

УНИВЕРЗИТЕТ У БЕОГРАДУ
ФАРМАЦЕУТСКИ ФАКУЛТЕТ
 СЕКРЕТАРИЈАТ

Примљено: 11.06.2022			
Фрт. јед.	Број	Прийе	Вредност
01	1188/11		

**UNIVERZITET U BEOGRADU – FARMACEUTSKI FAKULTET
 IZBORNOM VEĆU**

Na osnovu odluke Izbornog veća Univerziteta u Beogradu – Farmaceutskog fakulteta br. 804/3 od 15.04.2022. godine, imenovana je Komisija za pripremu referata o prijavljenim kandidatima po raspisanom konkursu za izbor jednog redovnog profesora za užu naučnu oblast Farmaceutska-medicinska hemija i strukturna analiza.

Komisija u sastavu:

1. Prof. dr Olivera Čudina, Univerzitet u Beogradu - Farmaceutski fakultet
2. Prof. dr Zorica Vujić, Univerzitet u Beogradu - Farmaceutski fakultet
3. Prof. dr Katarina Anđelković, Univerzitet u Beogradu - Hemijski fakultet

podnosi sledeći

R E F E R A T

Na konkurs objavljen 27.04.2022. godine u listu "Poslovi", broj 984-985, za jednog redovnog profesora za užu naučnu oblast Farmaceutska-medicinska hemija i strukturna analiza prijavio se jedan kandidat, dr Katarina Nikolić, vanredni profesor na Katedri za farmaceutsku hemiju Univerziteta u Beogradu – Farmaceutskog fakulteta,
 Na osnovu priložene dokumentacije utvrđeno je da kandidat ispunjava opšte uslove konkursa, pa Komisija Izbornom veću Farmaceutskog fakulteta podnosi detaljan izveštaj, kao i konačno mišljenje i zaključak.

U prilogu:

Obrazac 2: Predlog za izbor u zvanje redovnog profesora

Obrazac 4B. Sažetak Referata Komisije o prijavljenim kandidatima za izbor u zvanje redovnog profesora

Obrazac 5. Izjava o izvornosti

Biografski podaci

Katarina Nikolić je rođena 1975. godine u Sremskoj Mitrovici. U Rumi je završila osnovnu školu kao nosilac Vukove diplome i gimnaziju prirodno-matematičkog smera sa odličnim uspehom.

Farmaceutski fakultet u Beogradu je upisala 1993. godine i diplomirala septembra 1998. godine sa prosečnom ocenom 9,23. Povodom jubileja Univerziteta u Beogradu je 1999. godine dobila *nagradu za najboljeg studenta Farmaceutskog fakulteta* u školskoj 1997/98. godini.

Školske 1998/99. godine je upisala magistarske studije iz molekularne spektroskopije na Fakultetu za fizičku hemiju u Beogradu. Položila je sve ispite predviđene nastavnim programom sa prosečnom ocenom 9,75 i odbranila magistarsku tezu pod nazivom: "Primena bliske infracrvene spektroskopije u kvantitativnoj analizi Hidrokortizon Natrijum Sukcinata za injekcije", u martu 2001. godine.

Doktorsku disertaciju pod nazivom: "Molekulsko modeliranje i *in vitro* ispitivanje antioksidativnih osobina fenilselenosukcinil- α -tokoferil estara sa potencijalnim antiproliferativnim dejstvom" je odbranila u aprilu 2007. godine na Katedri za Farmaceutsku hemiju i analitiku lekova, Farmaceutskog fakulteta u Beogradu, pod mentorstvom dr Danice Agbaba.

Specijalistički rad na zdravstvenoj specijalizaciji Ispitivanje i kontrola lekova pod nazivom "Hemometrijsko ispitivanje hromatografskog ponašanja rivastigmina, selegilina i galantamina □ Farmakologija rivastigmina, selegilina i galantamina" je odbranila u oktobru 2021. na Farmaceutskom fakultetu u Beogradu.

Dr Katarina Nikolić je bila na studijskom boravku (FP7/COST-STSM-CM1103-10295) na *University of St Andrews, St Andrews, UK (Dr John Mitchell, EaStCHEM School of Chemistry)* pod nazivom: *Theoretical prediction of the pharmaceutical targets of the examined multitarget compounds* u periodu 11-20. jun 2012.

U okviru bilateralnog projekta *Hubert Curien Partnership Project for collaboration France-Serbia 2020-2022* pod nazivom: *Identification of novel DOT1L and DNMT1/3A inhibitors*, dr Katarina Nikolić je bila na studijskom boravku na *Intitute Pasteur* u Parizu u periodu 24.11 - 4. 12.2021. godine.

Pohađala je Trening školu: *Perspectives in Clinical Proteomics Training Workshop, Held at: Wellcome Trust Conference Centre Wellcome Trust Genome Campus Hinxton Cambridge UK*, 15-17. 03. 2012. godine.

Akademsko angažovanje i radno iskustvo

U periodu 1998-2002. godine dr Katarina Nikolić je radila u kontroli kvaliteta lekova, razvoju i validaciji novih analitičkih metoda fabrike lekova *Medochemie/Biogen* na Kipru.

Od 2001. do 2005. godine je bila angažovana kao istraživač saradnik na međunarodnom projektu pod rukovodstvom prof. dr. Anastasiosa Keramidasa na Hemijskom fakultetu Univerziteta u Nikoziji, Kipar. Od oktobra 2005. do januara 2007. godine je predavala hemiju na osnovnim studijama, *KES College-Nikozija*, Kipar.

Dr Katarina Nikolić je od 2007. godine angažovana kao naučni saradnik na projektu finansiranom od strane Ministarstva nauke Republike Srbije, na Katedri za

farmaceutsku hemiju Farmaceutskog fakulteta u Beogradu. U zvanje viši naučni saradnik izabrana je 2009. godine, a 2015. je izabrana u zvanje naučni savetnik.

Od januara 2013. godine zaposlena je na Farmaceutskom fakultetu u Beogradu u zvanju docenta, od novembra 2017. godine u zvanju vanrednog profesora na Katedri za farmaceutsku hemiju.

OBAVEZNI USLOVI ZA IZBOR U ZVANJE REDOVNOG PROFESORA

1. NASTAVNA AKTIVNOST

1.1. ISKUSTVO U PEDAGOŠKOM RADU SA STUDENTIMA

Dr Katarina Nikolić ima 10 godina pedagoškog iskustva u radu sa studentima. Učestvuje u realizaciji praktične i teorijske nastave u okviru integrisanih akademskih studija-studijski program *Farmacija* na obaveznim predmetima *Farmaceutska hemija 1*, *Farmaceutska hemija 2* i *Farmaceutska hemija 3* i na izbornom predmetu *Odabrana poglavlja farmaceutske hemije*.

Učestvuje u izvođenju praktične i teorijske nastave (predmeti *Pharmaceutical chemistry 2* i *Pharmaceutical chemistry 3*) u okviru integrisanih akademskih studija na engleskom jeziku na Farmaceutskom fakultetu u Beogradu.

Učestvovala je u izvođenju nastave na Doktorskim akademskim studijama-modul Farmaceutska hemija (program akreditovan 2013.) na predmetima *Metode u dizajniranju lekova*, *Hemometrijske metode u farmaceutskoj hemiji*, *Računarske metode u hemijskoj biologiji*, *Spektroskopske metode 2* i *Seminar 3*, kao i na predmetu *Hemijske i biološke interakcije biomolekula u razvoju novih lekova* (program akreditovan 2020.).

Od školske 2021/22. godine učestvuje u realizaciji nastave na novom master studijskom programu *Napredna analiza podataka*, akreditovanom na Univerzitetu u Beogradu. Za ovu master studiju je prof. dr Katarina Nikolić pripremila plan i program za akreditaciju i učestvuje u realizaciji na predmetu *Napredna analiza podataka u farmaceutskom istraživanju i razvoju*.

1.2. OCENA PEDAGOŠKOG RADA DOBIJENA U STUDENTSKIM ANKETAMA TOKOM CELOKUPNOG PROTEKLOG IZBORNOG PERIODA

Od izbora u zvanje vanredni profesor na studentskim anketama u praktičnoj i teorijskoj nastavi sa studentima Farmaceutskog fakulteta Univerziteta u Beogradu, na skali od 1 do 5, prof. dr Katarina Nikolić je ocenjena srednjom ocenom **4,73** (Tabela 1).

Tabela 1. Tabelarni prikaz prosečnih ocena za praktičnu i teorijsku nastavu za period nakon izbora u zvanje vanredni profesor.

