UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Biomolekularne simulacije
Course title:	Biomolecular Simulations

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

Vrsta predmeta / Course type	Izbirni / Elective
Univerzitetna koda predmeta / University course code:	NANO3-789

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. Janez Mavri
Jeziki / Languages: Predavanja / Lectures:	Slovenščina, angleščina / Slovenian, English
Vaje / Tutorial:	

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisits:**
Zaključen študij druge stopnje s področja naravoslovja ali tehnologije ali zaključen študij druge stopnje na drugih področjih z znanjem osnov s področja predmeta.	Completed second cycle studies in natural sciences or technologies or completed second cycle studies in other fields with knowledge of fundamentals in the field of this course.

Vsebina:	**Content (Syllabus outline):**
• Časovno odvisna in časovno neodvisna Schrödingerjeva enačba • Polje sile • Kemijske reakcije v plinski fazi • Molekulska dinamika in Monte Carlo simulacija • Refinement: Vključitev eksperimentalnih podatkov • Kako izračunati razlike v prostih energijah • Kemijska reakcija v encimski okolici • Simulacija nuklearnega tuneliranja • Design inhibitorjev na osnovi strukture prehodnega stanja • Modelna študija i) Simulacija kemijskega koraka monoaminske oksidaze • Modelna študija ii) Simulacija prenosa protona z integracijo po poti v encimskem	• Time-dependent and time-independent Schrödinger equation • Force field • Chemical reactions in the gas phase • Molecular dynamics and the Monte Carlo simulation • Refinement: Incorporation of experimental data • How to calculate free energy differences • Chemical reaction in an enzymatic environment • Simulation of nuclear tunnelling • Design of inhibitors on the basis of the transition- state structure • Model study i) Simulation of chemical step of monoamine oxidase • Model study ii) Path integral simulation of

centru • Modelna študija iii) Simulacija reakcije v vodni raztopini	proton transfer in the enzyme center • Model study iii) Simulation of a chemical reaction in aqueous soution

Temeljni literatura in viri / Readings:

- Warshel, A. (1991): Computer modeling of chemical reactions in enzymes and solutions. J. Wiley
- Field, M.J. (2002): Simulating enzyme reactions: Challenges and Perpectives. J. Comp. Chem. 23, str: 48 – 58.
- https://www.nobelprize.org/nobel_prizes/chemistry/laureates/2013/warshel-lecture.html

Cilji in kompetence:

Študent bo dobil vpogled v probleme biomolekularnih simulacij: kvantno mehanske metode, metode na osnovi molekulske mehanike, ki omogočajo termično povprečenje, modeliranje kemijskih reakcij v raztopinah, encimatske reakcije in načrtovanje inhibitorjev. Sestavni del predmeta je praktično delo z računalnikom.

Splošne kompetence:

- obvladanje raziskovalnih metod, postopkov inprocesov, razvoj kritične in samokritične presoje,
- 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 uporabo znanja s področja biomolekularnih simulacij.

Objectives and competences:

Students will gain insight into the problems of intermolecular simulations: quantum-mechanical methods, molecular mechanics-based methods enabling thermal averaging, the modelling of chemical reactions in solutions, enzymatic reactions and theplanning of inhibitors. Practical work involving the use of computers constitutes an integral part of this course.

General Competences:

- The student will master research methods, procedures and processes
- The student will develop critical thinking
- 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 apply knowledge of biomolecular simulations.

Predvideni študijski rezultati:

Študent bo dobil vpogled v probleme biomolekularnih simulacij.
Študent bo sposoben uporabljati pridobljeno znanje v svojem raziskovalnem delu.

Intended learning outcomes:

The student will gain insight into the problems of intermolecular simulations.
Students will be able to apply the obtained knowledge in their research work.

Metode poučevanja in učenja:

- Predavanja
- Seminarji
- Konzultacije
- Laboratorijsko delo

Learning and teaching methods:

- Lectures
- Seminar work
- Consultations
- Laboratory work

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
• seminar	50 %	• seminar
• ustni izpit	50 %	• oral exam

Reference nosilca / Lecturer's references:

- PREGELJC, Domen, JUG, Urška, MAVRI, Janez, STARE, Jernej. Why does the Y326I mutant of monoamine oxidase B decompose an endogenous amphetamine at a slower rate than the wild type enzyme? Reaction step elucidated by multiscale molecular simulations. *PCCP. Physical chemistry chemical physics: a journal of European chemical societies*, ISSN 1463-9076, Feb. 2018, vol. 20, iss. 6, str. 4181-4188
- **J**UG, Urška, PREGELJC, Domen, MAVRI, Janez, VIANELLO, Robert, STARE, Jernej. Elementary SN2SN2 reaction revisited. Effects of solvent and alkyl chain length on kinetics of halogen exchange in haloalkanes elucidated by Empirical Valence Bond simulation. *Computational and theoretical chemistry*, ISSN 2210-271X, 15 Sep. 2017, vol. 1116, str. 96-101
- OANCA, Gabriel, STARE, Jernej, VIANELLO, Robert, MAVRI, Janez. Multiscale simulation of monoamine oxidase catalyzed decomposition of phenylethylamine analogs. *European Journal of Pharmacology*, ISSN 0014-2999. [Print ed.], Dec. 2017, vol. 817, str. 46-50
- OANCA, Gabriel, STARE, Jernej, MAVRI, Janez. How fast monoamine oxidases decompose adrenaline? Kinetics of isoenzymes A and B evaluated by empirical valence bond simulation. *Proteins*, ISSN 0887-3585. [Print ed.], Dec. 2017, vol. 85, iss. 12, str. 2170-2178
- KISOVEC, Matic, REZELJ, Saša, KNAP, Primož, CAJNKO, Miša Mojca, CASERMAN, Simon, FLAŠKER, Ajda, ŽNIDARŠIČ, Nada, REPIČ, Matej, MAVRI, Janez, RUAN, Yi, SCHEURING, Simon, PODOBNIK, Marjetka, ANDERLUH, Gregor. Engineering a pH responsive pore forming protein. *Scientific reports*, ISSN 2045-2322, Feb. 2017, vol. 7, str. 42231-1-42231-13