UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	SPEKTROSKOPSKE METODE V BIOKEMIJI
Course Title:	SPECTROSCOPIC METHODS IN BIOCHEMISTRY

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
UŠP Biokemija, 1. stopnja	**/**	**3.**	**5.**
USP Biochemistry, 1st Cycle	**/**	**3rd**	**5th**

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: BK130

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30	**10**	**35 SV**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: prof. dr. Janez Košmrlj / Dr. Janez Košmrlj, Full Professor

Jeziki / Languages:

Predavanja / Lectures:	**slovenski / Slovenian**
Vaje / Tutorial:	**slovenski / Slovenian**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	Prerequisites:
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	Content (Syllabus outline):
Splošen uvod v spektroskopijo: elektromagnetno valovanje in interakcija z materijo, energetska stanja, prehodi med njimi, resonančni pogoj, absorpcija in emisija energije. Masna spektrometrija: princip delovanja masnega spektrometra, izotopska sestava, fragmentacije, ionizacijske metode, MS visoke ločljivosti, masni spektri spojin z velikimi molekulskimi masami. UV/Vis spektroskopija: vibracijski in elektronski nivoji molekule, prehodi med njimi, UV/Vis spektroskopija, polarimetrija, kirooptične metode (optična rotacijska disperzija (ORD) in cirkularni dihronizem (CD)), fluorescenca	General introduction to spectroscopy: Physical background of spectroscopic methods (electromagnetic radiation, interaction of light with matter, energy levels and transitions between them, absorption and emission of energy). Mass spectrometry (principles of measuring molecular mass, ionization techniques, ion mass analysis, low- and high-resolution MS, mass spectra of molecules with high molecular weight). UV/Vis spectroscopy: vibration and electron levels, transitions, UV/Vis spectroscopy, polarimetry, optical rotary dispersion (ORD) and circular dichroism (CD), fluorescence (emission,

(emisijski, ekscitacijski spekter, korekcija spektra, Stokesov premik, absolutni in relativni kvantni izkoristek). Vibracijska in rotacijska spektroskopija: Ramanska, IR in mikrovalovna spektroskopija, uporaba. Nuklearna magnetna resonanca (NMR): Osnove NMR eksperimenta, kemijski premik, multipliciteta in sklopitvena konstanta, integral, primerjava zveznega in pulznega načina snemanja NMR spektrov, osnove modernih 1D in 2D NMR tehnik. Elektronska paramagnetna resonanca (EPR): Principi EPR, hiperfina struktura, primeri uporabe EPR. Metode strukturnega in funkcionalnega slikanja: MRI (Magnetic Resonance Imaging), slikanje strukture organov in tkiv, principi delovanja, pozitronska emisijska tomografija (PET), principi metode, uporaba PET v raziskavah biokemijskih procesov v živih organizmih, konfokalna mikroskopija, principi, uporaba. Vaje: Urjenje v uporabi spektrometrov in interpretaciji spektrov za določanju struktur modelnih molekul in pri vsakodnevnem delu v (biokemijskem) laboratoriju.	excitation spectrum, correction for PMT response, Stokes shift, absolute and relative quantum yield. Vibration and rotation spectroscopy: Raman, IR and microwave spectroscopy, application in biochemistry. Nuclear magnetic resonance (NMR): basics of NMR experiments, chemical shift, homonuclear and heteronuclear coupling, integration, continuous wave versus pulse experiments, basics of modern 1D and 2D NMR methods. Electron paramagnetic resonance (EPR): principles of EPR experiments, hyperfine splitting, application. Methods of structural and functional imaging: Magnetic Resonance Imaging (MRI), imaging of tissues and organs, principles and application, positron emission tomography (PET), principles and application, confocal optical fluorescence microscopy, principles and application. Practical spectroscopy: sample preparation, basic instrumental procedures, one-dimensional experiments (1H, 13C, X), two-dimensional experiments (COSY, TOCSY, HMQC, HMBC).

Temeljna literatura in viri / Readings:

- M. Hesse, H. Meier, B. Zeeh, Spectroscopic Methods in Organic Chemistry, Thieme, 2008; 453 str.

Dodatna literatura / Additional reading:

- G.M. Lampman, D. L. Pavia, G. S. Kriz, J. R. Vyvyan, Spectroscopy, Brooks/Cole 2010 Int. Ed.; 656 str.
- A. Petrič, Spektroskopske metode v biokemiji (interno študijsko gradivo), UL FKKT, Ljubljana, 2012 (167 str.).