	Predmet						
Školska godina	Farmaceutska hemija 1		Farmaceutska hemija 2		Farmaceutska hemija 3		Odabrana pog. FH
	Teorijska nastava	Praktična nastava	Teorijska nastava	Praktična nastava	Teorijska nastava	Praktična nastava	Teorijska nastava
2017/18.	-	4,71	-	-	4,66	4,67	4,92
2018/19.	-	4,64	4,70	4,67	4,64	4,67	4,53
2019/20.	-	4,66	4,64	4,67	4,55	4,65	5,00
2020/21.	-		-	4,74	4,94	4,94	4,95
2021/22.	-		-	-	4,75	4,74	5,00
Σ		4,67	4,67	4,69	4,71	4,73	4,88
Σ	4,73						

1.3. MENTORSTVO I ČLANSTVO U KOMISIJAMA ZA ODBRANU ZAVRŠNIH RADOVA NA INTEGRISANIM AKADEMSKIM STUDIJAMA

Dr Katarina Nikolić bila je mentor ukupno 10 završnih radova na integrisanim akademskim studijama i član komisije za odbranu 4 završna rada. Od izbora u zvanje vanrednog profesora bila je mentor 4 završna rada.

U zvanju docenta dr Katarina Nikolić je bila mentor za odbranu 6 završnih radova na Farmaceutskom fakultetu u Beogradu.

1. Teodora Đikić (februar 2013.) Farmaceutski fakultet u Beogradu
2. Jelena Oluić (avgust 2015.) Farmaceutski fakultet u Beogradu
3. Svetlana Erić (jun 2016.) Farmaceutski fakultet u Beogradu
4. Nemanja Đoković (septembar 2016.) Farmaceutski fakultet u Beogradu
5. Milica Radan (septembar 2017.) Farmaceutski fakultet u Beogradu
6. Mirjana Antonijević (jul 2017.) Farmaceutski fakultet u Beogradu

Od izbora u zvanje vanredni profesor dr Katarina Nikolić je bila mentor 4 završna rada:

1. Milan Jovanovic (septembar 2018.) "3D-QSAR studija selektivnih inhibitora PI3Kα kinaze kao potencijalnih antineoplastika", Farmaceutski fakultet u Beogradu
2. Aleksandar Rajkovic (septembar 2019.) "3D-QSAR studija i analiza struktura farmakofore inhibitora ABL1 tirozin kinaza", Farmaceutski fakultet u Beogradu
3. Milan Beljkaš (avgust 2020.) "Molekulsko modelovanje, sinteza i ispitivanje antimigratornih i antiinvazivnih osobina novih derivata 1-benzhidrilnog piperazina", Farmaceutski fakultet u Beogradu - **Prva Konkursna nagrada Fond Nenada M. Kostića za najbolje diplomske i master radove odbranjene u periodu od 1. aprila 2020. do 31. marta 2021. godine iz oblasti hemijskih nauka**
4. Ana Postolović (jul 2021.) "Racionalni dizajn inhibitora sirtuina 2 primenom analize strukture farmakofore i molekulskog dokinga", Farmaceutski fakultet u Beogradu

1.4. MENTORSTVO I ČLANSTVO U KOMISIJAMA ZA PRIJAVU, OCENU I ODBRANU DOKTORSKE DISERTACIJE

Dr Katarina Nikolić je bila mentor ukupno 7 doktorskih disertacija i član komisije za odbranu 10 doktorskih disertacija. Od izbora u zvanje vanredni profesor je mentor 4 doktorske disertacije i bila je član komisije za odbranu 3 doktorske disertacije.

U zvanju docenta dr Katarina Nikolić je bila mentor 3 odbranjene doktorske disertacije:

1. Dipl. farm. Slavica Filipić (21.3.2013. godine) na Farmaceutskom fakultetu u Beogradu, pod nazivom: "Kvantitativni odnosi strukture, aktivnosti i retencionih osobina liganada imidazolinskih i alfa2 adrenergičkih receptora".
2. Dipl. farm. Marija Čarapić (7.9.2015. godine) na Farmaceutskom fakultetu u Beogradu, pod nazivom: „Razvoj hromatografskih metoda za određivanje sadržaja, stepena čistoće i retencionih karakteristika ziprazidona primenom eksperimentalnog dizajna“.
3. Dipl. farm. Nataša Đorđević Filijović (25.12.2015. godine) na Farmaceutskom fakultetu u Beogradu, pod nazivom: „Karakterizacija i procena kritičnih parametara stabilnosti tableta olanzapina i aripiprazola primenom eksperimentalnog dizajna“.

U zvanju docenta dr Katarina Nikolić je bila član komisije za odbranu 7 doktorskih disertacija:

- Mag. farm. Branka Ivković (20.3.2013.) na Farmaceutskom fakultetu u Beogradu
- Dipl. farm. Brankica Filipić (14.11.2013.) na Farmaceutskom fakultetu u Beogradu.
- Dipl. farm. Marija Popović (3.9.2015.) na Farmaceutskom fakultetu u Beogradu.
- Dipl. farm. Vladimir Dobričić (22.12.2014.) na Farmaceutskom fakultetu u Beogradu.
- Dipl. farm. Miralem Smajić (22.9.2016.) na Farmaceutskom fakultetu u Beogradu.
- Dipl. biol. Branislava Gemović (3.4.2015.) na Biološkom fakultetu u Beogradu.
- Dipl. farm. Musbah Shenger (13.4.2017.), na Farmaceutskom fakultetu u Beogradu

Od izbora u zvanje vanredni profesor dr Katarina Nikolić je mentor jedne odbranjene, jedne ocenjene i dve prijavljene doktorske disertacije:

1. Mast. hem. Strahinja Stevanović (odbranjena 25. 03. 2022.), na Farmaceutskom fakultetu u Beogradu pod nazivom: "*In silico* selekcija i *in vitro* ispitivanja prirodnih i sintetskih inhibitora rasta parazita *Leishmania* spp."
2. Mag. farm. Dušan Ružić na Farmaceutskom fakultetu u Beogradu pod nazivom: „Racionalni dizajn, sinteza i *in vitro* ispitivanja selektivnih inhibitora histon deacetilaze 6“. Izveštaj Komisije za ocenu i odbranu završene doktorske disertacije je prihvaćen na sednici NNV 14.04.2022. godine.
3. Mag. farm. Nemanja Đoković na Farmaceutskom fakultetu u Beogradu pod nazivom: „Simulacije molekulske dinamike, dizajn, sinteza i *in vitro* ispitivanje inhibitora epigenetskih proteina kao potencijalnih antineoplastika“. Tema doktorske disertacije je odobrena na sednici VNOMN 24.12.2020.
4. Mag. farm. Milica Radan na Farmaceutskom fakultetu u Beogradu pod nazivom: „Određivanje strukture farmakofore, dizajn i *in vitro* ispitivanje liganada sa višestrukim dejstvom kao potencijalno efikasnijih terapeutika složenih neuroloških i mentalnih oboljenja“. Tema doktorske disertacije je odobrena na sednici VNOMN 24.12.2020.

Od izbora u zvanje vanredni profesor dr Katarina Nikolić je bila član komisije 3 odbranjene doktorske disertacije:

1. Mag. farm. Darija Obradović (20.06.2021.), na Farmaceutskom fakultetu u Beogradu, pod nazivom: „Modelovanje retencionog ponašanja liganada imidazolinskih i serotoninских receptora i srodnih jedinjenja u različitim hromatografskim uslovima“.
2. Mag. farm. Žarko Gagić (13.04.2018.), na Farmaceutskom fakultetu u Beogradu pod nazivom: „Određivanje strukture farmakofore, dizajn, sinteza i ispitivanje antiproliferativne aktivnosti derivata α -tokoferola i γ -tokotrienola“, član komisije i mentor
3. Mag. farm. Jelica Vučićević (10.01.2020.), na Farmaceutskom fakultetu u Beogradu pod nazivom: „Heminformatička analiza, dizajn i ispitivanje proapoptotske aktivnosti novih liganada imidazolinskih receptora“, član komisije i mentor

1.5. UDŽBENICI, ZBIRKE ZADATAKA, PRAKTIKUMI

Dr Katarina Nikolić je koautor jednog pomoćnog udžbenika i jednog osnovnog udžbenika za predmet *Farmaceutska hemija 3*.

1. PRAKTIKUM IZ FARMACEUTSKE HEMIJE III

Autori: Katarina Nikolić, Slavica Filipić, Milkica Crevar Sakač

Farmaceutski fakultet, Univerzitet u Beogradu, Beograd, 2014. ISBN 978-86-6273-021-3

2. ADRENERGICI, ANTIANGINALNI LEKOVI I VAZODILATATORI

Autor: Katarina Nikolić

Farmaceutski fakultet, Univerzitet u Beogradu, Beograd, 2022. ISBN: 978-86-6273-078-

1.6. PODRŠKA VANNASTAVNIM AKADEMSKIM AKTIVNOSTIMA STUDENATA

Dr Katarina Nikolić je bila mentor 17 studentskih istraživačkih radova (od izbora u zvanje vanredni profesor 7 radova) i član Stručne Komisije Studenskog Mini-kongresa na Farmaceutskom fakultetu u Beogradu (2013, 2014. i 2017. godine).

