Course title	Panel: advanced synthetic methods
Organizational unit	Faculty of Chemistry
ECTS credit allocation	2
Contact hours	24
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Part 1: Pseudopolymorphism in coordination polymers (8 h)

Coordinator: dr hab. Beata Nowicka, prof. UJ

Objective: Presentation of the possibilities of post-synthetic modification of coordination polymers by removal or exchange of guest molecules in their structure; presentation of the gravimetric dynamic vapour sorption method and its application in the studies of pseudopolymorphic forms.

Description: Dynamic vapor sorption method applied to hydrates and solvates allows the observation of phase transitions between different pseudopolymorphic forms and assessment of their stability regions. In coordination polymers and MOF-type structures it enables to predict the possibility of post-synthetic modifications involving reorganization of the structure upon removal or inclusion of guest molecules or exchange of labile ligands. The practical exercise will include sorption studies for a selected coordination polymer, followed by a post-synthetic modification and observation of differences in properties between the original and the modified form of the compound.

Recommended reading:

1. S. Kitagawa, R. Kitaura, S. Noro, *Angew. Chem. Int. Ed.*, **2004**, *43*, 2334–2375.

Part 2: Magnetic materials (8 h)

Coordinator: dr hab. D. Pinkowicz, prof. UJ

Objective: The participants will learn the theoretical and practical aspects of modern air-free synthesis and handling of organometallic and coordination compounds sensitive to trace amounts of oxygen and moisture.

Description: The course begins with a review of the basic concepts of organometallic compounds in the field of molecular magnetism and then moves towards their design and synthesis using organometallic and coordination chemistry methods. The course will cover synthesis and handling of compounds sensitive to O_2 and H_2O concentration as low as 10 ppm. The following air-free methods will be discussed and demonstrated: state-of-the-art Schlenk techniques, glovebox workstation and automated solvent purification system. The participants will synthesize a model organometallic compound with extremely high sensitivity to oxygen using glovebox workstation and then perform several operations on the solution of this compound using Schlenk techniques. The compound will be crystallized and characterized by means of single-crystal and powder X-ray diffraction analysis.

Recommended reading:

1. D. F. Shriver, M. A. Drezdzon, "The manipulation of air-sensitive compounds", Wiley 1986
2. D. Yeung, J. Penafiel, H. S. Zijlstra, J. S. McIndoe, "Oxidation of titanocene(III): the deceptive implicity of a color change", *Inorg. Chem.* **2018**, *57*, 457-461.
3. S. J. N. Burgmayer, "Use of a titanium metallocene as a colorimetric indicator for learning inert atmosphere techniques", *J. Chem. Educ.* **1998**, *75*, 460

Part 3: Advanced methods of organic synthesis (8 h)

Coordinator: dr. B. Trzewik

Objective: Presentation of modern and non-standard methods of organic synthesis.

Description: Sometimes you do not need heat to form a compound - non-standard methods of supplying energy to reaction systems. The vast majority of chemical transformations take place only when a sufficient number of substrate molecules or substrates obtain required energy. In many reactions, at room temperature, only a small number of molecules have the energy to overcome the activation barrier, making the rate of such reactions slow or undetectable. The most common and classic way to initiate or shorten the time of a chemical transformation is to provide energy by heating the reaction mixture. Although simple, this method has significant drawbacks, such as high heat losses for higher reaction temperatures, uneven distribution in the system or uncontrolled boiling of reactants. Fortunately, reactant molecules can be excited in many other ways by providing energy other than thermal. This can be achieved, for example, by performing mechanical work, the action of electromagnetic waves of different wavelengths: light or microwaves, by ultrasounds or electric current. In many cases, the use of such non-standard methods of supplying energy to the reaction system can drastically reduce reaction times, increase their yield and purity of the resulting products, or avoid the need for a solvent. Examples of the use of such methods will be presented, their comparison with the classical heating of reaction mixtures, combined with a short practice in the form of laboratory workshop.

Recommended reading:

1. Baig, R. B. N., Varma, R. S. *Chem. Soc. Rev.* **2012**, *41*, 1559–1584
2. Hernández, J. G., Bolm C. *J. Org. Chem.* **2017**, *82*, 4007–4019
3. Bruckmann, A.; Krebs, A., Bolm, C. *Green Chem.* **2008**, *10*, 1131–1141
4. Romero, N. A., Nicewicz, D. A. *Chem. Rev.* **2016**, *116*, 10075–10166

Part 4: Organic synthesis using the Schlenk line (8 h)

Coordinator: dr hab. Miłosz Pawlicki, prof. UJ

Goal: The main goal of the course is the presentation of the basis of construction of the Schlenk line and the peripheries crucial for conducting reaction in an inert atmosphere. The practical part focuses on presentation of techniques necessary for the effective utilisation of the argon-vacuum line in the synthesis but also shows the possibilities of using them in preparation of samples requiring analysis in an inert atmosphere.

