UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	INTERAKCIJE BIOLOŠKIH MOLEKUL
Course Title:	INTERACTIONS OF BIOLOGICAL MOLECULES

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Biokemija, 2. stopnja	**/**	**1.**	**2.**
USP Biochemistry, 2nd Cycle	**/**	**1st**	**2nd**

Vrsta predmeta / Course Type: obvezni / Mandatory

Univerzitetna koda predmeta / University Course Code: BI2I05

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
30	**15**	**30 LV**	**/**	**/**	**75**	**5**

Nosilec predmeta / Lecturer: doc. dr. Marko Novinec / Dr. Marko Novinec, Assistant 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):
Vezava ligandov v bioloških sistemih. Kooperativnost vezave in alosterija. Modifikacija encimske aktivnosti: mehanizmi reverzibilne in ireverzibilne inhibicije, esencialna in neesencialna aktivacija, določanje mehanizma delovanja modifikatorjev encimske aktivnosti, inhibicija s substratom in produktom. Alosterična regulacija encimske aktivnosti. Napredna encimska kinetika: reakcije z več substrati in encimi. Reakcije v heterogenih sistemih (pretvorba netopnih substratov, reakcije na fazni meji lipid-voda). Kinetika hitrih reakcij. Kinetika predravnotežnega	Ligand binding in biological systems. Cooperativity of binding and allostery. Modification of enzyme activity: mechanisms of reversible and irreversible inhibition, essential and nonessential activation, determination of the mechanism of enzyme activity modification, substrate and product inhibition. Allosteric regulation of enzyme activity. Advanced enzyme kinetics: multi-substrate and multi-enzyme reactions. Reactions in heterogeneous systems (turnover of insoluble substrates, reactions at the lipid-water interface). Fast reaction kinetics. Pre-steady-state kinetics.

stanja. Tesne interakcije. Vpliv okolja na medmolekulske interakcije. Računalniške metode analize in napovedi molekulskih interakcij. Računalniško načrtovanje regulatorjev delovanja bioloških molekul. Povezava med strukturo in aktivnostjo načrtovanih biološko aktivnih molekul. *Pri vseh obravnavanih vsebinah je poudarek na povezavi med strukturo in funkcijo bioloških molekul ter matematičnih modelih za opis interakcij.* *<u>Seminarske naloge</u> na osnovi vrhunskih aktualnih člankov s področja obravnavane tematike.*	Tight interactions. Environmental effects on molecular interactions. Computational methods for the analysis and prediction of molecular interactions. Computational design of novel regulators of biological molecules. Structure-activity relationship of designed biologically active substances. *The course is designed to emphasize the structure-function relationship involved in biological interactions as well as the mathematical models used to describe these interactions.* *<u>Seminar work</u> based on state-of-the-art scientific papers with content related to this course.*

Temeljna literatura in viri / Readings:

- Fundamentals of Enzyme Kinetics. Cornish-Bowden, A. Fourth Edition. 2012. Wiley-Blackwell. 516 strani (60 %)

<u>Dopolnilna literatura:</u>

- Enzyme Kinetics: Behavior and Analysis of Rapid Equilibrium and Steady-State Enzyme Systems Segel, I.H. 1975. John Wiley & Sons, Inc, 957 strani

Cilji in kompetence:	**Objectives and Competences:**
Predmet obravnava medmolekulske interakcije in encimsko katalizirane kemijske reakcije z vidika povezave med strukturo in funkcijo bioloških molekul ter interpretacije mehanizmov interakcij. Študenti bodo sposobni samostojno preučevati interakcije med molekulami, encimsko katalizirane reakcije in njihovo regulacijo ter rezultate ustrezno interpretirati.	The course focuses on intermolecular interactions and enzyme-catalyzed chemical reactions from the perspective of the relationship between structure and function of biological molecules, and the interpretation of the mechanisms of interaction. Students will gain the competence to independently study intermolecular interactions, enzyme-catalyzed reactions and their regulation, and interpretation.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Študenti pridobijo znanje o interpretaciji mehanizmov interakcij med molekulami in encimsko kataliziranih reakcij ter njihove	<u>Knowledge and Comprehension</u> Students learn to interpret the mechanisms of intermolecular interactions and enzyme-catalyzed reactions. They integration this

regulacije. Pridobljeno znanje poveže s predhodnim znanjem o strukturi in funkciji proteinov in drugih bioloških molekul.	knowledge with prior knowledge of the structure and function of proteins and other biological molecules.
Uporaba Sposobnost določanja mehanizmov medmolekulskih interakcij ter delovanja in regulacije encimov je ključnega pomena pri študijah bioloških sistemov na molekulskem nivoju. Obenem je ključnega pomena pri dizajnu farmakoloških učinkovin, ki delujejo preko modifikacije aktivnosti različnih encimov ali drugih proteinov.	Application The ability to determine mechanisms of intermolecular interactions and the kinetics of enzyme catalysis and its regulation is a prerequisite for studying biological systems at the molecular level. It is also key to successful design of pharmacologically active substances that act by modifying the activity of enzymes and other proteins.
Refleksija Študenti povežejo predhodno znanje z novim znanjem.	Analysis Students reflect on prior knowledge and integrate it with new knowledge.
Prenosljive spretnosti Sposobnost načrtovanja eksperimentov in interpretacije rezultatov, sposobnost uporabe literature in drugih virov, sposobnost ustnega in pisnega poročanja.	Skill-transference Ability Ability to plan experiments and interpret the results, ability to use literature and other sources, ability of written and oral reporting.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, raziskovalni seminarji, laboratorijske vaje.	Lectures, seminars based on scientific research papers, laboratory tutorial.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Kolokvij iz laboratorijskih vaj Seminarska naloga Pisni izpit		Laboratory tutorial colloquium Seminar work Written examination

Reference nosilca / Lecturer's references:

- **NOVINEC, Marko**, KORENČ, Matevž, CAFLISCH, Amedeo, RANGANATHAN, Rama, LENARČIČ, Brigita, BAICI, Antonio. A novel allosteric mechanism in the cysteine peptidase cathepsin K discovered by computational methods. Nature communications, ISSN 2041-1723, feb. 2014, vol. 5, art. no. 3287
- **NOVINEC, Marko**, KOVAČIČ, Lidija, LENARČIČ, Brigita, BAICI, Antonio. Conformational flexibility and allosteric regulation of cathepsin K. Biochemical journal, ISSN 0264-6021, 2010, vol. 429, no. 2, p. 379-389
- **NOVINEC, Marko**, GRASS, Robert N., STARK, Wendelin J., TURK, Vito, BAICI, Antonio, LENARČIČ, Brigita. Interaction between human cathepsins K, L, and S, Mechanism of elastinolysis and ihibition by macromolecular inhibitors. The Journal of biological chemistry, ISSN 0021-9258, 2007, vol. 282, no. 11, str. 7893-78902