1. student Aleksandar Rajkovic, naziv rada: "Molekulsko modelovanje, 3D-QSAR studija i analiza struktura farmakofore inhibitora ABL1 tirozin kinaza", XI Mini-kongres studenata Farmaceutskog fakulteta, april 2018. godine, KSBMNS, Kopaonik, 26-30. april 2018. godine, p. 983.
2. student Alen Čebzan, naziv rada: "Molekulsko modelovanje, 3D-QSAR studija i analiza struktura farmakofore inhibitora MAPK1 (mitogen-aktivirane protein kinaze-1)", XI Mini-kongres studenata Farmaceutskog fakulteta, april 2018. godine.
3. student Milan Jovanović, naziv rada: "Molekulsko modelovanje, 3D-QSAR studija i analiza struktura farmakofore inhibitora kinaze PI3K- α ", XI Mini-kongres studenata Farmaceutskog fakulteta, april 2018. godine.
4. student Ana Postolović, naziv rada: "Molekulsko modelovanje inhibitora sirtuina 2 primenom molekuskog dokinga i analiza strukture farmakofore", XIV Mini-kongres studenata Farmaceutskog fakulteta, april 2021. godine.
5. student Branko Radović, naziv rada: "Sinteza i molekulsko modelovanje novog derivata fenitoina kao potencijalnog inhibitora humanie histon deacetilaze 6", XIV Mini-kongres studenata Farmaceutskog fakulteta, april 2021. godine - **najbolji rad na sesiji Farmaceutske hemije**
6. student Marija Radiša, naziv rada: „Sinteza, molekulsko modelovanje i ispitivanje citotoksičnih aktivnosti paroksetina i njegovog derivata na odabranim tumorskim ćelijama“, XV Mini-kongres studenata Farmaceutskog fakulteta, april 2022. godine.
7. student Alen Čebzan, naziv rada: „Kompjuterski dizajn novih MAPK inhibitora komparativnom analizom rezultata 3D-QSAR modelovanja i molekuskog dokinga“, XV Mini-kongres studenata Farmaceutskog fakulteta, april 2022. godine.

1.7. VREDNOVANJE NASTAVNOG I PEDAGOŠKOG RADA (PREMA ČLANU 9. PRAVILNIKA O BLIŽIM USLOVIMA ZA IZBOR NASTAVNIKA NA FARMACEUTSKOM FAKULTETU)

Tabela 2. Vrednovanje nastavnog i pedagoškog rada za period nakon izbora u zvanje vanredni profesor, osim za nastavnu literaturu koja se odnosi na celokupnu nastavnu karijeru.

Naziv	Vrednost
Zbirna ocena nastavne aktivnosti (teorijska, praktična nastava) dobijena na studentskoj anketi	5
Učešće u realizaciji nastave:	
Farmaceutska hemija 2 – teorijska nastava (preuzela nastavni program)	1
Farmaceutska hemija 3 – teorijska nastava (preuzela nastavni program)	1
Farmaceutska hemija 1 – praktična nastava (preuzela nastavni program)	1
Farmaceutska hemija 2 – praktična nastava (preuzela nastavni program)	1
Farmaceutska hemija 3 – praktična nastava (dopunila nastavni program)	2
Odabrana poglavlja farmaceutske hemije (dopunila nastavni program)	2
Metode u dizajniranju lekova – DAS (dopunila nastavni program)	4
Spektroskopske metode 2 – DAS (dopunila nastavni program)	4
Hemometrijske metode u farmaceutskoj hemiji – DAS (dopunila nastavni program)	4
Seminar 3 – DAS (dopunila nastavni program)	4
Računarske metode u hemijskoj biologiji – DAS (dopunila nastavni program)	4
Hemijske i biološke interakcije biomolekula u razvoju novih lekova – DAS (dopunila nastavni program)	4
Napredna analiza podataka u farmaceutskom istraživanju i razvoju – master studije	6
Praktikum	15
Udžbenik, knjiga	25
Mentor odbranjenog završnog rada IAS – 4x0,5	2
Član komisije za odbranu doktorske disertacije – 3x3	9
Mentor odbranjene doktorske disertacije – 1x10	10
UKUPNO	104

2. NAUČNO-ISTRAŽIVAČKA AKTIVNOST

2.1. RUKOVOĐENJE ILI UČEŠĆE U NAUČNO-ISTRAŽIVAČKIM PROJEKTIMA

Dr Katarina Nikolić je učestvovala u radu 3 nacionalna i 10 međunarodnih naučno-istraživačkih projekata. Od izbora u zvanje vanredni profesor učestvuje u radu 2 nacionalna i 8 međunarodnih naučno-istraživačkih projekata.

2.1.1. Nacionalni projekti

Od januara 2006. godine Katarina Nikolić učestvuje kao saradnik na projektima koje finansira Ministarstvo nauke Srbije:

- 2006-2010. Naziv projekta: *"Sinteza, kvantitativni odnos između strukture/osobina i aktivnosti, fizičko-hemijska karakterizacija i analiza farmakološki aktivnih supstanci"*
Broj projekta: 142071, Farmaceutski fakultet, Univerzitet u Beogradu
Rukovodilac projekta: Prof. dr Danica Agbaba
- 2010-2019. Naziv projekta: *„Sinteza, kvantitativni odnos između strukture i dejstva, fizičko-hemijska karakterizacija i analiza farmakološki aktivnih supstanci“*
Broj projekta: 172033, Farmaceutski fakultet, Univerzitet u Beogradu
Rukovodilac projekta: Prof. dr Danica Agbaba
- 2010-2019. Naziv projekta: *„Primena EIIP/ISM bioinformatičke platforme u otkrivanju novih terapijskih targeta i potencijalnih terapijskih molekula“*
Broj projekta: 173001, Institut za Nuklearne nauke Vinča
Rukovodilac projekta: Prof. dr Veljko Veljković

Od 2019. godine, nakon prelaska na institucionalno finansiranje naučnoistraživačkog rada, prof. dr Katarina Nikolić je imenovana za rukovodioca istraživačke grupe Farmaceutskog fakulteta Univerziteta u Beogradu, koja se sastoji od 11 članova.

2.1.2. Međunarodni projekti

1. Saradnik, član upravnog odbora i rukovodilac radne grupe za kompjutersku hemiju (WG-1) na evropskom projektu FP7/COST (European Cooperation in the field of Scientific and Technical Research) pod nazivom: *"Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain."* Action CM1103, 2011-2015.
http://www.cost.eu/COST_Actions/cmst/Actions/CM1103
2. Saradnik i član upravnog odbora na evropskom projektu FP7/COST (European Cooperation in the field of Scientific and Technical Research) pod nazivom GLISTEN: GPCR-Ligand Interactions, Structures, and Transmembrane Signaling: a European Research Network Action CM1207, 2013-2017.
http://www.cost.eu/COST_Actions/cmst/Actions/CM1207

3. Učesnik i član upravnog odbora EU projects: FP7/COST CM1406 action (2015-2019): *Epigenetic Chemical Biology (EPICHEM)*: http://www.cost.eu/COST_Actions/cmst/Actions/CM1406
4. Učesnik EU projects: HORISON 2020/COST Action CA15135 (2016-2020): *Multi-target paradigm for innovative ligand identification in the drug discovery process (MuTaLig)*. http://www.cost.eu/COST_Actions/ca/CA15135
5. Učesnik EU projects: HORISON 2020/COST Action CA16205 (2017-2021): *European Network on Understanding Gastrointestinal Absorption-related Processes (UNGAP)*: http://www.cost.eu/COST_Actions/ca/CA16205
6. Učesnik EU projects: Horison 2020/ COST CA17104 action (2018-2022): *New diagnostic and therapeutic tools against multidrug resistant tumors*: http://www.cost.eu/COST_Actions/ca/CA17104
7. Učesnik i član upravnog odbora EU projects: Horison 2020/ COST action CA18133 (2019-2023): *European Research Network on Signal Transduction*. <https://www.cost.eu/actions/CA18133/#tabsName:overview>
8. Učesnik i član upravnog odbora EU projects: Horison 2020/ COST action CA18240 (2019-2023): *ADHEsion GPCR Network: Research and Implementation Set the path for future Exploration*. <https://www.cost.eu/actions/CA18240/#tabsName:overview>
9. Rukovodilac istraživanja: Bilateral project, Hubert Curien Partnership Project for collaboration France-Serbia 2020-2022 (Program Pavle Savic 2020): *Identification of novel DOT1L and DNMT1/3A inhibitors*, with Epigenetic Chemical Biology, Institut Pasteur, CNRS UMR3523, Paris 75015 France (Prof Paola Arimondo research group).
10. Rukovodilac istraživanja: *Deutsche Forschungsgemeinschaft (DFG)* project named: *Control of epigenetic states through light-triggered protein-protein interaction mediators*, 2020-2023 PI Asst. Prof. Olalla Vázquez, Fachbereich Chemie Philipps-Universität Marburg, Germany.

