

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, 3 rd Cycle	/	1 st	1 st and 2 nd

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:

Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.

Prerequisites:

The course has to be assigned to the student.

Vsebina:

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 usmeritvam posameznega študenta. Vsebine je

Content (Syllabus outline):

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 course can be tailor-made to the level which

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.

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:

Študent teoretično in praktično spozna sodobne tehnike nuklearne magnetne resonance in njihovo uporabnost za reševanje znanstvenih problemov (praviloma) povezanih z njegovim lastnim raziskovalnim delom.

Objectives and Competences:

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:

Znanje in razumevanje

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.

Uporaba

Predmet je podlaga za razumevanje molekularno in strukturno usmerjenih raziskovalnih pristopov in metod, ki jih bo študent uporabljal na različnih strokovnih področjih.

Refleksija

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 prednosti in pomanjkljivosti v primerjavi s komplementarnimi metodami.

Intended Learning Outcomes:

Knowledge and Comprehension

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.

Application

The course is the basis for understanding molecular and structure oriented research approaches and methods that student will use in various professional areas.

Analysis

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 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 (pisмено 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:

Predavanja, seminar, delo na NMR spektrometru na praktičnih primerih praviloma na študentovih lastnih vzorcih.

Learning and Teaching Methods:

Lectures, seminars, hands-on experiments at the NMR spectrometer on student's own samples.

Delež (v %) /

Načini ocenjevanja:

Weight (in %) **Assessment:**

Izdelava in predstavitev seminarja	50 %	Presentation of seminar
Ustni izpit ob diskusiji projekta, ki ga je študent opravil	50 %	Oral examination with discussion on the project carried out by the student

Reference nosilca / Lecturer's references:

- V. Kocman, J. Plavec, A tetrahelical DNA fold adopted by tandem repeats of alternating GGG and GCG tracts, *Nat. Commun.* **2014**, *5*, art. no.: 5831.
- S. Čeru, P. Šket, I. Prislán, J. Lah, J. Plavec, A new pathway of DNA G-quadruplex formation, *Angew. Chem. Int. Ed.* **2014**, *53*, 4881.
- N. Busschaert, L. E. Karagiannidis, M. Wenzel, C. J. E. Haynes, N. J. Wells, P. G. Young, D. Makuc, J. Plavec, K. A. Joliffe, P. A. Gale, Synthetic transporters for sulfate: a new method for the direct detection of lipid bilayer sulfate transport, *Chem. Sci.* **2014**, *5*, 1118.
- M. Marušič, R. N. Veedu, J. Wengel, J. Plavec, G-rich VEGF aptamer with locked and unlocked nucleic acid modifications exhibits a unique G-quadruplex fold, *Nucleic Acids Res.* **2013**, *41*, 9524.
- M. Trajkovski, M. Webba da Silva, J. Plavec, Unique Structural Features of Interconverting Monomeric and Dimeric G-Quadruplexes Adopted by a Sequence from the Intron of the N-myc Gene, *J. Am. Chem. Soc.* **2012**, *134*, 4132.