Cilji in kompetence:	**Objectives and Competences:**
Cilji: Namen predmeta je posredovati študentu osnove in ga izuriti v uporabi spektroskopskih metod s posebnim poudarkom na uporabi v biokemiji. Absolvent predmeta je sposoben načrtovati uporabo in izbiro ter interpretirati rezultate	**Objectives**: To teach students theory and practice of spectroscopic methods with the emphasis on the application in biochemistry. After the course, the student is capable of designing and selection of appropriate experiments in solving spectroscopic problems

spektroskopskih metod pri reševanju strokovnih problemov na področju biokemije. **Kompetence:** Sposobnost načrtovanja, izvedbe in interpretacije spektroskopskih eksperimentov za uporabo v biokemiji.	in the field of biochemistry. **Competences**: Ability to design, perform, and interpret spectroscopic experiments for biochemical applications.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Razumevanje osnovnih principov spektroskopskih in spektrometričnih tehnik, prenosa energije elektromagnetnega valovanja na materijo in izkoriščanja tega efekta za določanje strukture molekul.	Knowledge and Comprehension Understanding the basic principles of spectroscopic methods, interaction of matter and electromagnetic waves, and utilization of this interaction in molecular structure elucidation.
Uporaba Uporaba naučenih principov oziroma zakonitosti za analizo oziroma določanje strukture molekul s pomočjo spektroskopskih in spektrometričnih tehnik.	Application Student will be able to apply the acquired knowledge in solving analytical problems.
Refleksija Zavedanje, da sicer podatki, pridobljeni s spektroskopskimi ali spektrometričnimi metodami, vsebujejo informacije o strukturi molekul, da pa je potrebno te podatke kritično uporabiti. Rezultat spektroskopske analize mora ustrezati vsem pridobljenim spektroskopskim lastnostim hkrati.	Analysis Being aware that data, acquired by spectroscopic methods contain information on molecular structure but they must be critically evaluated. All measured spectroscopic characteristics must uniformly support the proposed solution of the problem.
Prenosljive spretnosti Pri predmetu se študenti z reševanjem znanih in neznanih problemov izurijo v uporabi spektroskopskih in spektrometričnih tehnik, analitičnega mišljenja in uporabe literaturnih virov.	Skill-transference Ability Using known and unknown examples the student is trained in utilization of spectroscopic methods, analytical thinking and using literature sources.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminarske in laboratorijske vaje.	Lectures and problem solving seminars.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni izpit Ocene: 6-10 (pozitivno), 1-5 (negativno).		Written exam Grades: 6-10 (positive), 1-5 (negative)

Reference nosilca / Lecturer's references:

1) A. Demšar, **J. Košmrlj**, S. Petriček: Variable-temperature nuclear magnetic resonance spectroscopy allows direct observation of carboxylate shift in zinc carboxylate complexes. J. Am. Chem. Soc. 2002, 124, 3951–3958.
2) J. Košmrlj, S. Kafka, I. Leban, M. Grad: Formation and Structure Elucidation of Two Novel

Spiro[2H-indol]-3(1H)-ones, Magn. Reson. Chem. 2007, 45, 700–704.
2) B. Pinter, A. Demšar, D. Urankar, F. De Proft, **J. Košmrlj**: Conformational Fluxionality in a Palladium(II) Complex of Flexible Click Chelator 4-phenyl-1-(2-picolyl)-1,2,3-triazole. A dynamic NMR and DFT study. Polyhedron 2011, 30, 2368–2373.
4) K. Proisl, S. Kafka, D. Urankar, M. Gazvoda, R. Kimmel, **J. Košmrlj**: Fischer indolisation of N-(α-ketoacyl)anthranilic acids into 2-(indol-2-carboxamido)benzoic acids and 2-indolyl-3,1-benzoxazin-4-ones and their NMR study. Org. Biomol. Chem. 2014, 12, 9650–9664.
5) M. G. Sommer, P. Kureljak, D. Urankar, D. Schweinfurth, N. Stojanović, M. Bubrin, M. Gazvoda, M. Osmak, B. Sarkar, **J. Košmrlj**: Combining [Arene–Ru] with Azocarboxamide to Generate a Complex with Cytotoxic Properties. Chem. Eur. J. 2014, 20, 17296–17299.