2.2. OBJAVLJENI RADOVI

Prof. dr Katarina Nikolić je do sada ukupno objavila 107 radova u časopisima od međunarodnog značaja (M_{20}), 3 poglavlja u knjizi međunarodnog značaja (M_{13} i M_{14}), 8 radova u domaćim časopisima (M_{50}), 122 saopštenja na međunarodnim naučnim skupovima (M_{30}) i 16 saopštenja na nacionalnim naučnim skupovima (M_{64}). Od izbora u zvanje vanredni profesor publikovala je 29 radova (M_{20}): 5 M_{21a} , 10 M_{21} , 12 M_{22} , i 2 M_{23} , 2 poglavlja u knjizi međunarodnog značaja (M_{14}), 3 rada u domaćem časopisu M_{52} , 52 saopštenja na međunarodnim naučnim skupovima (M_{30}): 1 M_{31} , 12 M_{32} , 6 M_{33} i 33 M_{34} i 7 saopštenja na nacionalnim naučnim skupovima (M_{64}).

Kumulativni IF objavljenih radova Katarine Nikolić (u poslednjih 5 godina) je 130,326. Prvi autor ili nosilac rada je u 9 radova sa kumulativnim IF 31,365. Ukupan broj citata bez autocitata je 1110 (Scopus), a H-indeks 17 (Scopus),

SPISAK OBJAVLJENIH PUBLIKACIJA I SAOPŠTENJA

Poglavlje u istaknutoj monografiji međunarodnog značaja (M₁₃)

Pre izbora u zvanje vanredni profesor

1. Danica Agbaba and Katarina Nikolic: Chapter 26: TLC of Antihypertensive and Antihypotensive drugs (p.481-527) In: Thin layer chromatography in drug analysis, Edited by Łukasz Komsta, Monika Waksmundzka-Hajnos and Joseph Sherma. Published by CRC Press (Taylor & Francis) December 20, 2013. ISBN 978-1-4665-0715-9.

Poglavlje u monografiji međunarodnog značaja (M₁₄)

Posle izbora u zvanje vanredni profesor

2 x 4 = 8

1. Ruzic D., Djokovic N., Nikolic K. (2021) Fragment-Based Drug Design of Selective HDAC6 Inhibitors. pages 155-170 In: Ballante F. (eds) Protein-Ligand Interactions and Drug Design. Methods in Molecular Biology, vol 2266. Humana Press-Springer Protocols, New York, NY. https://doi.org/10.1007/978-1-0716-1209-5_9
2. T. Djikic, Z. Gagic, K. Nikolic. Molecular Docking for Computer-Aided Drug Design, Chapter 16 - Design and Discovery of Kinase Inhibitors Using Docking Studies. Fundamentals, Techniques, Resources and Applications 2021, Pages 337-365. Academic Press <https://doi.org/10.1016/B978-0-12-822312-3.00009-6>

Objavljeni radovi međunarodnog značaja (M₂₀):

Radovi u međunarodnom časopisu izuzetnih vrednosti (M_{21-a})

Pre izbora u zvanje vanredni profesor

1. Butini S, Nikolic K, Kassel S, Brückmann H, Filipic S, Agbaba D, Gemma S, Brogi S, Brindisi M, Campiani G, Stark H. Polypharmacology of dopamine receptor ligands. *Progress in Neurobiology* 142, 68-103 (2016) <https://doi.org/10.1016/j.pneurobio.2016.03.011> (IF 2016: 13.217, Neurosciences 7/259).
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151, 4–34 (2017) <https://doi.org/10.1016/j.pneurobio.2015.12.003> (IF 2017: 14.163, *Neurosciences* 8/261).

Posle izbora u zvanje vanredni profesor

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2. S. Abás, S. Rodríguez-Arévalo, A. Bagán, C. Griñán-Ferré, F. Vasilopoulou, I. Brocos-Mosquera, C. Muguruza, B. Pérez, E. Molins, F. Javier Luque, P. Pérez-Lozano, S. de Jonghe, D. Daelemans, L. Naesens, J. Brea, M. Isabel Loza, E. Hernández-Hernández, J. A. García-Sevilla, M. Julia García-Fuster, M. Radan, T. Djikic, K. Nikolic, M. Pallàs, L. F. Callado, C. Escolano. Bicyclic α -iminophosphonates as High Affinity Imidazoline I2 Receptor Ligands for Alzheimer's Disease. *J. Med. Chem.* 2020, 63, 7, 3610–3633. <https://doi.org/10.1021/acs.jmedchem.9b02080> (IF 2020: 7.446, *Chemistry, Medicinal* (3/63)) – **nagrada Farmaceutskog fakulteta za izuzetan doprinos naučnoistraživačkom radu**
3. I. Asanovic, E. Strandback, A. Kroupova, Dj. Pasajlic, A. Meinhart, P. Tsung-Pin, N. Djokovic, D. Anrather, T. Schuetz, M.J. Suskiewicz, S. Sillamaa, T. Kocher, R. Beveridge, K. Nikolic, A. Schleiffer, M. Jinek, M. Hartl, T. Clausen, J. Penninger, P. Macheroux, S. Weitzer, J. Martinez. The oxidoreductase PYROXD1 uses NAD(P)⁺ as an antioxidant to sustain tRNA ligase activity in pre-tRNA splicing and unfolded protein response. *Molecular Cell* 81 (12), P2520-2532.E16, June 17, 2021. DOI: <https://doi.org/10.1016/j.molcel.2021.04.007> (IF 2020: 17.970, *Biochemistry & Molecular Biology* (6/296)) – **nagrada Farmaceutskog fakulteta za izuzetan doprinos naučnoistraživačkom radu**
4. S. Rodriguez-Arévalo, A. Bagán, Christian G. Ferré, F. Vasilopoulou, M. Pallàs, I. Brocos-Mosquera, L.F. Callado, M. Isabel Loza, A.L. Martínez, J. Brea, B. Pérez, E. Molins, S. De Jonghe, D. Daelemans, M. Radan, T. Djikic, K. Nikolic, E.H. Hernández, M.J. García-Fuster, J.A. García-Sevilla, C. Escolano, Benzofuranyl-2-imidazoles as imidazoline I2 receptor ligands for Alzheimer's disease, *European Journal of Medicinal Chemistry* 2021, 222, 113540, <https://doi.org/10.1016/j.ejmech.2021.113540> (IF 2020: 6.514, *Chemistry, Medicinal* (5/63)) – **nagrada Farmaceutskog fakulteta za izuzetan doprinos naučnoistraživačkom radu**
5. Albert L, Nagpal J, Steinchen W, Zhang L, Werel L, Djokovic N, Ruzic D, Hoffarth M, Xu J, Kaspareit J, Abendroth F, Royant A, Bange G, Nikolic K, Ryu S, Dou Y, Essen LO, Vázquez O. Bistable Photoswitch Allows in Vivo Control of Hematopoiesis. *ACS Cent. Sci.* 2022, 8, 57–66. <https://doi.org/10.1021/acscentsci.1c00434> (IF 2020: 14.553, *Chemistry, Multidisciplinary* (17/178)).

Radovi u vrhunskom međunarodnom časopisu (M₂₁)

Pre izbora u zvanje vanredni profesor

1. K. Nikolic, QSAR Study of Aromatic Organochalcogens with Glutathione Peroxidase – like Antioxidant Activity, *QSAR & Combinatorial Science*, 26 (3), 358-367 (2007). <https://doi.org/10.1002/qsar.200610013> (IF 2006: 1.987, Computer Science/Interdisciplinary Application (16/86), Chemistry Multidisciplinary (33/124))
2. K. Nikolic, Design and QSAR study of analogs of alpha-tocopherol with enhanced antiproliferative activity against human breast adenocarcinoma cells, *Journal of Molecular Graphics and Modelling*, 26, 868–873 (2008). <https://doi.org/10.1016/j.jmgm.2007.05.008> (IF 2008: 2.347, Computer Science, Interdisciplinary Applications 12/94)
3. S. Filipic, K. Nikolic, M. Krizman, and D. Agbaba, The Quantitative Structure-Retention Relationship (QSRR) analysis of some centrally acting antihypertensives and diuretics, *QSAR & Combinatorial Science*, 27, 1036 – 1044 (2008). <https://doi.org/10.1002/qsar.200710161> (IF 2008: 2.594, Computer Science, Interdisciplinary Applications 10/94)
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17. O. M. B. Aguilera, G. Esteban, I. Bolea, K. Nikolic, D. Agbaba, I. Moraleda, I. Iriepa, A. Samadi, E. Soriano, M. Unzeta, J. M. Contelles. Design, synthesis, pharmacological evaluation, QSAR analysis, molecular modeling and ADMET of novel donepezileindolyl hybrids as multipotent cholinesterase/monoamine oxidase inhibitors for the potential treatment of Alzheimer's disease. *European Journal of Medicinal Chemistry* 63, 239-255, (2013) <https://doi.org/10.1016/j.ejmech.2013.12.028> (IF 2012: 3.499, Chemistry, Medicinal 13/59).
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 24. Z. Gagic, **K. Nikolic**, B. Ivkovic, S. Filipic, D. Agbaba. QSAR studies and design of new analogs of vitamin E with enhanced antiproliferative activity on MCF-7 breast cancer cells. *J. Taiwan Institute of Chemical Engineers* Volume 59, February 2016, Pages 33-44, <http://dx.doi.org/10.1016/j.jtice.2015.07.019>. (IF 2016: **4.217**, Engineering, Chemical **16/135**)
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Posle izbora u zvanje vanredni profesor

