

UČNI NAČRT PREDMETA / COURSE SYLLABUS

Predmet: MODERNE NMR METODE
Course Title: MODERN NMR METHODS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	/	2.	3.
USP Chemistry, 2 nd Cycle	/	2 nd	3 rd

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I10

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	/	30 LV	/	/	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:

Uvod. Osnove NMR eksperimenta, kemijski premik, sklopitve, integrali, običajno merjeni nuklidi, klasične in pulzne tehnike.

Magnetne lastnosti jeder. Jedro v magnetnem polju, Energetski nivoji, relaksacijski časi, vektorski opis vzorca, laboratorijski in rotirajoč koordinatni sistem, pulz.

Sklopitvena konstanta. Spektri prvega in drugega reda, kemijska in magnetna ekvivalenca jeder, predznak in velikost sklopitvene konstante, sklopitev preko ene, dveh, treh in več vezi.

Povezava strukture spojine in kemijskih premikov. Vplivi na kemijske premike ¹H in ¹³C, programska oprema za napoved kemijskih premikov.

Merjenje NMR spektra. Magnet, CW in pulzni

Content (Syllabus outline):

Basics of NMR experiment, chemical shift, coupling, integral, frequently measured nuclei, classical pulse sequences.

Magnetic properties of nuclei. A nucleus in magnetic field, energy levels, relaxation times, vector description of a sample, laboratory and rotating frame coordinate system, pulse.

Coupling constant. First and higher order spectra, chemical and magnetic equivalence, sign and magnitude of coupling constant, one-, two, or more-bond coupling.

Relation between structure and chemical shifts.

Chemical shift dependence on molecular structure, NMR spectral prediction software.

Acquisition of NMR spectra. Magnet, Continuous wave and pulse mode, data acquisition, FID, Fourier transformation,

način, zajemanje podatkov, FID, Fourierjeva transformacija, matematične manipulacije FID, **Študij dinamičnih procesov z NMR.**

Moderne pulzne NMR tehnike. Manipulacija magnetizacije, spin-echo pulzna sekvenca in njene posledice; prenos polarizacije in editiranje spektrov; nuklearni Overhauserjev efekt; uvod v dvo- in večdimenzionalne NMR eksperimente.

Dvodimenzionalne NMR tehnike. Pregled principov in uporabe dvodimenzionalnih NMR metod pri določanju kemijske strukture in konformacije molekul v raztopini COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC, NOESY.

Vaje

Priprava vzorca in inštrumenta; 1D eksperimenti (^1H , ^{13}C , X); 2D eksperimenti (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).

mathematical manipulation of FID.

Study of Dynamic processes by NMR.

Modern pulse NMR. Manipulation of magnetization, spin-echo pulse sequence, polarization transfer and spectral editing, nuclear Overhauser effect, introduction to two- and more-dimensional NMR experiments.

Two-dimensional NMR techniques. Overview of principles and application of 2D NMR methods in structure elucidation and conformational studies

in solution, COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC, NOESY.

Practical spectroscopy: sample preparation, basic instrumental procedures, one-dimensional experiments (^1H , ^{13}C , X), two-dimensional experiments (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).

Temeljna literatura in viri / Readings:

- J. B. Lambert, *Nuclear Magnetic Resonance Spectroscopy. An Introduction to Principles, Applications, and Experimental Methods*, Pearson Education Inc., New Jersey, 2003; 293 od 341 strani.

Praktikum

- S. Braun, H.-O. Kalinowski, S. Berger, *150 and More Basic NMR Experiments*, Wiley-VCH Publishers, Weinheim, 1998.

Dodatna literatura

- R. S. Macomber: *A Complete Introduction to Modern NMR Spectroscopy*, J. Wiley & Sons, Inc., New York, 1998.

- E. Derome, *Modern NMR Techniques for Chemistry Research*, Pergamon Press, Oxford, 1987.

