UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Od kristalov do 3D strukture makromolekul
Course title:	From Crystals to 3D Structure of Macromolecules

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Nanoznanosti in nanotehnologije, 3. stopnja	Bioznanosti	1	1
Nanosciences and Nanotechnologies, 3rd cycle	Biosciences	1	1

Vrsta predmeta / Course type	Izbirni / Elective
Univerzitetna koda predmeta / University course code:	NANO3-820

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Laboratory work	Druge oblike	Samost. delo Individ. work	ECTS
30	**30**			**30**	**210**	**10**

**Navedena porazdelitev ur velja, če je vpisanih vsaj 15 študentov. Drugače se obseg izvedbe kontaktnih ur sorazmerno zmanjša in prenese v samostojno delo. / This distribution of hours is valid if at least 15 students are enrolled. Otherwise the contact hours are linearly reduced and transfered to individual work.*

Nosilec predmeta / Lecturer:	Prof. dr. Dušan Turk
Jeziki / Languages: Predavanja / Lectures:	slovenščina, angleščina / Slovenian, English
Vaje / Tutorial:	

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisites:**
Zaključena druga stopnja bolonjskega študija ali diploma univerzitetnega študijskega programa. Potrebno je poznavanje osnov biokemije, molekularne biologije in fizike. Študent mora biti vključen v raziskave s področja strukturne biologije na osnovi kristalografije.	Completed Bologna second cycle study program or an equivalent pre-Bologna university study program. Basic knowledge of biochemistry, molecular biology and physics is also requested. The student must be involved in structural biology research based on crystallography.

Vsebina:	**Content (Syllabus outline):**
Preverjanje čistosti in stabilnosti makromolekul **Kristalizacija makromolekul** Snemanje in procesiranje podatkov **Faziranje** kristalografskih struktur z vsaj eno od metod: - molekularne zamenjave - multi valovna anomalna disperzija (MAD,SAD) - multipla in enojna izomorfna zamenjava (MIR,SIR) **Modifikacija elektronske gostote:** - identifikacija proteinske regije in topila - postopki modifikacije regije proteina in topila - uporaba ne kristalografske simetrije	**Verifying purity** and stability of macromolecules **Crystallization of macromolecules**. Data collection and processing. **Phasing** of crystallographic data by at least one method: - molecular replacement (MR) - multi-wavelength anomalous dispersion technique (MAD, SAD) - multiple and single isomorphous replacement (MIR and SIR) **Modifications of density maps**: - identification of protein and solvent regions

- povprečenje elektronske gostote Interpretacija elektronske gostote - avtomatsko in - manualno grajenje molekularnih modelov **Fitanje** in predelovanje modelov - tarčne funkcije (metoda najmanjših kvadratov in maksimalne podobnosti) - počasno in hitro ohlajanje pregretih modelov **Analiza in preverjanje struktur** **Biološka interpretacija modelov:** - pisanje članka - zastavitev nadaljnjih raziskav	- separate procedures for solvent and protein regions - exploiting non-crystallographic symmetry: electron density averaging **Interpretation** of electron density maps: - automated and - manual model building **Refinement** and model rebuilding - target functions (least square and maximum-likelihood targets) - "slow" (simulated annealing) and "fast" cooling minimization techniques **Analysis and validation** of 3-D models **Model interpretation**: - manuscript preparation - basis for further investigations

Temeljna literatura in viri / Readings:

Crystallography of biological macromolecules: International Tables for Crystallography, Volume F, 2nd Edition, edited by Michael G. Rossmannm, Daniel M. Himmel and Eddy Arnold (2012). Wiley, ISBN 978-0-470-66078-2

Protein crystallography. Editors: Wlodawer, Alexander, Dauter, Zbigniew, Jaskolski, Mariusz (Eds.) Springer International Publishing AG. 2017. ISBN 978-1-4939-7000-1. Methods in Molecular Biology Series Ed.: **Walker**, John M. ISSN: 1064-3745

Tekoča relevantna literatura iz problematike/ Relevant current articles from the field (Biological Crystallography, Applied Crystallography, Structure, Journal of Molecular Biology, Nature, Science, Current Opinion of Structural Biology, ...)