10 x 8 = 80

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Pre izbora u zvanje vanredni profesor

1. J. Letica, S. Markovic, J. Zirojevic, **K. Nikolic**, D. Agbaba, High-Performance Liquid Chromatographic Determination of Pantoprazole and Its Main Impurities in Pharmaceuticals. *Journal of AOAC International*, 93 (4): 1121-1128 (2010). (IF 2010: 1.229, Chemistry/Analytical 46/73)
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Posle izbora u zvanje vanredni profesor

12 x 5 = 60

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3. Čarapić M, **Nikolic K**, Marković B, Petković M, Pavlovic M, Agbaba D. Ultra□ performance liquid chromatography tandem mass spectrometry for the rapid, simultaneous analysis of ziprasidone and its impurities. *Biomedical Chromatography* 2019 Feb;33(2):e4384. <http://dx.doi.org/10.1002/bmc.4384> Epub 2018 Oct 17. (IF 2017: **1.688**, Chemistry, Analytical **47/81**)
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27. D. Obradović, S. Oljačić, **K. Nikolic**, D. Agbaba. Influence of selected mobile phase properties on the TLC retention behavior of ziprasidone and its impurities. *J. Liq. Chrom. Rel. Techn.* 2017, VOL. 40, NOS. 5–6, 247–251. <http://dx.doi.org/10.1080/10826076.2017.1298026> (IF 2016: 0.697, Chemistry, Analytical 68/76).

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29. J. Oluić, **K. Nikolic**, J. Vucicevic, Z. Gagic, S. Filipic, D. Agbaba. 3D-QSAR, Virtual Screening, Docking and Design of Dual PI3K/mTOR Inhibitors with Enhanced Antiproliferative Activity. *Combinatorial Chemistry & High Throughput Screening* 2017, 20 (4), 292-303. <https://doi.org/10.2174/1386207320666170427143858> (IF 2017: **1.205**, Pharmacology & Pharmacy 226/261)
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2 x 3 = 6

1. D. Obradović, D. Jovanović, S. Pešić, J. Tomić, S. Oljačić, **K. Nikolić**, D. Agbaba. Analysis of the retention behavior of selected antiarrhythmics by means of thin-layer chromatography. *Journal of Liquid Chromatography & Related Technologies*. Volume 42, 2019, Issue 9-10: Thin Layer Chromatography. 317-323 <https://doi.org/10.1080/10826076.2019.1585613>. (IF 2019: **0.992**, Chemistry, Analytical 75/86)
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Naučni radovi objavljeni u nacionalnom časopisu (M₅₂)

Pre izbora u zvanje vanredni profesor

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3. **Nikolic K**, Filipic S, Agbaba D. Polypharmacology of dopamine D1-like receptor antagonists. *Arhiv za farmaciju* 2015; 65: 287-303. <https://scindeks.ceon.rs/article.aspx?artid=0004-19631505287N>

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5. Antonijević M, Nikolić K, Vučićević J, Oljačić S, Agbaba D. 3D-QSAR modelovanje i analiza farmakofore antagonista serotonininskih 5-HT_{2A} receptora. *Arhiv za farmaciju* 2017, vol. 67, br. 4, str. 233-247. <https://scindeks.ceon.rs/article.aspx?artid=0004-19631704233A>

Posle izbora u zvanje vanredni profesor

3 x 1,5 = 4,5

1. Jovanović M, Nikolić K, Gagić Ž, Agbaba D. Molekulska modelovanje i analiza 3D-strukture farmakofore selektivnih PI3K-α inhibitora kao antitumorskih agenasa. *Arhiv za farmaciju* 68: 860 – 873 (2018). <https://doi.org/10.5937/ArhFarm1804860J>
2. Radan M, Bošković J, Dobričić V, Čudina O, Nikolić K. Current computer-aided drug design methodologies in discovery of novel drug candidates for neuropsychiatric and inflammatory diseases. *Archives of Pharmacy* 2021, 71, 4. <https://doi.org/10.5937/arhfarm71-32523>
3. Ružić, D., Đoković, N., Nikolić, K., Vujić, Z. (2021). Medicinska hemija inhibitora histon deacetilaza. *Archives of Pharmacy* 2021, 71(2), 73-100. <https://doi.org/10.5937/arhfarm71-30618>

Zbornici međunarodnih naučnih skupova (M₃₀):

Pre izbora u zvanje vanredni profesor

Predavanje po pozivu sa međunarodnog skupa štampano u celini (M₃₁):

1. Nikolic K, Vucicevic J, Popovic M, Filipic S, Obradovic D, Dobričić V, Agbaba D. Study of blood-brain barrier permeation using parallel artificial membrane permeability assay and quantitative-structure permeability relationship modeling. 11th Central European Symposium on Pharmaceutical Technology. September 22-24, 2016, Belgrade, Serbia. Book of Abstracts, *Arh. farm.* 2016; 66/Special Issue, Invited lectures, IL 08, 25-26p.

Posle izbora u zvanje vanredni profesor

Predavanje po pozivu sa međunarodnog skupa štampano u celini (M₃₁): 3 poena

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12 x 1,5 = 18,0

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Posle izbora u zvanje vanredni profesor

33 x 0,5 = 16,5

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7 x 0, 2 = 1,4 poena

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2.3. ANALIZA RADOVA OBJAVLJENIH POSLE IZBORA U ZVANJE VANREDNI PROFESOR

U okviru naučno-istraživačkog rada dr. Katarina Nikolić se bavi računarskom hemijom i kompjuterskim dizajnom novih antineoplastika, epigenetičkih modulatora, antihipertenziva, CNS lekova, antiparazitika i antivirusa, kao i njihovom sintezom i ispitivanjem u cilju otkrića potencijalno efikasnijih terapeutika. Razvojem novih metoda kompjuterskog dizajna lekova (*Computer-Aided Drug Design*, CADD) baziranih na strukturama liganada (*Ligand Based Drug Design*, LBDD) ili na strukturama ciljnog mesta dejstva aktivnih jedinjenja (*Structure Based Drug Design*, SBDD) omogućena je detaljna analiza farmakofora liganada, ključnih interakcija liganada sa receptorom i detaljna procena uticaja strukturnih modifikacija na aktivnost dizajniranih jedinjenja. Deo naučno-istraživačke aktivnosti dr. Katarine Nikolić se odnosi na hemometrijsku i QSPR/QSRR (*Quantitative Structure Property/Retention Relationship*) analizu retencionog ponašanja, fizičko-hemijskih i farmakokinetičkih osobina ispitivanih grupa farmakološki aktivnih supstanci i novosintetisanih jedinjenja primenom regresionih metoda (multilinearna regresija - *Multiple Linear Regression* (MLR), postupna multilinearna regresija - *Stepwise Multiple Linear Regression* (sMLR), metoda parcijalnih najmanjih kvadrata - *Partial Least Square Regression* (PLSR), analiza glavne komponente - *Principal Component Analysis* (PCA)) i naprednih metoda mašinskog učenja (metoda podržavajućih vektora - *Support Vector Machine* (SVM), veštačke neuronske mreže - *Artificial Neural Networks* (ANN)).

