UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	SODOBNI NMR PRISTOPI V KARAKTERIZACIJI SPOJIN
Course Title:	MODERN NMR APPROACHES IN CHARACTERIZATION OF COMPOUNDS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
DR Kemijske znanosti, 3. stopnja	**/**	**1.**	**1. in 2.**
Doctoral programme in Chemical Sciences, 3rd Cycle	**/**	**1st**	**1st and 2nd**

Vrsta predmeta / Course Type: izbirni/Elective

Univerzitetna koda predmeta / University Course Code: KZ313

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30	**45**	**/**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: prof. dr. Janez Plavec /Dr. Janez Plavec, 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):**
Jedrski spin, NMR eksperiment, relaksacija, kompozitni pulzi, heteronuklearno razklapljanje, ”spin lock”, selektivno vzbujanje, gradientni pulzi, difuzija, obdelava NMR spektrov, heteronuklearni eksperimenti, editiranje spektrov, prenos polarizacije, večdimenzionalni NMR eksperimenti, povezave preko vezi in preko prostora, asignacija spektrov, računanje strukture iz NMR podatkov, ravnotežja in dinamične lastnosti molekul, NMR v trdnem agregatnem stanju, polimorfizem in solvatacija. Vsebina oz. program izvajanja predmeta bosta individualno prilagojena raziskovalnim	Nuclear spin, NMR experiment, relaxation, composite pulses, heteronuclear decoupling, spin lock, selective excitation, gradient pulses, diffusion, processing and interpretation of NMR spectra, heteronuclear experiments, spectral editing, polarisation transfer, multidimensional NMR experiments, correlations through bonds and through space, spectral assignment, NMR restraint molecular modelling, equilibrium and dynamic properties of molecules, solid state NMR, polymorphism and solvation. Contents and the program of the course will be individually adjusted as per requests and scientific interests of individual students. The

usmeritvam posameznega študenta. Vsebine je mogoče prilagoditi do te mere, da bo študent lahko sodobne NMR pristope po uspešno opravljenem predmetu samostojno uporabljal na organskih, anorganskih, farmacevtskih, biokemijskih in ostalih vzorcih tako v trdnem kot v tekočem agregatnem stanju.	course can be tailor-made to the level which will allow students to independently use NMR spectroscopy in later studies of organic, inorganic, pharmaceutical, biochemical and other samples in solid as well as in liquid states.

Temeljna literatura in viri / Readings:

- T.D.W. Claridge, High-resolution NMR techniques in organic chemistry, 1999, Pergamon
- N.E. Jacobsen, NMR spectroscopy explained, 2007, Wiley
- M. H. Levitt, Spin Dynamics-Basics of Nuclear Magnetic Resonance, 2001, Wiley.
- I. Bertini, K. S. McGreevy, G. Parigi (Eds.), NMR of Biomolecules, Wiley, 2012
- Novejši (pregledni) članki iz primarne znanstvene literature.

Cilji in kompetence:	**Objectives and Competences:**
Študent teoretično in praktično spozna sodobne tehnike nuklearne magnetne resonance in njihovo uporabnost za reševanje znanstvenih problemov (praviloma) povezanih z njegovim lastnim raziskovalnim delom.	Introducing students with up-to-date techniques of nuclear magnetic resonance, both theoretically and practically. Students will be able to apply knowledge in solving scientific problems (preferably) associated with the student's own research work.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Študent se seznani z raznovrstnimi NMR metodami, ki dajejo strukturno informacijo o (bio)(makro)molekulah na različnih nivojih ločljivosti s ciljem potrditve strukturne identitete ali pridobitve statičnih oziroma dinamičnih informacij o prostorski strukturi. Študent je seznanjen s prednostmi in komplementarnostmi posameznih NMR eksperimentov v primerjavi z informacijami iz drugih strukturnih tehnik.	<u>Knowledge and Comprehension</u> The student gets acquainted with a number of NMR methods which provide structural information on (bio)(macro)molecules at different levels of resolution with a goal to confirm structural identity or provide a static or dynamic insights into three-dimensional structure. The student is familiarized with the advantages and complementarities of individual NMR experiments with respect to information from other structural techniques.
<u>Uporaba</u> Predmet je podlaga za razumevanje molekularno in strukturno usmerjenih raziskovalnih pristopov in metod, ki jih bo študent uporabljal na različnih strokovnih področjih.	<u>Application</u> The course is the basis for understanding molecular and structure oriented research approaches and methods that student will use in various professional areas.
<u>Refleksija</u> Študent pridobi vpogled v NMR in njegovo uporabo v študijah strukture, dinamike, interakcij med malimi in/ali makromolekulami, reakcijskih mehanizmov, itd, ter razvije kritičen pogled na	<u>Analysis</u> The student gains insight into NMR and its use in studies of structure, dynamics, interactions among small and/or macromolecules, reaction mechanisms, etc. as well as develops critical

prednosti in pomanjkljivosti v primerjavi s komplementarnimi metodami.	view on advances and limitations with respect to complementary methods.
Prenosljive spretnosti Timsko delo pri spektrometru. Uporaba tuje literature. Podajanje poročil o opravljenem delu in prebrani literaturi (pismeno in ustno).	Skill-transference Ability Teamwork at spectrometer. The use of foreign literature. Submission of written reports on lab results and literature survey (written and oral).

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, seminar, delo na NMR spektrometru na praktičnih primerih praviloma na študentovih lastnih vzorcih.	Lectures, seminars, hands-on experiments at the NMR spectrometer on student's own samples.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Izdelava in predstavitev seminarja Ustni izpit ob diskusiji projekta, ki ga je študent opravil	50 % 50 %	Presentation of seminar Oral examination with discussion on the project carried out by the student

Reference nosilca / Lecturer's references:

1. Li, Q., Trajkovski, M., Fan, C., Chen, J., Zhou, Y., Lu, K., Li, H., Su, X., Xi, Z., Plavec, J. in sod. (2022) 4'-SCF3-Labeling Constitutes a Sensitive 19F NMR Probe for Characterization of Interactions in the Minor Groove of DNA. Angew. Chem. Int. Ed., 61, e202201848.
2. Ghosh, A., Trajkovski, M., Teulade-Fichou, M.-P., Gabelica, V. in Plavec, J. (2022) Phen-DC3 Induces Refolding of Human Telomeric DNA into a Chair-Type Antiparallel G-Quadruplex through Ligand Intercalation. Angew. Chem. Int. Ed., 61, e202207384.
3. Takahashi, S., Kotar, A., Tateishi-Karimata, H., Bhowmik, S., Wang, Z.-F., Chang, T.-C., Sato, S., Takenaka, S., Plavec, J. in Sugimoto, N. (2021) Chemical Modulation of DNA Replication along G-Quadruplex Based on Topology-Dependent Ligand Binding. J. Am. Chem. Soc., 143, 16458-16469.
4. Peterková, K., Durník, I., Marek, R., Plavec, J. in Podbevšek, P. (2021) c-kit2 G-quadruplex stabilized via a covalent probe: exploring G-quartet asymmetry. Nucleic Acids Res., 49, 8947-8960.
5. Lago, S., Nadai, M., Ruggiero, E., Tassinari, M., Marušič, M., Tosoni, B., Frasson, I., Cernilogar, F.M., Pirota, V., Doria, F., Plavec J. in sod. (2021) The MDM2 inducible promoter folds into four-tetrad antiparallel G-quadruplexes targetable to fight malignant liposarcoma. Nucleic Acids Res., 49, 847-863.