Description: Contemporary organic synthesis finds its foundations in application of all available reactions leading to structural changes in the skeletons of organic compounds. A wide spectrum of potential modifications allows a formation of every type of connectivity in the frames of hydrocarbons that, because of the strict structural design, allows for a precise addressing of the obtained derivatives into concrete applications starting from classic medicinal chemistry endingup in modern molecular materials with an applicability as luminophores. This wide scope of possible applications requires increasing of the precision and efficiency of synthetic paths which utilisation leads to effective formation of target derivatives. Currently it can be easily noticed that a substantial weight is placed on application of the synthetic paths catalyzed with transition metal opening a request for using argon-vacuum line allowing to perform processes in an inert atmosphere. Schlenk techniques are broadly used for conducting the syntheses in an atmosphere protected from moisture and air. During the planned classes the foundations of construction of Schlenk line (argon-vacuum line) as well as a necessary equipment (glassware, high vacuum pumps, traps) will be discussed. In the practical part of the subject crucial techniques allowing for work in an inert atmosphere and conduction in the lab space reactions protected from the moisture and air will be discussed. Beside the fundamental techniques of solvents degassing (*pump-thaw approach*) the cannulation of degassed solvent to the sample will be also presented. The prepared sample will be analysed spectroscopically to show the quality of conducted experiments with application of Schlenk-line.

Recommended reading:

1. Herrmann, W. A. et al.: 1996 Synthetic Methods of Organometallic and Inorganic Chemistry (Herrmann/Brauer): Literature, Laboratory Techniques, and Common Starting Materials
2. Shriver, D. F.; Drezdzon, M. A. The Manipulations of Air-Sensitive Compounds, 2nd ed.; Wiley: New York, 1986

Course title	Panel: advanced computational methods
Organizational unit	Faculty of Chemistry
ECTS credit allocation	2
Contact hours	24
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Coordinator: dr hab. A. Eilmes, prof. UJ

Description:

1. numerical stability of algorithms
2. linear algebra
   - solving systems of linear equations; methods based on triangular factorizations
   - singular value decomposition of a matrix; solving overdetermined systems of equations
   - eigenvalues and eigenvectors
   - practical implementation on contemporary computer architectures; BLAS and Lapack libraries
3. solving nonlinear equations and systems of nonlinear equations
4. differential equations
   - ordinary differential equations and systems of ODEs; stiff systems
   - examples of solving partial differential equations
5. optimization
   - simplex method; gradient-based methods
   - finding a global minimum; simulated annealing; genetic algorithms

Recommended reading:

Mandatory: D. Kincaid, W. Cheney, Analiza numeryczna, WNT

Additional: Z. Fortuna, B. Macukow, J. Wąsowski, Metody numeryczne, WNT; documentation available on the Internet.

Course title	Panel: advanced microscopic methods
Organizational unit	Faculty of Chemistry
ECTS credit allocation	4
Contact hours	40
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Part 1: SEM and TEM microscopy (20 h)

Coordinator: prof. dr. hab. Zbigniew Sojka

Objective: The electron microscopy course aims to provide theoretical background and experimental experience on the use of electron microscopy techniques for investigations into the structure, morphology and chemical composition of inorganic materials and heterogeneous catalysts, which is required to interpret the SEM and S/TEM images, electron diffraction patterns, and for quantitative EDX and EELS analysis.

Description: The lecture covers the physical basics of geometrical, wave and Fourier optics. Basics of coherent and incoherent imaging, transmission function of the optical system. Electron optics and basic types of electron guns. The interaction of the electron beam with the material and types of generated signals. Construction and operation modes of the electron microscope. Image formation mechanism and types of contrast. Imaging on a micro- and nano-metric scale (morphology). Methods of grain shape analysis. High-resolution electron microscopy and picometric scale imaging (atomic structure). Methods for analysing the size and dispersion of grain sizes. Phase composition analysis - electron diffraction from a selected area (SAED), interpretation of electron diffraction patterns in kinematic and dynamic terms. X-ray characteristic energy dispersion spectroscopy (EDX/EDS), quantification methods and composition mapping. Electron energy filtration - application in imaging and diffraction. Electron energy loss spectroscopy (EELS), composition analysis with chemical resolution, spectral imaging in the micro and nano scale.

As part of the workshop the course participants will be trained in the method of preparing samples for microscopic examinations on selected examples. Participants will learn about the operating modes of the microscope and the practice of making measurements as well as the types of obtained information. They will be trained in computer processing and analysis of results, interpretation of images and electron diffractograms, including the use of simulation techniques and quantitative chemical analysis (EDX/EELS data quantification).