Posttranslacione modifikacije histona obuhvataju kovalentnu modifikaciju amino kiselinskih rezidua histona acetil, benzoil formil, krotonil, metil, sukcinil ili nekim drugim grupama, koje vrše kontrolu organizacije hromatina i aktivaciju ili represiju transkripcije gena. Nivo acetilacije lizinskih rezidua histona regulisan je ravnotežnom aktivnošću enzima histon acetiltransferaza (HAT) i histon deacetilaza (HDAC) što utiče na remodelovanje hromatina i regulaciji genske ekspresije. Acetillovani lizini histona predstavljaju epigenetičke markere koji pomoću proteina čitača, poput bromodomena, mogu pokrenuti proces transkripcije odgovarajućih gena. Histon deacetilaze su epigenetski enzimi koji utiču na aktivaciju onkogenih i onkosupresivnih mehanizama regulacije ćelijskog ciklusa, pa se zbog toga danas intenzivno ispituju inhibitori histon deacetilaza. Do sada je potvrđena klinička efikasnost i registrovano je pet inhibitora histon deacetilaza za terapiju hematoloških tipova kancera. Sa druge strane, značaj aktivacije određenih proteinskih i lipidnih kinaza u procesima nastanka i rasta ćelija karcinoma doveo je do velikog interesovanja za razvijanje novih antitumorskih lekova koji inhibiraju signalni put onih kinaza kod kojih je pokazana njihova izmenjena aktivnost na određenim tipovima karcinoma. U poglavljima monografija međunarodnog značaja M₁₄: 1-2, kao i u radovima M_{21a}-1; M₂₁: 5, 10; M₅₂: 2, 3, dat je detaljan pregled, uporedna i kritička analiza najnovijih rezultata istraživanja antineoplastika iz grupe epigenetičkih modulatora i inhibitora kinaza. U okviru ovih publikacija analizirani su rezultati određivanja kvantitativnog odnosa strukture i dejstva farmakološki aktivnih jedinjenja (*Quantitative Structure Activity Relationship*, QSAR), ispitivanja 3D-strukture farmakofora, molekulske dinamičke simulacije ligand-receptor kompleksa, analize načina vezivanja i ključnih interakcija liganda i receptora određenih virtuelnim dokingom, sistemskog pretraživanja baza hemijskih jedinjenja u odnosu na predloženi

ligand (*Ligand-Based Virtual Screening*) ili u odnosu na ciljno mesto (*Structure-Based Virtual Screening*), kao i različitih metoda racionalnog ili kompjuterskog dizajna, sinteze i ispitivanja potencijalno efikasnijih i bezbednijih antineoplastika iz grupe epigenetičkih modulatora i inhibitora kinaza.

Enzimi iz familije histon deacetilaza su podeljeni u 4 klase, od kojih su klase I, II i IV cink-zavisne hidrolaze, dok su histon deacetilaze III klase NAD⁺ zavisne oksido-reduktaze. Histon deacetilaza 6 (HDAC6) je u najvećoj meri lokalizovana u citoplazmi gde hidrolizuje acetil-lizin rezidue citoplazmatskih proteina poput α -tubulina, peroksiredoksina, *heat shock* proteina 90 (Hsp90), kortaktina, kao i poliubikvitiranih proteina. Uzimajući u obzir navedene biohemijske uloge HDAC6 u organizaciji i dinamici ćelije, ova izoforma enzima je potvrđena kao važno ciljno mesto dejstva savremenih antikancerskih terapeutika iz grupe epigenetskih modulatora. Određivanjem 3D-strukture farmakofore (3D-QSAR), QSAR analizom formiranih modela i ispitivanjem ključnih ligand-receptor interakcija molekulskim dokingom odabranih inhibitora histon deacetilaza po prvi put su detaljno definisane specifične strukturne determinante ovih jedinjenja koje su neophodne za selektivnu inhibiciju određene izoforme histon deacetilaza, poput HDAC-6. Za 3D-QSAR modelovanje su upotrebljene bioaktivne konformacije ispitivanih liganada, koje su prethodno formirane primenom različitih metoda molekulske dinamike i virtuelnog dokinga. Kompjuterski dizajn selektivnih inhibitora određenih izoformi histon deacetilaza je bio baziran na kombinaciji rezultata 3D-QSAR analize, molekulskog dokinga i virtuelnog skrininga (baziranog na strukturi liganda, fragmenta ili ciljnog mesta dejstva) što je omogućilo sintezu, karakterizaciju i *in vitro* ispitivanje novih tipova modulatora epigenetičkih enzima iz grupe histon deacetilaza kao potencijalno efikasnijih i bezbednijih antikancerskih terapeutika (radovi M₂₁: 3, 4; M₂₂: 12).

Ispitivanjem molekulske dinamike i mehanizama ligand-receptor interakcija na dva epigenetska targeta, DOT1-slične histon H3K79 metiltransferaze (DOT1L) i WD ponavljajući domen 5 proteina (WDR5), obuhvaćena je analiza uticaja konformacione dinamike ova dva proteina na racionalni dizajn novih DOT1L ili WDR5 inhibitora, kao novih tipova antineoplastika za hematološke tipove karcinoma. Histon metiltransferaza DOT1L katalizuje mono-, di- i trimetilaciju histona 3 lizinske rezidue 79 (H3K79). Pošto je hipermetilacija H3K79 povezana sa razvojem akutne leukemije (MLLr ćelije) inhibicija metilacije H3K79 usporava proliferaciju MLLr ćelija. Specifični DOT1L inhibitor pinometostat je bio u kliničkim ispitivanjima (faza Ib/II). U okviru publikovane studije izvršen je dizajn, sinteza i ispitivanje novih nanomolarnih inhibitora humanog DOT1L enzima efikasnih u MLLr ćelijama koji su pokazali sličnu inhibitornu aktivnost na DOT1L enzimu, ali poboljšanu metaboličku stabilnost u odnosu na pinometostat. WDR5 protein učestvuje kroz protein-protein interakcije u formiranju različitih multiproteinskih kompleksa. Zbog velike složenosti istraživanja ovih sistema, sa aspekta eksperimentalnih i računarskih metoda, tek su u prethodnih par godina počeli uspešno da se ispituju peptidomimetski inhibitori koji se dovoljno efikasno vezuju sa fleksibilnom dodirnom površinom ovih protein-protein interakcija. Razvijene su nove metode i protokoli ispitivanja ligand-protein interakcija pomoću naprednih metoda molekulske dinamike, molekulskog dokinga i virtuelnog skrininga, pa je tako omogućena analiza veoma kompleksnih sistema u kojima učestvuju WDR5 epigenetski proteini. Kompjuterski dizajn novih modulatora različitih epigenetičkih proteina je omogućilo

sintezu, karakterizaciju i *in vitro* ispitivanje potencijalno efikasnijih i bezbednijih antikancerskih terapeutika (radovi M_{21a}: 5; M₂₂: 2, 9).

U publikovanoj PYROXD1 studiji je pokazano da ova oksidoreduktaza štiti tRNA-LC (njegovu subjedinicu RTCB), kao i da se jasno uočava međusobna zavisnost PYROXD1 enzima i RTCB u ćelijskim linijama različitih tipova karcinoma. Razvijene su nove metode i protokoli ispitivanja ligand-receptor interakcija pomoću naprednih metoda modelovanja strukture proteina, virtuelnog dokinga, molekulske dinamike i metadinamike čime je omogućena analiza veoma složenih i dinamičnih sistema poput PYROXD1 enzima. (rad M_{21a}: 3).

Kombinovanjem rezultata 3D-QSAR analize i virtuelnog dokinga derivata ksantena i tetrahidropiridina definisane su strukturne determinante ispitivanih jedinjenja neophodne za snažniju antikancersku aktivnost na HeLa, A549 i LS174 ćelijskim linijama. Kompjuterski dizajn novih derivata ksantena i tetrahidropiridina je omogućilo sintezu, karakterizaciju i *in vitro* ispitivanje potencijalno efikasnijih i bezbednijih antineoplastika (radovi M₂₂: 5, 11).

Određivanjem 3D-strukture farmakofore (3D-QSAR) i QSAR analizom formiranih modela inhibitora COX-2/LOX i PI3K enzima definisane su strukturne determinante ispitivanih jedinjenja neophodne za optimalnu aktivnost. Za 3D-QSAR modelovanje su upotrebljene bioaktivne konformacije ispitivanih liganada, koje su prethodno formirane primenom različitih metoda molekuskog dokinga. Kombinovanjem rezultata 3D-QSAR analize i virtuelnog dokinga inhibitora COX-2/LOX i PI3K enzima definisane su strukturne determinante ispitivanih jedinjenja neophodne za snažniju antikancersku aktivnost. Kompjuterski dizajn novih COX-2/LOX i PI3K inhibitora omogućava sintezu, karakterizaciju i *in vitro* ispitivanje potencijalno efikasnijih i bezbednijih antikancerskih terapeutika (radovi M₂₃: 2; M₅₂: 1).

Razvijen je složeni protokol za dizajn i ispitivanje novih tipova: dualnih antagonista serotoninskih 5-HT_{2A} i dopaminskih D₂ receptora, sa smanjenim afinitetom za histaminski H₁ receptor; potentnih i selektivnih liganada imidazolskih I₂ receptora, kao i novih liganada dopaminskih D₂ i D₃ receptora. Formirana je opšta *in silico* platforma za određivanje dodatnih (*off-target*) interakcija ispitivanih liganada sa G-protein kuplovanim receptorima (*G-Protein Coupled Receptors*, GPCR) primenom metoda molekuskog ukrštenog dokinga i dokinga veoma visoke preciznosti. Poredbenom analizom rezultata 3D-strukture farmakofore (3D-QSAR), QSAR modelovanja, molekulske dinamike, virtuelnog dokinga/skrininga, *in vitro/in silico* ispitivanja ADMET (*Absorption, Distribution, Metabolism, Excretion, and Toxicity*) osobina i kompjuterskog dizajna novih liganada GPCR i imidazolskih I₂-R je usmereno istraživanje ka sintezi i ispitivanju novih potencijalno efikasnijih i bezbednijih CNS terapeutika (radovi M_{21a}: 2 i 4; M₂₁: 6; M₂₂: 4, 7).

