Univerza v Mariboru

Fakulteta za naravoslovje in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	**Atomistične simulacije biomolekul**
Course title:	**Atomistic simulations of biomolecules**

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
FIZIKA		1. ali 2.	**1., 2. ali 4.**
PHYSICS		1. or 2.	**1., 2. or 4.**

Vrsta predmeta / Course type Izbirni za vse module

Univerzitetna koda predmeta / University course code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Lab. vaje Laboratory work	Terenske vaje Field work	Samost. delo Individ. work	ECTS
10	**5**				**165**	**6**

Nosilec predmeta / Lecturer: **Franci Merzel**

Jeziki / Languages:	
Predavanja / Lectures:	slovenski/Slovenian in/and angleški s slovenskim prevodom/English with translation in Slovenian
Vaje / Tutorial:	slovenski/Slovenian in/and angleški s slovenskim prevodom/English with translation in Slovenian

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

Ni posebnih zahtev.

Prerequisits:

No special prerequisites.

Vsebina:

- Opis kvantnih in klasičnih prostostnih stopenj ter interakcij pri biomolekularnih sistemih
- Simulacije različnih statistično-mehanskih porazdelitev
- Napredne metode in algoritmi za simulacije

Content (Syllabus outline):

- Description of quantum and classical degrees of freedom and corresponding interactions in biomolecular systems
- Simulating various statistical-mechanical ensambles - Advanced simulation methods and algorithms
- Structure, dynamics and function of biomolecules

• Struktura, dinamika in funkcija biomolekul • Analiza normalnih načinov nihanja • Povezava z glavnimi eksperimentalnimi tehnikami za določanje strukture (rentgenska kristalografija, NMR spektroskopija) in dinamike (IR in nevtronska spektroskopija) • Računanje proste energije pri biokemijskih procesih (vezava ligandov) • Problem zvijanja proteinov • Simulacije agregacije polipeptidov	• Normal mode analysis • Simulation methods versus experimental techniques for structure determination (X-ray crystallography, NMR) and for studying dynamics (light and neutron spectroscopy) • Calculating free energies in biochemical processes (ligand binding) • Protein folding problem • Simulating polypeptide aggregation

Temeljni literatura in viri / Readings:

1) A. R. Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001.
2) D. Frenkel, B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2002.
3) M. Daune, Molecular biophysics: Structures in motion, Oxford, University Press, 1999.

Cilji in kompetence:	**Objectives and competences:**
Študenti poglobijo znanje s področja modeliranja v molekularni biofiziki. Študenti so sposobni uporabiti metode molekularnega modeliranja pri konkretnih problemih iz molekularne biofizike. Spoznajo pomembnost povezanosti računalniških simulacij z eksperimentalnimi metodami. Spoznajo najnovejše raziskave in delo raziskovalnih skupin na tem področju po svetu in v regiji.	Students acquire advanced knowledge in the field of modeling in molecular biophysics. Students are able to apply methods of molecular modeling to solve various problems in molecular biophysics. They learn about the importance of the link between computer simulations and experimental methods. Students get familiar with up-todate research work and research teams working in that field in the region and worldwide.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanje in razumevanje: Poglobljeno razumevanje in sposobnost formulacije problemov iz molekularne biofizike na atomskem nivoju ter njihovo reševanje s sodobnimi računalniškimi metodami. Prenesljive/ključne spretnosti in drugi atributi:	Knowledge and understanding: Deeper understanding of - and abilities to formulate - problems in molecular biophysics on atomic-detail level and solving these problems using modern computational methods. Transferable/Key Skills and other attributes:

Sposobnost razvoja in uporabe izvirnih znanstvenih rešitev pri konstruiranju matematičnih modelov molekularne biofizike ter njihova predstavitev v mednarodni znanstveni periodiki.	Skills for development and implementation of original scientific solutions in constructing mathematical models of molecular biophysics. Presentation of acquired knowledge and research results in international scientific journals.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja, seminar in izdelava samostojnih raziskovalnih/seminarskih nalog.	Lectures, seminar and work out of individual research seminars.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Način (pisni izpit, ustno izpraševanje, naloge, projekt)		Type (examination, oral, coursework, project):
Seminarska naloga	**50%**	Coursework
Ustni izpit	**50%**	Oral exam

Reference nosilca / Lecturer's references:

1. GRDADOLNIK, Jože, MERZEL, Franci, AVBELJ, Franc. Origin of hydrophobicity and enhanced water hydrogen bond strength near purely hydrophobic solutes. *Proceedings of the National Academy of Sciences of the United States of America*, ISSN 0027-8424, Jan. 2017, vol. 114, iss. 2, str. 322-327 http://www.pnas.org/content/early/2016/12/23/1612480114.full.pdf?sid=4d626f7e-b9fa-446e-aeb6-b9080c59ce6a, doi: 10.1073/pnas.1612480114. [COBISS.SI-ID 6068250]

2. MIRTIČ, Andreja, MERZEL, Franci, GRDADOLNIK, Jože. The amide III vibrational circular dichroism band as a probe to detect conformational preferences of alanine dipeptide in water. *Biopolymers*, ISSN 0006-3525, Jul. 2014, vol. 101, iss. 7, str. 814-818, ilustr. http://onlinelibrary.wiley.com/doi/10.1002/bip.22460/pdf, doi: 10.1002/bip.22460. [COBISS.SI-ID 5482522]

3. PODOBNIK, Marjetka, SIDDIQUI, Nida, REBOLJ, Katja, NAMBI, Subhalaxmi, MERZEL, Franci, VISWESWARIAH, Sandhya S. Allostery and conformational dynamics in cAMP-binding acyltransferases. *The Journal of biological chemistry*, ISSN 0021-9258, Jun. 2014, vol. 289, iss. 23, str. 16588-16600. http://www.jbc.org/content/289/23/16588.abstract, doi: 10.1074/jbc.M114.560086. [COBISS.SI-ID 5463578]

4. NANDI, Sisir, MONESI, Alessandro, DRGAN, Viktor, MERZEL, Franci, NOVIČ, Marjana. Quantitative structure-activation barrier relationship modeling for Diels-Alder ligations utilizing quantum chemical structural descriptors. *Chemistry central journal*, ISSN 1752-153X, Oct. 2013, vol. 7, str. 1-13, ilustr. http://journal.chemistrycentral.com/content/pdf/1752-153X-7-171.pdf, doi: 10.1186/1752-153X-7-171. [COBISS.SI-ID 5382426]

5. GODEC, Aljaž, SMITH, Jeremy C., MERZEL, Franci. Soft collective fluctuations governing hydrophobic association. *Physical review letters*, ISSN 0031-9007. [Print ed.], Sep. 2013, vol. 111,

iss. 12, str. 127801-1 - 127801-5. http://link.aps.org/doi/10.1103/PhysRevLett.111.127801, doi: 10.1103/PhysRevLett.111.127801. [COBISS.SI-ID 36953605]