Recommended reading:

1. Gryboś, J., Indyka, P., Sojka, Z., (2021) Transmission Electron Microscopy and Elemental Analysis *chapter* in Metal Oxide Nanoparticles. Formation, Functional Properties and Interfaces,: Morphology, Structure, and Chemical Composition:, Wiley-Blackwell, ISBN 978-1-119-43678-2
2. Carter, C.B. and Williams, D.B. (2016). Transmission Electron Microscopy: A Textbook for Materials Science. Switzerland: Springer International Publishing.
3. Egerton, R.F. (2005). Physical Principles of Electron Microscopy. An Introduction to TEM, SEM and AEM. Springer.
4. Kirkland, E.J. (2010). Advanced Computing in Electron Microscopy. Springer.
5. Egerton, R.F. (2011). Electron Energy-Loss Spectroscopy in the Electron Microscope. Springer.

Part 2: AFM and fluorescence microscopy (20 h)

Coordinator: prof. dr. hab. Szczepan Zapotoczny

Objective: The aim of the course is gaining knowledge regarding the use of selected advanced microscopic methods in the characterization of materials and acquisition of the skills of sample preparation, measurement and processing of results in case of atomic force microscopy and confocal fluorescence microscopy.

Description: The workshop covers issues related to the advanced applications of microscopic research techniques such as atomic force microscopy (AFM) and confocal fluorescence microscopy. During the theoretical part, several issues will be discussed: the principle of operation and the structure of an atomic force microscope, advantages and disadvantages of AFM, applications, measurement possibilities and limitations, as well as the basic and advanced operating modes of the microscope. Examples of selected samples from various material groups will be used to carry out measurements by atomic force microscopy in advanced modes of operation, such as: surface topography mapping in air and in the liquid phase, thickness measurements of thin organic layers, mapping of mechanical and electrical properties, imaging of biological samples in aqueous solutions. The collected AFM micrographs will be subjected to appropriate processing and detailed analysis. In addition, workshop participants will be introduced to the most common sources of problems that occur when working with AFM microscopy. The classes also include a brief overview of the principles of operation of the advanced modes of the fluorescence and confocal microscopes and the presentation of general methods of preparing samples for observation using optical microscopy methods. On the examples of selected samples, students will carry out measurements in advanced modes of operation such as: three-dimensional imaging and measurements of the fluorescence spectra of micro-objects. Methods used for analysis of the obtained microscopic images will be presented as well.

Recommended reading:

1. Voigtländer, B. Atomic Force Microscopy, Springer Nature Switzerland AG **2019,** 1-331.
2. Nguyen-Tri, P.; Ghassemi, P.; Carriere, P.; Nanda, S.; Assadi, A.A.; Nguyen, D.D. Recent applications of advanced atomic force microscopy in polymer science: A review. *Polymers* **2020**, *12*, 1–28.
3. Jalili, N.; Laxminarayana, K. A review of atomic force microscopy imaging systems: Application to molecular metrology and biological sciences. *Mechatronics* **2004**, *14*, 907–945.
4. Howland, R.; Benatar, L.; A practical guide to scanning probe microscopy, Park scientific instruments, **1996,** 1-79**.**
5. Dazzi, A.; Prater, C.B. AFM-IR: Technology and applications in nanoscale infrared spectroscopy and chemical imaging. Chem. Rev. 2017, 117, 5146–5173.
6. Collazo, A.; Bricaud, O.; Desai, K. Use of confocal microscopy in comparative studies of vertebrate morphology. *Methods Enzymol.* **2005**, *395*, 521–543.
7. Furrer, P.; Gurny, R. Recent advances in confocal microscopy for studying drug delivery to the eye: Concepts and pharmaceutical applications. *Eur. J. Pharm. Biopharm.* **2010**, *74*, 33–40.
8. Chestnut, M.H. Confocal microscopy of colloids. *Curr. Opin. Colloid Interface Sci.* **1997**, *2*, 158–161.
9. Paddock, S.W. Principles and Practices of Laser Scanning Confocal Microscopy. *Mol. Biotechnol.* **2000**, *16*, 127–150.
10. Webb, R.H. Confocal optical microscopy: Reports on progress in physics. *Rep. Prog. Phys* **1996**, *59*, 427–471.

Course title	Panel: advanced spectroscopic methods
Organizational unit	Faculty of Chemistry
ECTS credit allocation	2
Contact hours	24
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Part 1: Advanced techniques of EPR spectroscopy (6 h)

Coordinator: dr. hab. P. Pietrzyk, prof. UJ

Objective: The aim of this part of the course is to acquaint students with the methodology of continuous-wave EPR studies of anisotropic systems and analysis of the obtained spectra as well as research possibilities of pulsed EPR spectroscopy. Research possibilities of the family of EPR techniques and chemical information contained in the spectra will be illustrated on the examples of recent literature reports.