Definisanje 3D-strukture farmakofore (3D-QSAR), QSAR analiza, virtuelni doking/skrining, kao i kompjuterski dizajn novih inhibitora specifičnih enzima mikroorganizama (virusi, paraziti) je omogućilo sintezu, karakterizaciju i *in vitro* ispitivanje novih potencijalno efikasnijih i bezbednijih antivirusika i antiparazitika (radovi M₂₁: 7; M₂₂: 6, 8, 10).

Modelovanje retencionog i elektrohemijskog ponašanja, razvoj novih HPLC analitičkih metoda, hemometrijske studije i *in silico/in vitro* ADMET skrining (*Parallel Artificial Membrane Permeability Assay* (PAMPA), *Biomimetic Chromatography*

(BMC), *Hydrophilic Interaction Liquid Chromatography* (HILIC)) ispitivanih grupa liganada imidazolinskih receptora, G-protein kuplovanih receptora i novosintetisanih jedinjenja je omogućio hemometrijsku i QSPR/QSRR analizu retencionog ponašanja, fizičko-hemijskih i farmakokinetičkih osobina ispitivanih grupa farmakološki aktivnih supstanci i novosintetisanih jedinjenja i formiranje prediktivnih hemometrijskih modela za dalju selekciju najboljih kandidata za sintezu. U ovim hemometrijskim i QSPR/QSRR studijama su korišćene različite kombinacije regresionih metoda (MLR, sMLR, PLSR i PCA) i naprednih metoda mašinskog učenja (SVM i ANN), kao i virtuelni doking i molekulska dinamika (radovi M_{21} : 1, 2, 8, 9; M_{22} : 1, 3; M_{23} : 1).

2.4. VREDNOVANJE NAUČNO-ISTRAŽIVAČKOG RADA PREMA PRAVILNIKU O STICANJU ISTRAŽIVAČKIH I NAUČNIH ZVANJA

Tabela 3. Vrsta i kvantifikacija rezultata naučnoistraživačke aktivnosti.

Kategorija časopisa	Od izbora u prethodno zvanje broj/bodova	Ukupno broj/bodova
Poglavlje u monografiji međunarodnog značaja – M13	0/0	1/6
Poglavlje u monografiji međunarodnog značaja – M14	2/8	2/8
Međunarodni časopisi izuzetnih vrednosti – M21-a	5/50	7/70
Vrhunski međunarodni časopisi – M21	10/80	44/360
Istaknuti međunarodni časopisi – M22	12/60	22/110
Međunarodni časopisi – M23	2/6	32/96
Predavanje po pozivu sa međunarodnog skupa štampano u celini – M31	1/3	2/6
Predavanje po pozivu sa međunarodnog skupa štampano u izvodu – M32	12/18	23/34,5
Saopštenje sa međunarodnog skupa štampano u celini – M33	6/6	14/14
Saopštenje sa međunarodnog skupa štampano u izvodu – M34	33/16,5	82/41
Rad u istaknutom nacionalnom časopisu – M52	3/4,5	8/12
Rad u nacionalnom časopisu – M53	0/0	0/0
Predavanje po pozivu sa skupa nacionalnog značaja štampano u celini – M61	0/0	0/0
Saopštenje sa skupa nacionalnog značaja štampano u izvodu – M64	7/1,4	16/3,2
Doktorska disertacija – M71	0/0	1/6
Novo tehničko rešenje – M85	0/0	0/0
Učešće na nacionalnim projektima	2/4	3/6
Učešće na međunarodnim projektima	8/32	10/40
UKUPNO BODOVA	289,4	806,7

IZBORNI USLOVI

VREDNOVANJE IZBORNIH USLOVA

2. DOPRINOS AKADEMSKOJ I ŠIROJ ZAJEDNICI

3. Članstvo u stručnim ili naučnim asocijacijama u koje se član bira ili koje imaju ograničen broj članova.

- Dr Katarina Nikolić je od 2019. godine, na predlog Srpskog hemijskog društva, predstavnik Srbije u okviru *European Chemical Society (EuChemS) Division of Computational and Theoretical Chemistry (DCTC)*: <https://www.euchems.eu/divisions/computational-chemistry-2/>
- Dr Katarina Nikolić je 2022. godine, na predlog predsednika EuChemMS-DCTC udruženja, postala član i sekretar Komisije za dodelu nagrade: *The EuChemS Walter Thiel Award In Computational and Theoretical Chemistry*, pri EuChemS Division of Computational and Theoretical Chemistry.

4. Uređivanje časopisa ili monografija priznatih od strane resornog ministarstva za nauku.

- Dr Katarina Nikolić je tokom 2021. i 2022. godine aktivna kao urednik tematskog izdanja časopisa *Frontiers in Endocrinology* pod nazivom: *Physiology and Pathophysiology of GPCR Signal Transduction*
- Dr Katarina Nikolić je 2022. godine izabrana za *Review Editor on the Editorial Board of Protein Biochemistry for Basic and Applied Sciences* (specialty section of *Frontiers in Chemistry* and *Frontiers in Molecular Biosciences*).

8. Recenzentske aktivnosti u priznatim časopisima i monografijama (dodatni izborni uslov prema Pravilniku o bližim uslovima za izbor u zvanje nastavnika na Farmaceutskom fakultetu)

Od izbora u zvanje vanrednog profesora dr Katarina Nikolić je bila recenzent 23 rada u međunarodnim časopisima kategorije M20 i recenzent tri poglavlja u monografiji međunarodnog značaja M13.

9. Rukovođenje ili angažovanje u radu stručnih tela i organizacionih jedinica Fakulteta i/ili Univerziteta (dodatni izborni uslov prema Pravilniku o bližim uslovima za izbor u zvanje nastavnika na Farmaceutskom fakultetu)

Dr Katarina Nikolić je od 2019. godine član Komisije Farmaceutskog fakulteta za ocenu studentskih anketa

10. Predsedavanje ili članstvo u stručnim i naučnim odborima nacionalnih ili međunarodnih skupova

Dr Katarina Nikolić je bila član Naučnog odbora međunarodog skupa: e-EuCo-CTC 2021, Online conference, EuChemS Division of Computational and Theoretical Chemistry, November 18-19 2021.

1. SARADNJA SA DRUGIM VISOKOŠKOLSKIM, NAUČNO-ISTRAŽIVAČKIM USTANOVAMA, ODNOSNO USTANOVAMA KULTURE ILI UMETNOSTI U ZEMLJI I INOSTRANSTVU

4. Učešće na naučno-istraživačkim projektima

- Učesnik i član upravnog odbora EU projects: FP7/COST CM1406 action (2015-2019): *Epigenetic Chemical Biology (EPICHEM)*: http://www.cost.eu/COST_Actions/cmst/Actions/CM1406
- Učesnik EU projects: HORIZON 2020/COST Action CA15135 (2016-2020): *Multi-target paradigm for innovative ligand identification in the drug discovery process (MuTaLig)*. http://www.cost.eu/COST_Actions/ca/CA15135
- Učesnik EU projects: HORIZON 2020/COST Action CA16205 (2017-2021): *European Network on Understanding Gastrointestinal Absorption-related Processes (UNGAP)*: http://www.cost.eu/COST_Actions/ca/CA16205
- Učesnik EU projects: Horizon 2020/ COST CA17104 action (2018-2022): *New diagnostic and therapeutic tools against multidrug resistant tumors*: http://www.cost.eu/COST_Actions/ca/CA17104
- Učesnik i član upravnog odbora EU projects: Horizon 2020/ COST action CA18133 (2019-2023): *European Research Network on Signal Transduction*. <https://www.cost.eu/actions/CA18133/#tabs|Name:overview>
- Učesnik i član upravnog odbora EU projects: Horizon 2020/ COST action CA18240 (2019-2023): *ADHEsion GPCR Network: Research and Implementation Set the path for future Exploration*. <https://www.cost.eu/actions/CA18240/#tabs|Name:overview>
- Rukovodilac istraživanja: Bilateral project, Hubert Curien Partnership Project for collaboration France-Serbia 2020-2022 (Program Pavle Savic 2020): *Identification of novel DOT1L and DNMT1/3A inhibitors*, with Epigenetic Chemical Biology, Institut Pasteur, CNRS UMR3523, Paris 75015 France (Prof Paola Arimondo research group).
- Rukovodilac istraživanja: *Deutsche Forschungsgemeinschaft (DFG)* project named: *Control of epigenetic states through light-triggered protein-protein interaction mediators*, 2020-2023 PI Asst. Prof. Olalla Vázquez, Fachbereich Chemie Philipps-Universität Marburg, Germany.

