UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Analiza in predikcija 3D struktur proteinov
Course title:	Analysis and Prediction of 3D Protein Structure

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

Vrsta predmeta / Course type	Izbirni / Elective
Univerzitetna koda predmeta / University course code:	NANO3-788

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	Samost. delo Individ. work	ECTS
15	**15**			**15**	**105**	**5**

**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. Veronika Stoka Prof. dr. Andrej Šali
Jeziki / Languages: Predavanja / Lectures:	slovenščina, angleščina / Slovenian, English
Vaje / Tutorial:	

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisits:**
Osnovno znanje biologije. kemije in fizike s poudarkom na biokemiji in molekularni biologiji na dodiplomskem nivoju.	Basic knowledge in biology, chemistry, and physics in particular biochemistry and molecular biology at the undergraduate level.

Vsebina:	**Content (Syllabus outline):**
Pri predmetu bomo proteinske strukture raziskovali z dveh zornih kotov: zakonov fizike in teorije evolucije. Z vidika fizike je nativna struktura proteina rezultat sil, ki delujejo na atome proteina in topila med procesom njegovega zvijanja, z biološke perspektive pa je nativna struktura proteina rezultat evolucije. Obe osnovni načeli sta tudi temelj metod, ki napovedujejo strukturo proteinov. Prvi način, de novo ali ab initio metode, poskuša napovedati strukturo proteinov le iz njihove sekvence, ne nanašajoč se na podobnost na nivoju zvitja med modelirano sekvenco proteina in znanimi strukturami. Drugi razred metod, ki vključuje primerjalno modeliranje, pa sloni na podobnosti večjega dela sekvence modeliranega	Within this course, protein structures will be researched from two basic aspects: the laws of physics and the theory of evolution. From the aspect of physics, the native structure of proteins is the result of forces acting on the atoms of protein and solvent in the process of its folding, while from the biological aspect the native structure of protein is the result of evolution. Both basic principles also form the foundation for the protein structure prediction methods. The first, i.e., de novo or ab initio methods attempt to predict the structure of proteins from their sequence alone, not referring to the similarity at the level of folding between the modelled protein sequence and known structures. The second class of methods, which includes

proteina z vsaj eno že znano strukturo. Raziskovali bomo naravo sil, ki kontrolirajo nastanek določene proteinske strukture, nekatere vidike procesa zvijanja proteinov, primerjali proteinske sekvence, strukture proteinov, na vse načine modelirali proteine ter raziskovali strukturno genomiko in možnosti napovedi funkcije proteinov na osnovi predikcije njihove strukture.	comparative modelling, is based on the similarity between the major part of the sequence of modelled protein and at least one known structure. We will research the nature of forces controlling the formation of a particular protein structure and certain aspects of the protein folding process, compare protein sequences, and protein structures, model proteins in many different ways, and research structural genomics and the possibilities for predicting the functions of proteins by predicting their structure.

Temeljni literatura in viri / Readings:

- Structural Bioinformatics, 2nd Edition (2009) J. Gu & P.E. Bourne (Eds.), Wiley-Blackwell
- Webb B, Sali A. (2014) Comparative Protein Structure Modeling Using MODELLER. Curr Protoc Bioinformatics 47:5.6.1-5.6.32.
- Schneidman-Duhovny D, Pellarin R, Sali A. (2014) Uncertainty in integrative structural modeling. Curr Opin Struct Biol. 28:96-104.
- Ryan CJ, Cimermančič P, Szpiech ZA, Sali A, Hernandez RD, Krogan NJ. (2013) High-resolution network biology: connecting sequence with function. Nat Rev Genet. 14:865-79.
- Szilagyi A, Zhang Y. (2014) Template-based structure modeling of protein-protein interactions. Curr Opin Struct Biol. 24:10-23.
- Bordoli L, Kiefer F, Arnold K, Benkert P, Battey J, Schwede T. (2009) Protein structure homology modeling using SWISS-MODEL workspace. Nat Protoc. 4:1-13.
- Pavlopoulou A, Michalopoulos I. (2011) State-of-the-art bioinformatics protein structure prediction tools (Review). *Int J Mol Med.* 28:295-310.