Description:

1. Insights into continuous wave EPR spectroscopy:
   - anisotropy and symmetry of EPR spectra,
   - spectra of polycrystalline samples,
2. Pulse EPR spectroscopy
   - the basics of the spin echo phenomenon,
   - relaxation processes,
   - hyperfine sublevel spectroscopy.
3. Applications of EPR spectroscopy in chemical and material research - literature examples

Recommended reading:

1. Spektroskopia EPR w chemii i biochemii, M. Symons, PWN (1987)
2. Spektroskopia EPR. Zastosowania w chemii, R. Kirmse, J. Stach, Wyd. UJ, Kraków 1994
3. EPR Spectroscopy: Fundamentals and Methods, D. Goldfarb, S. Stoll (ed.) John Wiley & Sons; (2018)
4. Electron Paramagnetic Resonance Spectroscopy of Inorganic Materials (str. 225-300), P. Pietrzyk, T. Mazur, Z. Sojka, w Local Structural Characterisation: Inorganic Materials Series, John Wiley & Sons (2013)
5. Electron Paramagnetic Resonance Spectroscopy (str. 343-406), P. Pietrzyk, Z. Sojka, E. Giamello, in: Characterization of Solid Materials and Heterogeneous Catalysts - From Structure to Surface Reactivity, Tom 1, Wiley-VCH Verlag (2012)

Part 2: Advanced techniques of Raman spectroscopy (6 h)

Coordinator: prof. dr. hab. M. Barańska; dr hab. K. Małek, prof. UJ

Objective: Introducing students to the physical basics of advanced methods of Raman scattering spectroscopy allowing the analysis of objects at micro- and nanoscopic scale. Research possibilities of Raman techniques will be illustrated on the examples of the latest literature reports and at demonstration.

Description: The panel consists of a 4-hour lecture and a 2-hour demonstration of one of the discussed Raman spectroscopy technique. Raman imaging, nonlinear techniques for fast imaging (Coherent Anti-Stokes Raman Scattering - CARS and Stimulated Raman Scattering - SRS), plasmonic enhancement of the Raman effect (Surface Enhanced (SERS) and Tip Enhanced (TERS) Raman Spectroscopy) will be presented. PhD students will learn about the scope of application of these techniques for the chemical characterization of new materials, tracing of chemical processes, detection at the molecular level.

Recommended reading:

1. Chapters 2, 4.4, 5, 7.13, 7.14 in *Vibrational spectroscopy. From theory to practice*, K. Malek (ed.), PWN 2016
2. *Stimulated Raman Scattering Microscopy*, Ji-Xin Cheng, Wei Min, Yasuyuki Ozeki, Dario Polli (eds), Elsevier, 2021
3. *Confocal Raman Microscopy*, Jan Toporski, Thomas Dieing, Olaf Hollricher (ed.), Springer Series in Surface Sciences book series (SSSUR, vol.66), 2018
4. *Surface-Enhanced Raman Spectroscopy,* Sebastian Schlücker, Wiley-VCH Verlag GmbH & Co. KGaA, 2011

Part 3: Advanced techniques of FTIR spectroscopy (6 h)

Coordinator: prof. dr hab. K. Góra-Marek

Objective: Introducing PhD students to non-trivial applications of infrared spectroscopy.

Description: The course focus on issues related to the study of catalytic properties of porous materials by modern FTIR techniques. Rapid scanning IR measurements (phenomena in the 0.2 ms time domain) include research related to (i) diffusion of reagent molecules in materials with different topology and channel sizes, (ii) interaction of molecules with different properties (acidity/alkalinity/polarity) with active centres. Two-dimensional IR correlation spectroscopy will be also discussed, as well as the basics of catalytic measurements carried out in the operando mode, i.e. the coupling of IR spectroscopic measurements with studies of catalytic activity.

Recommended reading:

1. Two-dimensional correlation spectroscopy: applications in vibrational and optical spectroscopy, Isao Noda, Yukihiro Ozaki, John Wiley & Sons – introduction
2. In Situ and Operando Spectroscopy: A Powerful Approach Towards Understanding Catalysts; Johnson Matthey Technol. Rev., 2018, 62, (3), 316–331
3. Operando IR coupled to SSITKA for photocatalysis: reactivity and mechanistic studies, ACS Catalysis, 12, 2013, 2790-2798

Part 4: Advanced methods of NMR spectroscopy (6 h)

Coordinator: dr B. Musielak

Aim: Application of NMR spectroscopy in structural studies of small molecules and biomolecules.

Description: As part of the course, the doctoral student will learn: proper preparation of the sample for NMR analysis; TopSpin software - commands, spectrum processing; DEPT and APT techniques, 2D spectroscopy (COSY, HSQC, HMBC, TOCSY, NOESY, ROESY), methods suitable for investigation of protein-protein, and protein-inhibitor interactions.