2. *Internacionalizacija postojećih studijskih programa u okviru visokoškolskih ustanova.*

Učestvuje u izvođenju praktične i teorijske nastave (predmeti *Pharmaceutical chemistry 2* i *Pharmaceutical chemistry 3*) u okviru integrisanih akademskih studija na engleskom jeziku na Univerzitetu u Beogradu – Farmaceutskom fakultetu

6. *Izvođenje nastave ili mentorstvo u zajedničkim međunarodnim studijskim programima.*

Dr Katarina Nikolić je bila eksterni član komisije (external examiner): University of Eastern Finland, October 2020: "Exploring SIRT6 modulators and an indirect approach to modulate sirtuin activity" for the degree of Doctor of Science (Pharmacy). Doktorand: Jonna Tenhunen, Mentor: Prof. dr Maija Lahtela-Kakkonen

8. *Učestvovanje na međunarodnim kursevima ili školama za užu naučnu oblast za koju se bira*

Dr Katarina Nikolić je učestvovala je u okviru Trening škole (*Computational Methods in Drug Design*) sa predavanjem na temu: *Computer-aided design of histone deacetylase inhibitors*. Epigenetic Chemical Biology – Action CM1406, Training School 22-24 March 2018, Istanbul, Turkey.

MIŠLJENJE I PREDLOG

Na konkurs objavljen 27.04.2022. godine u listu "Poslovi" za jednog redovnog profesora za užu naučnu oblast Farmaceutska-medicinska hemija i strukturna analiza prijavio se jedan kandidat dr Katarina Nikolić, vanredni profesor na Katedri za Farmaceutsku hemiju, Farmaceutskog fakulteta, Univerziteta u Beogradu.

Dr Katarina Nikolić ispunjava sve obavezne i izborne uslove predviđene odredbama Zakona o visokom obrazovanju, Statuta Farmaceutskog fakulteta, Pravilnika o minimalnim uslovima za sticanje zvanja nastavnika na Univerzitetu u Beogradu i Pravilnika o bližim uslovima za izbor nastavnika na Farmaceutskom fakultetu u Beogradu, za izbor u zvanje redovni profesor za užu naučnu oblast Farmaceutska-medicinska hemija i strukturna analiza.

U okviru **nastavne aktivnosti**, dr Katarina Nikolić učestvuje u realizaciji teorijske i praktične nastave na Katedri za farmaceutsku hemiju u okviru integrisanih akademskih studija - studijski program Farmacija, u pripremi i izvođenju nastave u okviru doktorskih akademskih studija, kao i u pripremi i realizaciji nastave na master studijskom programu *Napredna analiza podataka*, akreditovanom na Univerzitetu u Beogradu. U studentskim anketama njen nastavni i pedagoški rad ocenjen je ocenom 4,73. Dr Katarina Nikolić je autor jednog osnovnog i jednog pomoćnog udžbenika za predmet Farmaceutska hemija 3.

Bila je mentor 7 doktorskih disertacija i član komisije za odbranu 10 doktorskih disertacija, od toga u zvanju vanredni profesor je mentor 4 doktorske disertacije i član komisije za odbranu 3 doktorske disertacije. Bila je mentor 10 završnih radova na integrisanim akademskim studijama i član komisije za odbranu 4 završna rada, od toga je bila mentor 4 završna rada u zvanju vanredni profesor. Bila je mentor 17 studentskih istraživačkih radova (od izbora u zvanje vanredni profesor 7 radova) i član Stručne Komisije na tri Studenska Mini-kongresa na Farmaceutskom fakultetu u Beogradu.

Vrednovanjem nastavnog i pedagoškog rada prema članu 9 Pravilnika o bližim uslovima za izbor nastavnika na Farmaceutskom fakultetu u Beogradu dr Katarina Nikolić je ostvarila ukupno 104 boda.

U domenu **naučne aktivnosti**, dr Katarina Nikolić je do sada ukupno objavila 107 radova u časopisima od međunarodnog značaja (M_{20}), 3 poglavlja u knjizi međunarodnog značaja (M_{13} i M_{14}), 8 radova u domaćim časopisima (M_{50}), 122 saopštenja na međunarodnim naučnim skupovima (M_{30}) i 16 saopštenja na nacionalnim naučnim skupovima (M_{64}). Od izbora u zvanje vanredni profesor publikovala je 29 radova (M_{20}): 5 M_{21a} , 10 M_{21} , 12 M_{22} , i 2 M_{23} , 2 poglavlja u knjizi međunarodnog značaja (M_{14}), 3 rada u domaćem časopisu M_{52} , 52 saopštenja na međunarodnim naučnim skupovima (M_{30}): 1 M_{31} , 12 M_{32} , 6 M_{33} i 33 M_{34} i 7 saopštenja na nacionalnim naučnim skupovima (M_{64}). Kumulativni IF objavljenih radova Katarine Nikolić (u poslednjih 5 godina) je 130,326. Prvi autor ili nosilac rada je u 9 radova sa kumulativnim IF 31,365. Ukupan broj citata bez autocitata je 1110 (Scopus), a H-indeks 17 (Scopus), Dr Katarina Nikolić je učestvovala u radu 3 nacionalna i 10 međunarodnih naučno-istraživačkih projekata, od toga od izbora u zvanje vanredni profesor učestvuje u radu 2 nacionalna i 8 međunarodnih naučno-istraživačkih projekata.

Vrednovanjem naučno-istraživačkog rada prema Pravilniku o sticanju istraživačkih i naučnih zvanja dr Katarina Nikolić je ostvarila 289,4 bodova od izbora u zvanje vanredni profesor.

U okviru **izbornih uslova**, u domenu *Doprinos akademskoj i široj zajednici*, dr Katarina Nikolić je izabrana za predstavnika Srbije u okviru *European Chemical Society (EuCheMS) Division of Computational and Theoretical Chemistry (DCTC)*, kao i za člana Komisije za dodelu nagrade: *The EuChemS Walter Thiel Award In Computational and Theoretical Chemistry*, pri *EuCheMS Division of Computational and Theoretical Chemistry*. Dr Katarina Nikolić je tokom 2021. i 2022. godine bila aktivna kao urednik tematskog izdanja časopisa *Frontiers in Endocrinology*. Dr Katarina Nikolić je 2022. godine izabrana za *Review Editor on the Editorial Board of Protein Biochemistry for Basic and Applied Sciences*. Od izbora u zvanje vanrednog profesora recenzent je 23 rada u međunarodnim časopisima kategorije M_{20} i tri poglavlja u monografiji međunarodnog značaja kategorije M_{13} . Od 2019. godine je član Komisije Farmaceutskog fakulteta za ocenu studentskih anketa. Bila je član 1 naučnog odbora međunarodnog skupa.

U domenu *Saradnje sa drugim visokoškolskim, naučno-istraživačkim ustanovama*, dr Katarina Nikolić učestvuje u radu 8 međunarodnih naučno-istraživačkih projekata. Učestvovuje je u izvođenju praktične i teorijske nastave u okviru integrisanih akademskih studija na engleskom jeziku na Farmaceutskom fakultetu u Beogradu. Bila je eksterni član komisije za odbranu doktorske disertacije na *Faculty of Pharmacy, University of Eastern Finland*, 2020. Učestvovala je u realizaciji Trening škole (*Computational Methods in Drug Design*) 2018, Istanbul, Turska.

Na osnovu uvida u priloženu dokumentaciju o nastavnom i naučno-istraživačkom radu, kao i izbornim uslovima, Komisija je zaključila da dr Katarina Nikolić ispunjava sve uslove predviđene odredbama Zakona o visokom obrazovanju, Statuta Farmaceutskog fakulteta, Pravilnika o minimalnim uslovima za sticanje zvanja nastavnika na Univerzitetu u Beogradu i Pravilnika o bližim uslovima za izbor nastavnika na Farmaceutskom fakultetu u Beogradu, za izbor u zvanje redovnog profesora.

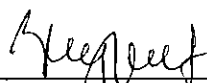
Na osnovu ovakvog zaključka, Komisija predlaže Izbornom veću Farmaceutskog fakulteta Univerziteta u Beogradu da usvoji pozitivan referat i uputi predlog Veću naučnih oblasti medicinskih nauka Univerziteta u Beogradu da dr Katarinu Nikolić izabere u zvanje redovni profesor za užu naučnu oblast Farmaceutska-medicinska hemija i strukturna analiza.

Beograd, 01. jun 2022.

Članovi Komisije



Dr Olivera Čudina, redovni profesor
Predsedavajući Komisije
Univerzitet u Beogradu -- Farmaceutski
Fakultet



Dr Zorica Vujčić, redovni profesor
Univerzitet u Beogradu – Farmaceutski
Fakultet



Dr Katarina Andelković, redovni
profesor
Univerzitet u Beogradu – Hemijski
fakultet