

MODERNE NMR METODE

UČNI NAČRT PREDMETA/COURSE SYLLABUS

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| Predmet: | Moderne NMR metode |
| Course title: | Modern NMR methods |
| Članica nosilka/UL Member: | UL FKKT |

| Študijski programi in stopnja | Študijska smer | Letnik | Semestri | Izbirnost |
|-----------------------------------|---------------------------------|-------------------------|----------|-----------|
| Kemija, druga stopnja, magistrski | Ni členitve (študijski program) | 1. letnik, 2. letnik | | izbirni |

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| Univerzitetna koda predmeta/University course code: | 0072221 |
| Koda učne enote na članici/UL Member course code: | K2I10 |

| Predavanja /Lectures | Seminar /Seminar | Vaje /Tutorials | Klinične vaje /Clinical tutorials | Druge oblike študija /Other forms of study | Samostojno delo /Individual student work | ECTS |
|-------------------------|---------------------|--------------------|---|---|---|------|
| 30 | | 45 LV | | | 75 | 5 |

Nosilec predmeta/Lecturer: prof. dr. Janez Plavec

Vrsta predmeta/Course type: izbirni strokovni/Elective Professional

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| Jeziki/Languages: | Predavanja/Lectures: | Slovenščina |
| | Vaje/Tutorial: | Slovenščina |

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti: **Prerequisites:**

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| Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost. | The course has to be assigned to the student. |
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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.

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,

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| <p>Merjenje NMR spektra. Magnet, CW in pulzni način, zajemanje podatkov, FID, Fourierjeva transformacija, matematične manipulacije FID, Študij dinamičnih procesov z NMR.</p> <p>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.</p> <p>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.</p> <p>Vaje Priprava vzorca in inštrumenta; 1D eksperimenti (1H, 13C, X); 2D eksperimenti (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).</p> | <p>Continuous wave and pulse mode, data acquisition, FID, Fourier transformation mathematical manipulation of FID.</p> <p>Study of Dynamic processes by NMR.</p> <p>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.</p> <p>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.</p> <p>Practical spectroscopy: sample preparation, basic instrumental procedures, one-dimensional experiments (1H, 13C, X), two-dimensional experiments (COSY, TOCSY, HMQC, HMBC, gs-COSY, gs-HMQC, gs-HMBC).</p> |
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Temeljna literatura in viri/Readings:

1. James Keeler Understanding NMR Spectroscopy, ISBN: 0-470-01787-2, oktober 2005
2. Thomas C. Pochapsky & Susan Sondej Pochapsky, NMR for Physical and Biological Scientists, ISBN: 0 8153 4103 2, 2007
3. Neil E. Jacobsen, NMR Spectroscopy Explained, ISBN: 978-0-471-73096-5, John Wiley & Sons, 2007

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 NMR 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.

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:

Learning and teaching methods:

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| Predavanja in vaje | Lectures and practical laboratory work |
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Načini ocenjevanja:
Delež/Weight Assessment:

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| Ustni izpit in praktični preskus. 10 (odlično), 9 in 8 (prav dobro), 7 (dobro), 6 (zadostno), 5-1 (nezadostno) | | |
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Reference nosilca/Lecturer's references:

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| <ul style="list-style-type: none"> - Li, Q., Trajkovski, M., Fan, C., Chen, J., Zhou, Y., Lu, K., Li, H., Su, X., Xi, Z., Plavec, J. <i>et al.</i> (2022) 4'-SCF3-Labeling Constitutes a Sensitive ¹⁹F NMR Probe for Characterization of Interactions in the Minor Groove of DNA. <i>Angew. Chem. Int. Ed.</i>, 61, e202201848. - Ghosh, A., Trajkovski, M., Teulade-Fichou, M.-P., Gabelica, V. and Plavec, J. (2022) Phen-DC3 Induces Refolding of Human Telomeric DNA into a Chair-Type Antiparallel G-Quadruplex through Ligand Intercalation. <i>Angew. Chem. Int. Ed.</i>, 61, e202207384. - Takahashi, S., Kotar, A., Tateishi-Karimata, H., Bhowmik, S., Wang, Z.-F., Chang, T.-C., Sato, S., Takenaka, S., Plavec, J. and Sugimoto, N. (2021) Chemical Modulation of DNA Replication along G-Quadruplex Based on Topology-Dependent Ligand Binding. <i>J. Am. Chem. Soc.</i>, 143, 16458-16469. |
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