Cilji in kompetence:	**Objectives and competences:**
Cilj predmeta je, da se študent seznani s teoretičnimi osnovami in praktičnimi pristopi k določevanju 3-dimenzionalne strukture makromolekul v kristalih. Pri svojem delu bo uporabljal najnovejšo tujo strokovno literaturo, kar bo izboljšalo njegove sposobnosti uporabe tujega jezika in kritičnega pogleda na objavljeno raziskovalno delo. Po uspešno zaključenem predmetu bi morale kompetence študentov doseči nivo samostojnega določevanja in interpretacije struktur makromolekul v kristalih. Splošne kompetence: - obvladanje raziskovalnih metod in postopkov, razvoj kritične in samokritične presoje, - sposobnost uporabe znanja v praksi, - razvoj komunikacijskih sposobnosti in spretnosti,	The goal of the course is to familiarize the student with theoretical background upgraded by practical work on crystal structure determination. During the study the newest scientific literature will be used, which will improve the student's foreign language skills and the ability to study the published research critically. The competencies of the students completing this course successfully should reach the level of independent determination of crystal structures of macromolecules and their interpretation. General Competences: - the student will master research methods and procedures and develop skills for critical assessment of his activities, - the student will be able to put his knowledge into practice,

posebej komunikacije v mednarodnem okolju, - kooperativnost, delo v skupini in tudi v mednarodnem okolju	- the student will develop communications skills to present research achievement in the international environment, - training for team work including the work in international environment

Predvideni študijski rezultati:	**Intended learning outcomes:**
Poznavanje in razumevanje pojmov, metod iz strukturne biologije, s poudarkom na določevanju in interpretaciji 3-dimenzionalnih struktur makromolekul s pomočjo kristalografije. Pregled različnih pristopov k reševanju relevantnih problemov in razumevanje omejitev metode.	Knowledge and understanding of the concepts and methods of structural biology with the emphasis on macromolecular crystallography. Overview of different approaches to solving relevant problems and understanding of limitations of the approach.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Konzultacije/Predavanja Seminarji Individualno laboratorijsko delo	Consultants/Lectures Seminar work Individual laboratory work

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Seminarska naloga	20 %	Seminar work
Uspešna določitev strukture makromolekule v kristalu	80 %	Successful completion of macromolecular crystal structure determination

Reference nosilca / Lecturer's references:

- TURK, Dušan. MAIN software for density averaging, model building, structure refinement and validation. *Acta crystallographica. Section D, Biological crystallography*, ISSN 0907-4449, 2013, vol. 69, part 8, str. 1342-1357, doi: 10.1107/S0907444913008408
- PRAŽNIKAR, Jure, TURK, Dušan. Free kick instead of cross-validation in maximum-likelihood refinement of macromolecular crystal structures. Acta crystallographica. D, Biological crystallography, ISSN 1399-0047, 2014, vol. 70, no. 12, str. 3124-3134. http://journals.iucr.org/d/issues/2014/12/00/lv5072/lv5072.pdf, doi: 10.1107/S1399004714021336.
- TURK, Dušan. Boxes of model building and visualization. V: WLODAWER, Alexander (ur.), DAUTER, Zbigniew (ur.), JASKOLSKI, Mariusz (ur.). Protein crystallography : methods and protocols, (Methods in molecular biology, 1607), (Springer protocols). New York: Humana Press: Springer, 2017, str. 491-548. [COBISS.SI-ID 30667303]
- USENIK, Aleksandra, RENKO, Miha, MIHELIČ, Marko, LINDIČ, Nataša, BORIŠEK, Jure, PERDIH, Andrej, PRETNAR, Gregor, MÜLLER, Uwe, TURK, Dušan. The CWB2 cell wall-anchoring module is revealed by the crystal structures of the Clostridium difficile cell wall proteins Cwp8 and Cwp6. Structure, ISSN 0969-2126. [Print ed.], 7 Mar. 2017, vol. 25, iss. 3, str. 514-21. http://www.sciencedirect.com/science/article/pii/S0969212616304269?via%3Dihub, doi: 10.1016/j.str.2016.12.018
- MIHELIČ, Marko, VLAHOVIČEK-KAHLINA, Kristina, RENKO, Miha, MESNAGE, Stephan, DOBERŠEK, Andreja, TALER-VERČIČ, Ajda, JAKAS, Andreja, TURK, Dušan. The mechanism behind the selection of two different cleavage sites in NAG-NAM polymers. *IUCrJ*, ISSN 2052-2525, 2017, vol. 4, part 2, str. 185-198, doi: 10.1107/S2052252517000367.