Recommended reading:

1. J. Keeler, Understanding NMR spectroscopy, J. Wiley 2010 http://www-keeler.ch.cam.ac.uk/
2. H. Gunther, NMR Spectroscopy: Basis Principles, Concepts and Applications in Chemistry, WILEY-VCH Verlag, GmbH&Co. KGaA. Weinheim, Germany, 2013.
3. R. M. Silverstein, F. X. Webster, D. J. Kremle, Spektroskopowe metody identyfikacji związków organicznych

Course title	Panel: advanced structural methods
Organizational unit	Faculty of Chemistry
ECTS credit allocation	4
Contact hours	40
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Part 1: Structural analysis of biomolecules (20 h)

Coordinator: prof. dr. hab. Krzysztof Lewiński

Objective: to familiarize PhD students with the structural analysis of biomolecules

Description: Advanced methods in CSD and PDB structural databases application. Statistical analysis of molecular conformation and intra-/intermolecular interactions in the crystal. Analysis of the 3D protein structure and the ligand binding site. Evaluation of the correctness of macromolecular structural data in the aspect of designing low-molecular-weight ligands. Preparation of the protein and ligands structure for docking procedures. Molecular docking methods, analysis of the scoring function results and the verification of the docked poses. Determination of interactions between the ligand and amino acids of the protein binding pocket – creation of the 2D ligand-protein interactions map (2D ligand plot).

Recommended reading:

1. S. K. Burley, et al. *RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences,* Nucleic Acids Research 49: D437–D451, 2021, DOI: 10.1093/nar/gkaa1038
2. I. J. Bruno, J. C. Cole, P. R. Edgington, M. Kessler, C. F. Macrae, P. McCabe, J. Pearson, R. Taylor, *New software for searching the Cambridge Structural Database and visualising crystal structures*, Acta Cryst., B58, 389-397, 2002, DOI: 10.1107/S0108768102003324
3. M. L. Verdonk, J. C. Cole, M. J. Hartshorn, C. W. Murray, R. D. Taylor, *Improved Protein-Ligand Docking Using GOLD,* Proteins, 52, 609-623, 2003, DOI: 10.1002/prot.10465

Part 2: Structural analysis of polycrystalline and antique materials (20 h)

Coordinator: prof. dr. hab. W. Łasocha

Objective: Presentation of the potential of diffraction methods to the investigation of the material properties, catalytic research, and antiques.

Description: Classic applications usually include qualitative and quantitative phase analysis and determination of crystallite size, while the new applications include:

- Powder diffraction under conditions of variable temperatures and pressures
- Measurements in reactive gas atmospheres (applications in catalysis)
- Texture analysis (preferred crystallite orientation)
- Full structural studies

Recommended reading:

1. Shankland, Kenneth, Markvardsen, Anders J. and David, William I. F.. "Powder diffraction based structural studies of pharmaceuticals" *Zeitschrift für Kristallographie - Crystalline Materials*, vol. 219, no. 12, 2004, pp. 857-865. https://doi.org/10.1524/zkri.219.12.857.55864
2. Altomare, Angela, Caliandro, Rocco, Camalli, Mercedes, Cuocci, Corrado, Giacovazzo, Carmelo, Moliterni, Anna Grazia Giuseppina, Rizzi, Rosanna, Spagna, Riccardo and González-Platas, Javier. "Towards EXPO2005" Zeitschrift für Kristallographie - Crystalline Materials, vol. 219, no. 12, 2004, pp. 833-837. https://doi.org/10.1524/zkri.219.12.833.55860
3. Favre-Nicolin, Vincent and Černý, Radovan. "A better FOX: using flexible modelling and maximum likelihood to improve direct-space *ab initio* structure determination from powder diffraction" *Zeitschrift für Kristallographie - Crystalline Materials*, vol. 219, no. 12, 2004, pp. 847-856. https://doi.org/10.1524/zkri.219.12.847.55869
4. David, W. I., Shankland, K., McCusker, L. B., & Baerlocher, C. (Eds.). (2006). Structure determination from powder diffraction data (Vol. 13). OUP Oxford.

Course title	Panel: advanced analytical methods
Organizational unit	Faculty of Chemistry
ECTS credit allocation	2
Contact hours	24
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

The classes will consist of 4 thematic blocks listed below. Each subject will be presented in the form of a lecture and a workshop (the proportion will depend on the specific topic and expectations of participants). The overall aim of the course is to familiarize PhD students with modern issues of analytical chemistry and research carried out in the laboratories of the Faculty of Chemistry.

Coordinator: dr hab. Renata Wietecha-Posłuszny, prof. UJ

Part 1: **Quality of analytical methods (6 h)**

Objective: To familiarize PhD students with the concepts of the quality of analytical methods: validation, models of comprehensive evaluation of the analytical method quality and their fitting to the principles of sustainable development, as well as "green" and "white" analytical chemistry. PhD students will be introduced to selected examples of analytical methods of high complex quality and consistent with the idea of "green" and "white" analytical chemistry.

Description: In the seminar part, a model of comprehensive evaluation of the analytical method based on the RGB colour mixing model will be demonstrated, in a basic version and adapted to the evaluation of methods in accordance with the idea of "white" analytical chemistry. On the example of selected analytical methods, participants will learn to use the RGB model in practice, which will allow them to assess the potential of their own methods, which they will in their work in the future.