- M. Hesse, H. Meier, B. Zeeh, *Spectroscopic Methods in Organic Chemistry*, G. Thieme Verlag, 2008

- A. Petrič: *Moderne NMR metode (interno študijsko gradivo)*, UL FKKT, 2012 (144 str.).

Cilji in kompetence:

Cilji: Študent pridobi znanja, ki so potrebna za razumevanje modernih NMR tehnik, načrtovanje in izvedbo eksperimentov njihovo uporabo in interpretacijo rezultatov.

Kompetence: Pridobljeno znanje študentu omogoča samostojno načrtovanje NMR eksperimentov, njihovo praktično izvedbo in interpretacijo rezultatov.

Objectives and Competences:

Objectives: To teach students theory and practice of modern NMR methods necessary to understand modern MMR techniques, planning and performing experiments and interpretation of the results.

Competences: Ability to design, perform, and interpret NMR experiments for the determination of structure and conformation of

	compounds in solution.
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Predvideni študijski rezultati:

Znanje in razumevanje

Poznavanje principov in praktične izvedbe modernih NMR eksperimentov za določanje strukture in konformacije spojin v raztopini.

Uporaba

Študent uporabi pridobljeno znanje NMR spektroskopskih tehnik pri reševanju raziskovalnih problemov.

Refleksija

Zavedanje, da z NMR tehnikami pridobimo pomembne informacije o strukturi in konformaciji molekul v raztopini in da so NMR tehnike najpomembnejša analitska metoda v organski kemiji.

Prenosljive spretnosti

Pri predmetu se študenti se izurijo v načrtovanju in izvedbi eksperimentov ter kritični interpretaciji rezultatov.

Intended Learning Outcomes:

Knowledge and Comprehension

Understanding the basic principles and practical knowledge about NMR experiments.

Application

Student utilizes the acquired knowledge in solving research problems

Analysis

Student applies the acquired NMR spectroscopy knowledge and skills in solving research problems.

Skill-transference Ability

Student is trained in planning and utilization of NMR spectroscopic methods, analytical thinking and using literature sources.

Metode poučevanja in učenja:

Predavanja in vaje

Learning and Teaching Methods:

Lectures and practical laboratory work

Delež (v %) /

Načini ocenjevanja:

Weight (in %) **Assessment:**

Ustni izpit in praktični preskus.

10 (odlično), 9 in 8 (prav dobro), 7 (dobro), 6 (zadostno), 5-1 (nezadostno)

Reference nosilca / Lecturer's references:

- KOTAR, Anita, WANG, Baifan, SHIVALINGAM, Arun, GONZALEZ-GARCIA, Jorge, VILAR, Ramon, **PLAVEC, Janez**. NMR structure of a triangulenium-based long-lived fluorescence probe bound to a G-quadruplex. *Angewandte Chemie*, ISSN 1433-7851. [Print ed.], Sep. 2016, vol. 55, iss. 40, str. 12508-12511, doi: [10.1002/anie.201606877](https://doi.org/10.1002/anie.201606877). [COBISS.SI-ID [5990426](https://www.cobiss.si/id/5990426)]
- GALER, Petra, WANG, Baifan, ŠKET, Primož, **PLAVEC, Janez**. Reversible pH switch of two-quartet G-quadruplexes formed by human telomere. *Angewandte Chemie*, ISSN 1433-7851. [Print ed.], Feb. 2016, vol. 55, iss. 6, str. 1993-1997, doi: [10.1002/anie.201507569](https://doi.org/10.1002/anie.201507569). [COBISS.SI-ID [5864474](https://www.cobiss.si/id/5864474)]
- MARUŠIČ, Maja, **PLAVEC, Janez**. The effect of DNA sequence directionality on G-quadruplex folding. *Angewandte Chemie*, ISSN 1433-7851. [Print ed.], Sep. 2015, vol. 54, iss. 40, str. 11716-11719, doi: [10.1002/anie.201505348](https://doi.org/10.1002/anie.201505348). [COBISS.SI-ID [5780506](https://www.cobiss.si/id/5780506)]