UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	MOLEKULARNA RAZLAGA BIOLOŠKIH SISTEMOV
Course Title:	MOLECULAR INTERPRETATION OF BIOLOGICAL SYSTEMS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Biokemija, 2. stopnja	**/**	**2.**	**4.**
USP Biochemistry, 2nd Cycle	**/**	**2nd**	**4th**

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: BI2I11

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

Nosilec predmeta / Lecturer: prof. dr. Barbara Hribar Lee / dr. Barbara Hribar Lee, 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:

Osnove: Opis mikroskopskega stanja in statistična vsota, kanonična porazdelitev, Boltzmannova porazdelitev, povprečja in kolebanja okoli povprečne vrednosti, povezava s termodinamiko, izoliran sistem, odprt sistem, koncentracijska kolebanja, stisljivost in stabilnost sistema.

Neodvisni podsistemi: Einsteinov model kristala, razredčeni plini, kemično ravnotežje, adsorbcija (Langmuirjeva izoterma).

Aplikacija na biokemijske sisteme: Vezanje ligandov na makromolekule (vezavne krivulje), kooperativnost-fazni prehodi biološko pomembnih makromolekul, lastnosti polimerov skozi mrežne modele ("lattice models"). Osnove zvijanja proteinov v naravno

Content (Syllabus outline):

Introduction: The description of microscopic state of the system; partition function; canonical ensemble; Boltzmann distribution; fluctuations; thermodynamic relations; isolated system; open system; compressibility and the system stability.

Independent subsystems: Einstein crystal; diluted gasses; chemical equilibrium; adsorption (Langmuir isotherm).

Application to biological systems: Ligand binding (adsorption isotherms), cooperativity – phase transitions of biological molecules; lattice models of polymers. Fundamentals of protein folding.

Classical statistical thermodynamics: Microscopic structure of liquids; distribution

konformacijo (“protein folding”). Klasična statistična termodinamika: Struktura tekočin in prostorske porazdelitvene funkcije, termodinamične količine (notranja energija, enačba stanja), povezava z eksperimentom, računalniške simulacije (metoda Monte Carlo, molekulska dinamika) kot orodje za študij obnašanja raztopin makromolekul. Vloga topila v bioloških sistemih: Lastnosti vode kot univerzalnega topila, solvatacija, hidrofobnost, stabilnost raztopin proteinov-Hofmeistrova vrsta.	functions; thermodynamic functions (internal energy, equation of state); experimental interpretation; computer simulations (Monte Carlo method, molecular dynamics) as tools for studying the properties of the solutions of macromolecules. Solvent in biological systems: Properties of water as universal solvent; salvation; hydrophobicity; protein stability – Hofmeister series.

Temeljna literatura in viri / Readings:

- Dill, K. A., Bromberg, S., Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology, New York: Garland Science, 2003.
- Friedman, H. L., A Course in Statistical Mechanics, New Jersey: Prantice-Hall, 1985.
- Hill, T. L., Introduction to Statistical Thermodynamics, Reading: Addison-Wesley, 1960.

Cilji in kompetence:	**Objectives and Competences:**
Veda, ki omogoča, da iz podatkov o lastnostih atomov in molekul ter sil med njimi izpelje makroskopske lastnosti snovi, je statistična termodinamika. Na ta način omogoča razumevanje naravnih zakonitosti in molekularno interpretacijo merskih podatkov. V prvem delu predmet obravnava osnove statistične termodinamike, le-te omogočajo globje razumevanje pojavov kot so toplota, entropija, termodinamično povprečje, kolebanje okoli povprečne vrednosti in drugi. Drugi del predmeta je namenjen prikazu primerov uporabe statistične termodinamike v kemiji s poudarkom na biološko pomembnih sistemih. Ker obnašanja raztopin biološko pomembnih molekul ne moremo razložiti brez upoštevanja vloge molekul topila, predmet na koncu posebej obravnava vodo kot najpomembnejše topilo v teh sistemih.	The statistical thermodynamics uses the properties of atoms and molecules to obtain from them the macroscopic properties of the systems. As such, it contributes to understanding of the natural laws, as well as the molecular interpretation of the experimental data. In the first part of the course the basics of the statistical thermodynamics is learned that enables the deeper understanding of the quantities such as heat, entropy, thermodynamic averages, fluctuations ... In the second part of the course, the statistical thermodynamics is applied to different problems taken from biologically important systems. The last part of the course is dealing with water as the most important solvent in the biological systems.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
Znanje in razumevanje Poznavanje osnov statistične termodinamike biološko pomembnih sistemov, ki jih	Knowledge and Comprehension The basic knowledge of the statistical thermodynamics enables a deeper

obravnava ta predmet, omogoča globlje razumevanje obnašanje teh sistemov na molekularnem nivoju in interpretacijo eksperimentalnih podatkov.	understanding of these systems on the molecular level, as well as the interpretation of the experimental data.
Uporaba Principi statistične termodinamike omogočajo konstrukcijo in študij modelov, kakršne široko uporabljajo v farmacevtski industriji, pa tudi pri načrtovanju različnih drugih tehnoloških procesov kot so ionska izmenjava, desalinacija vode ...	Application The principles of the statistical thermodynamics are the starting point for the construction and interpretation of the models, that are broadly used in the pharmaceutical industry, as well as in other technological processes, such as ion exchange, desalination, ...
Refleksija Znanja in veščine, ki jih študent osvoji pri tem predmetu, mu pomagajo pri kritičnem ovrednotenju merskih podatkov, boljšem razumevanju obnašanja bioloških sistemov in s tem do novih idej pri raziskavah.	Analysis The knowledge and skills that are gained in this course help the students critically assess the experimental data, and the understanding of the biological systems.
Prenosljive spretnosti Spretnosti uporabe domače in tuje literature in drugih virov, identifikacija in reševanje problemov, kritična analiza, refleksij na prebrano literaturo, uporaba različnih postopkov poročanja (ustno in pisno).	Skill-transference Ability The ability of using different literature, as well as other resources, identification and problem solving, critical evaluation of the results, the ability to present their results in the written and oral form.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja, individualno delo v obliki seminarjev.	-Lectures, -individual work in the form of seminars

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Seminar Ustni izpit		Seminar Oral exam

Reference nosilca / Lecturer's references:

- DILL, Ken A., TRUSKETT, Thomas Michael, VLACHY, Vojko, **HRIBAR-LEE, Barbara**. Modeling water, the hydrophobic effect, and ion solvation. Annu Rev Biophys Biomol Struct, 2005, vol. 34, str. 173-199.
- JARDAT, Marie, **HRIBAR, Barbara**, VLACHY, Vojko. Self-diffusion of ions in charged nanoporous media. *Soft matter*, 2012, vol. 8, no. 4, str. 954-964.
- **HRIBAR, Barbara**, LUKŠIČ, Miha, VLACHY, Vojko. Partly-quenched systems containing charges. Structure and dynamics of ions in nanoporous materials. *Annu. rep. prog. chem. Sect C. Phys. chem*, 2011, vol. 107, no. 1, str. 14-46