Recommended reading:

1. E. Bulska, Metrologia Chemiczna, rodz.: 4,7,9, Wydawnictwo Malamut, Warszawa 2008.
2. J. Namieśnik, P. Konieczka, B. Zygmunt, E. Bulska, i in., rodz.: 3,4,8, Ocena i kontrola jakości wyników pomiarów analitycznych, Wydawnictwo Naukowo-Techniczne, Warszawa, 2007
3. P.M. Nowak, P. Kościelniak, What color is your method? Adaptation of the RGB additive color model to analytical method evaluation, Analytical Chemistry, 91, 2019, 10343-10352, https://doi.org/10.1021/acs.analchem.9b01872
4. P.M. Nowak, R. Wietecha-Posłuszny, J. Pawliszyn, White Analytical Chemistry: An approach to reconcile the principles of Green Analytical Chemistry and functionality, Trends in Analytical Chemistry, 138, 2021, 116223, https://doi.org/10.1016/j.trac.2021.116223

Part 2: Preparation of samples for chemical and biochemical analysis (6 h)

Objective: Theoretical and practical introduction to modern methods of sample preparations of various materials for chemical analysis.

Description: The theoretical basis of the separation process will be presented (including: thermodynamic description, basic separation mechanisms and intermolecular interactions) and the concept of lipophilicity and the possibility of predicting molecular interactions. Issues related to modern methods of separating analytes (e.g. techniques requiring specialized apparatus or laboratory equipment: MAE, SPME and those in requires skills in pipetting: Cloud Point Extraction (CPE) and QuEChERS extraction , i.e. Quick, Easy, Cheap, Effective, Rugged and Safe extraction from a variety of non-biological and biological matrices. Modified methods of preparing biological matrices for inorganic analyses will be presented (including mineralization assisted by microwave radiation with minimal consumption of sample). Various modifications of these techniques (e.g. miniaturization) and their application in analytical practice will also be presented.

Recommended reading:

1. L. Ruchomski, QuEChERS – metoda wielopozostałościowa (cz. I), LAB 5, 2020
2. S. Yazdi, *Surfactant-based extraction methods,* Trends in Analytical Chemistry 30(6), 2011, 918-929
3. P. Stepnowski, E. Synak, B. Szafranek, Z. Kaczyński, *Techniki separacyjne*, Wydawnictwo Uniwersytetu Gdańskiego, Gdańsk 2010
4. S. Risticevic, D. Vuckovic, H. Lord, J. Pawliszyn, *Solid-Phase Microextraction*, Elsevier, 2012. doi:10.1016/B978-0-12-381373-2.10055-9
5. A. Wójtowicz, R. Wietecha-Posłuszny, *Contemporary Trends in Drug Analysis of Vitreous Humor: A critical review,* Trends in Analytical Chemistry, 129C (2020) 115935, doi: 10.1016/j.trac.2020.115935

Part 3: Multicomponent and Speciation Analysis (6 h)

Objective: To familiarize PhD students with the prospects of contemporary coupled techniques (LC-MS, GC-MS, CE-MS, LC-ICP-MS) in multicomponent and speciation analysis.

Description: Speciation and multicomponent analysis will be presented on the examples of investigations carried out in renowned laboratories, with an emphasis on the interdisciplinarity of methods. Methodology of working with coupled techniques will point on the multidimensionality of research, the need to combine multiple techniques in order to ensure complementarity of the obtained information. HPLC-ICP-MS, LC-Q-TOF-MS, CE-MS setup will be presented and requirements for the properties of analysed samples will be discussed.

Recommended reading:

1. C.F. Poole, *The Essence of Chromatography*, Elsevier 2003
2. M.S. Lee, *Mass Spectrometry Handbook*, Wiley 2012
3. H.H. Lauer and G.P. Rozing, *High Performance Capillary Electrophoresis,* Second edition, Agilent Technologies: https://www.agilent.com/cs/library/primers/public/5990-3777EN.pdf
4. Praca zbiorowa pod redakcją W. Żyrnicki, E. Borkowska-Brunecka, E. Bulska i E. Szmyd, *Metody analitycznej spektrometrii atomowej*, MALAMUT, Warszawa 2010.
5. John R. Dean, *Practical Inductively Coupled Plasma Spectroscopy*, Wiley 2005
6. Praca zbiorowa pod redakcją D. Barałkiewicz i E. Bulskiej, *SPECJACJA CHEMICZNA - Problemy i możliwości*, MALAMUT, Warszawa 2009.

Part 4: Chemical sensors and biosensors (6 h)

Objective: Understanding the basic issues related to sensors and biosensors.

Description: Definition of the sensor and biosensor, division of (bio) sensors, immobilizing matrices and composites modifying sensors, immunosensors. Examples of (bio) sensors and their application in medical diagnostics. In the seminar part, exemplary functional materials of electrochemical sensors will be presented.