Cilji in kompetence:	**Objectives and competences:**
Študenti spoznajo osnove bioinformatike, proteinskih struktur in se seznanijo z metodami za njihovo analizo in predikcijo. Splošne kompetence: • obvladanje raziskovalnih metod, postopkov in procesov, razvoj kritične in samokritične presoje pri generiranju hipotetičnih 3-D modelov proteinov, • sposobnost uporabe znanja v praksi, • razvoj komunikacijskih sposobnosti in spretnosti, posebej komunikacije v mednarodnem okolju, • kooperativnost, delo v skupini (in v mednarodnem okolju). Predmetnospecifične kompetence: Predmet pripravlja študente za delo s 3-dimenzionalnimi strukturami in njihovimi modeli v akademskih in industrijskih sredinah.	Students learn the basics of bioinformatics, protein structures, and become acquainted with methods for their analysis and prediction. General Competences: • The student will master research methods, procedures and processes in 3-D protein structure prediction. • The student be able to use the gained knowledge in research • The student will develop communications skills to present research achievement in the international environment • Work in team (in international environment) Course Specific Competences: This course prepares students to work with 3-dimensional molecular models of proteins in academic and industrial research environments.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanje in razumevanje: Študenti bodo sposobni uporabiti in presoditi relevantnost hipotetičnih 3-dimenzionalnih molekularnih modelov, generiranih s pomočjo programskih orodij.	Knowledge and Understanding: Students will learn to use and will be able to assess the relevance of the hypothetical 3-D molecular models generated by means of current software tools.

Metode poučevanja in učenja:	**Learning and teaching methods:**
• Predavanja • Seminarji • Konzultacije	• Lectures • Seminar work • Consultations

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Seminar	50 %	Seminar
Ustni izpit	50 %	oral exam

Reference nosilca / Lecturer's references:

- TALER-VERČIČ, Ajda, HASANBAŠIĆ, Samra, BERBIĆ, Selma, STOKA, Veronika, TURK, Dušan, ŽEROVNIK, Eva. Proline residues as switches in conformational changes leading to amyloid fibril formation. International journal of molecular sciences, ISSN 1661-6596, 2017, vol. 18, no. 3, str. 549-1-549-17, doi: 10.3390/ijms18030549
- BIDOVEC, Katja, BOŽIČ, Janja, DOLENC, Iztok, TURK, Boris, TURK, Vito, STOKA, Veronika. Tumor necrosis factor-αα induced apoptosis in U937 cells promotes cathepsin D-independent stefin B degradation. Journal of cellular biochemistry, ISSN 0730-2312, [in press] 2017, 23 str., doi: 10.1002/jcb.26152
- VIZOVIŠEK, Matej, VIDMAR, Robert, VAN QUICKELBERGHE, Emmy, IMPENS, Francis, ANDJELKOVIĆ, Uroš, SOBOTIČ, Barbara, STOKA, Veronika, GEVAERT, Kris, TURK, Boris, FONOVIĆ, Marko. Fast profiling of protease specificity reveals similar substrate specificities for cathepsins K, L and S. Proteomics, ISSN 1615-9853. [Print ed.], 2015, vol. 15, issue 14, str. 2479-2490, doi: 10.1002/pmic.201400460
- MAHER, Katarina, JERIČ KOKELJ, Barbara, BUTINAR, Miha, MIKHAYLOV, Georgy, MANČEK KEBER, Mateja, STOKA, Veronika, VASILJEVA, Olga, TURK, Boris, GRIGORYEV, Sergei A., KOPITAR-JERALA, Nataša. A role for stefin B (cystatin B) in inflammation and endotoxemia. The Journal of biological chemistry, ISSN 0021-9258, 2014, vol. 289, no. 46, str. 31736-31750, doi: 10.1074/jbc.M114.609396
- JERIČ KOKELJ, Barbara, DOLENC, Iztok, MIHELIČ, Marko, KLARIĆ, Martina, ZAVAŠNIK-BERGANT, Tina, GUNČAR, Gregor, TURK, Boris, TURK, Vito, STOKA, Veronika. N-terminally truncated forms of human cathepsin F accumulate in aggresome-like inclusions. *Biochimica et biophysica acta. BBA, Molecular cell research*, ISSN 0167-4889. [Print ed.], 2013, vol. 1833, no. 10, str. 2254-2266, doi: 10.1016/j.bbamcr.2013.05.007