation on selected new applications of spectroscopic techniques for investigating biosamples.		
Teaching staff and contact email	Dr. Habil. Agnieszka Kaczor (Professor JU): agnieszka.kaczor@uj.edu.pl		
Examination			