Recommended reading:

1. Z. Brzózka, E. Malinowska, W. Wróblewski, *Sensory chemiczne i biosensory*, PWN, Warszawa, 2022
2. P. Gründler, *Chemical Sensors*, Springer-Verlag Berlin Heidelberg, Lipsk, 2007 I link – dostęp on line: https://link.springer.com/content/pdf/10.1007/978-3-540-45743-5.pdf
3. J. Kochana, A. Pollap, M. Madej, rozdział: *Bioczujniki : zasada działania, receptory, detektory* w: Bioanalityka w nauce i życiu, Nowe strategie analityczne i rozwiązania aparaturowe, PWN, Warszawa, 2020.

Course title	Panel: BioPharma
Organizational unit	Faculty of Chemistry
ECTS credit allocation	2
Contact hours	24
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Part 1: Therapeutic antibodies as biopharmaceuticals (8 h)

Coordinator: Dr. Łukasz Skalniak

Objective: The aim of the course is to familiarize participants with the unique properties of therapeutic antibodies and explain the phenomenon of their use in both laboratory and biomedical procedures.

Description: The course (4h seminar, 4h laboratory) will address the biochemical nature of antibodies, their properties, natural biological functions, production in the body and in the laboratory, isolation and purification, laboratory and medical applications, as well as nomenclature. During the practical part, one of the laboratory procedures using antibodies and illustrating their biochemical properties will be performed.

Recommended reading:

1. *"An Introduction to Medicinal Chemistry",* Graham L. Patrick, Oxford University Press, ISBN 978-0-19-874969-1

Part 2: New drugs: from synthesis to clinical studies (8 h)

Coordinator: dr. hab. Janusz Dąbrowski, prof. UJ

Aim: The course will discuss the path that a chemical compound must follow from its discovery to the so-called pharmacy. Selected research on new drugs will be presented, both fundamental, as well as parts of preclinical and clinical studies. The course will also provide an understanding of how the chemical structure of biologically active compounds determines their physicochemical and pharmacological properties, and how their further modification may contribute to their use in medicine. In addition, the course is designed to provide the experimental basis for the use of a variety of research techniques to determine the basic pharmacological parameters and biological activity.

Description: Sources of new drugs include chemical compounds found in plants, animal organisms, but the greatest role in the drug discovery and development process is the synthesis of new chemical compounds with improved physicochemical and pharmacological properties and desired biological activity that can be used to treat or prevent disease. Substances are modified by substituting different chemical groups or metal ions into it, yielding several variants with more favorable properties compared to the parent drug. In this lecture, course participants will learn examples of basic, preclinical and clinical research. The scientific research process that potential drugs must undergo before reaching clinical trials will be examined. Cellular, tissue and animal models in preclinical practice will be discussed. The workshop will determine the basic pharmacological parameters (e.g. octanol/water partition coefficient, half-life) and biological properties (cytotoxicity, accumulation in cells) of potential drugs.

Recommended reading:

1. J.M. Dąbrowski, *Advances in Inorganic Chemistry* (2017) 70, 343-394.
2. B. Pucelik, A. Sułek, J.M. Dąbrowski, *Coord. Chem. Rev.* (2020) 416, 213340.
3. B. Pucelik, A. Sułek, A. Barzowska, J.M. Dąbrowski *Cancer Letters* (2020) 492, 116-135.

Part 3: Raman biospectroscopy (8 h)

Coordinator: prof. dr. hab. M. Barańska; dr. hab. K. Małek, prof. UJ

Objective: Introducing students to the methodology of Raman studies on biological samples and spectroscopic data analysis. Overview of confocal Raman imaging supported by atomic force microscopy (AFM), near-field optical microscopy (SNOM) and fluorescence microscopy as a modern approach to the comprehensive spectroscopic analysis of biological samples.

Description: The panel consists of a 6-hour lecture and a 2-hour demonstration of one of the discussed Raman spectroscopy techniques. Raman imaging and plasmonic enhancement of the Raman effect (Surface Enhanced (SERS) and Tip Enhanced (TERS) Raman Spectroscopy) will be presented as well as the coupling of these techniques with an optical confocal microscope or near field microscopies (AFM, SNOM). Raman Optical Activity (ROA) in combination with Circular Dichroism (CD) will also be presented as an alternative approach in the analysis of chiral samples and polymorphism. PhD students will learn about the application of these techniques in the analysis of biological, medical and pharmaceutical samples. In the demonstration part of the panel, PhD students will be familiarized with the practical aspects of working with biological samples during confocal Raman measurements and AFM imaging of cells.

Recommended reading:

1. Chapters 2, 4.4, 5, 7.13, 7.14 in *Vibrational spectroscopy. From Theory to practice*, K. Malek (ed.), PWN 2016
2. *Atomic Force Microscopy of Mammalial Cells* - materials will be provided.
3. *Confocal Raman Microscopy*, Jan Toporski, Thomas Dieing, Olaf Hollricher (editors), Springer Series in Surface Sciences book series (SSSUR, vol. 66), 2018
4. *Surface-Enhanced Raman Spectroscopy,* Sebastian Schlücker, Wiley-VCH Verlag GmbH & Co. KGaA, 2011

Course title	Panel: Technology and environmental chemistry
Organizational unit	Faculty of Chemistry
ECTS credit allocation	2
Contact hours	24
Teaching language	Polish
Type of class	workshop
Examination	credit with a grade

Part 1: Chemical synthesis on a technical scale (8 h)

Coordinator: prof dr. hab. Piotr Kuśtrowski

Objective: As part of the workshop, PhD students will learn about the possibilities and limitations of up-scaling chemical synthesis to a technical scale.

Description: Demonstration and discussion classes based on the analysis of typical processes carried out in the chemical industry. Reactor techniques as well as devices for unit operations used on an industrial scale will be presented on selected examples. PhD students will learn, among others, with the specificity of technology and the functioning of the installation for the production of synthesis gas, ammonia and nitric acid, nitrogen fertilizers, polymerization processes or obtaining materials in kilogram scale.

Recommended reading:

1. Jacob A. Moulijn, Michiel Makkee, Annelies Van Diepen, "Chemical Process Technology", John Wiley & Sons, 2013
2. Andreas Jess, Peter Wasserscheid, "Chemical Technology: From Principles to Products", Wiley-VCH, 2020
3. Krzysztof Schmidt-Szałowski, Mikołaj Szafran, Ewa Bobryk, Jan Sentek, "Technologia chemiczna", Wydawnictwo Naukowe PWN, 2013

Part 2: The challenges of sustainable chemistry (8 h)

Coordinator: dr hab. Katarzyna Hąc-Wydro, prof. UJ

Objective: The aim of the course is to present, based on the selected examples, the importance of chemical sciences in environmental and sustainability efforts.

Description:

Lecture (2h): Sustainable development, European Green Deal, actions and challenges for environmental protection and sustainable development on the examples of the European Strategy for Plastics in a Circular Economy, "Farm to Fork" strategy, cosmetics law;

Sustainable chemistry - research areas in chemical sciences for environmental protection and sustainable development, their importance and selected achievements (environmental monitoring and environmental analytics, new methods of removing harmful substances from various elements of the environment, methods of reducing emissions of environmentally harmful Substances);

Workshops (6h): 1. (3h) Preparation of lipid membrane models and their use to illustrate toxic effects of the substances emitted from plastics (e.g. bisphenol) on biological systems, 2. (3h) Detection of heavy metals in colored cosmetics - analysis and interpretation of the results in relation to the legal norms being in force.

Recommended reading:

1. M. Burchard-Dziubińska et al. *Zrównoważony rozwój – naturalny wybór*, rozdz. 1, wydawnictwo UŁ, 2014 (dostępna online)
2. Ch. Blum, et al, *The concept of sustainable chemistry: Key drivers for the transition towards sustainable development, Sustainable Chemistry and Pharmacy*, 5 (2017) 94- 104
3. P. Marion et al., *Sustainable chemistry: how to produce better and more from less?* Green Chem., 19 (2017) 4973

Part 3: Sustainable Li-ion energy storage technologies (8 h)

Coordinator: dr hab. Marcin Molenda, prof. UJ

Objectives: Participants will learn the practical aspects of design, scale-up and the elementals of implementation process of sustainable material technologies used in electrical energy storage based on Li-ion battery technology in the era of green energy transformation.

Description: Workshops (lecture and practical classes in "case study" formula). The principles of green chemistry designing of sustainable material technologies covering the entire product value chain will be discussed: raw materials-processing-application-management-recycling, aspect of environmental impact (carbon footprint), energy efficiency and economy as well as regulations. The technology scale-up process and the elementals of implementation process will be presented on the selected example of the active material technology (cathode or anode). As part of the practical "case study" classes, participants will conduct the process of synthesis of active material for Li-ion cells on a semi-technical scale of ca. 1 kg, for which they will perform a material and energy balance. The obtained product will be used to build demonstrators of Li-ion cells and their electrochemical validation.

Recommended reading:

1. M. Yoshio, R. Brodd, A. Kozawa: Lithium-Ion Batteries, Springer, 2009
2. A. Czerwiński: Akumulatory, baterie, ogniwa, WKŁ, 2005
3. FCAB National Blueprint Lithium Batteries.
   https://www.energy.gov/sites/default/files/2021-06/FCAB%20National%20Blueprint%20Lithium%20Batteries%200621_0.pdf
4. Batteries Europe: Strategic Research Agenda for batteries 2020.
   https://ec.europa.eu/energy/sites/default/files/documents/batteries_europe_strategic_research_agenda_december_2020__1.pdf