NAME AND FAMILY NAME: KATARINA NIKOLIĆ

Employment Information:
2017 - Associate Professor at the Department of
Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade
2015 - Scientific Adviser - Natural and Mathematical Sciences, Chemistry.
2012 - Assistant Professor
at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade .
2010 - Senior Research Associate on projects of the Ministry of Science of the Republic of Serbia under the leadership of prof. dr. DanicaAgbaba, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade (172033) and the Institute of NuclearSciences - Vinca, University of Belgrade (173001).
2007-2010 - Research associate on the project of the Ministry of Science of the Republic of Serbia under the leadership of prof. dr. DanicaAgbaba, Department of Pharmaceutical Chemistry and Drug Analysis, Faculty of Pharmacy , University of Belgrade. Assistant inexperimental and theoretical exercises in Pharmaceutical Chemistry II and III at the Faculty of Pharmacy, University of Belgrade ..
2005-2007 - Professor of Chemistry at *KES College* , Nicosia, Cyprus / *American Academy* , Limassol, Cyprus.
2004-2005 - Clinical Pharmacist, *Lemesos Medical Center* , Limassol, Cyprus.
2001-2005 - Research associate on an international project led by prof. dr. Anastasios Keramidas at the Faculty of Chemistry, University ofNicosia, Cyprus.
2001-2002 - Pharmacist in the laboratory for development and validation of analytical methods, Drug Factory - *Biogena Ltd,* Limassol,Cyprus.
1998-2000 - Pharmacist in drug quality control, Drug factory - *Medochemie Ltd* , Limassol, Cyprus.

Education:
2021 - Drug testing and control specialist. She defended her health specialization with the mentor prof. dr. Zorica Vujić, Department ofPharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade.
2007 - Doctor of Pharmacy - She defended her doctoral dissertation entitled: "Molecular modeling and *in vitro* testing of antioxidant propertiesof phenylselenosuccinyl-α-tocopheryl esters with potential antiproliferative effect"
with the mentor prof. dr. Danica Agbaba, Department ofPharmaceutical Chemistry and Drug Analysis, Faculty of Pharmacy , University of Belgrade.
2001 - Master of Physical Chemistry - Master's thesis entitled: "Application of close infrared spectroscopy in the quantitative analysis ofHydrocortisone Sodium Succinate for injection" was defended by the mentor prof. dr. Ubavke Mioč, at the Faculty of Physical Chemistry,University of Belgrade.
1998 - Graduated Pharmacist - graduated from the Faculty of Pharmacy, University of Belgrade with an average grade of 9.23.
1993 - graduated from the high school of natural sciences and mathematics in Ruma.

Training:
November **2021** - *Hubert Curien Partnership Project* bilateral cooperation with France (Pasteur Institute)
March **2018** - Training School: Epigenetic Chemical Biology - Action CM1406, Computational Methods in Drug Design, Istanbul, Turkey.
Jun **2012** . - study stay (FP7 / COST-STSM-CM1103-10295) at the University of St Andrews, UK (Dr John Mitchell, EaStCHEM School ofChemistry) entitled: *Theoretical prediction of the pharmaceutical targets of the examined multitarget compounds* .
March **2012** - Course at *The European Bioinformatics Institute* entitled **:** *Perspectives in Clinical Proteomics Training Workshop* - WellcomeTrust Genome Campus, Hinxton, Cambridge, UK

2001 - 2005 - Research associate on the international project: " *Synthesis, antioxidant and anticancer activities of mixed selenium-tocopherolantioxidants* " under the leadership of prof. dr. Anastasios Keramidas at the Faculty of Chemistry, University of Nicosia, Cyprus. The researchwork included molecular modeling and application of Nuclear Magnetic Resonance (NMR) spectroscopy in the structural and kinetic study ofsynthesized tocopherol derivatives. This scientific project was partly funded by the *Research Promotion Foundation of Cyprus, grand 13/1999*.

Academic awards and distinctions:
2021 - Nenad M. Kostić Fund Award for the best final work in the field of chemistry in 2021 (as mentor).
In 2020 and **2021**, the award of the Faculty of Pharmacy for outstanding contribution to scientific research.
1999 - award for the best student of the generation of the Faculty of Pharmacy for the school year 1997/98.

Teaching activities:
Since **2013**, she has been engaged in teaching several subjects in the field of computer chemistry, drug design and hemometry in doctoralstudies module - pharmaceutical chemistry, Faculty of Pharmacy, University of Belgrade

Since **2012**, she has been engaged in conducting experimental and theoretical exercises

and participates in conducting theoretical classes (lectures) at the Department of Pharmaceutical Chemistry (Pharmaceutical Chemistry II(antibiotics) and Pharmaceutical Chemistry III (adrenergic drugs), Selected chapters of pharmaceutical chemistry (drugs and substances thatcause addiction).
Since **2007**, she has been engaged in conducting experimental and theoretical exercises in Pharmaceutical Chemistry II and III integratedacademic studies at the Faculty of Pharmacy, University of Belgrade.

Teaching literature:
2021 - peer-reviewed textbook in Pharmaceutical Chemistry III entitled: Adrenergics, antianginal drugs and vasodilators. Faculty of Pharmacy,University of Belgrade.
2014 - Practicum for experimental exercises in Pharmaceutical Chemistry III, Faculty of Pharmacy, University of Belgrade.
2013 - Chapter: Danica Agbaba and Katarina Nikolic: " *TLC of Antihypertensive and Antihypotensive drugs* " in the Book: " *Thin layerchromatography in drug analysis* ", Edited by Lukasz Komsta, Monika Waksmundzka-Hajnos, Joseph Sherma. CRC Press Inc. 2013

Activities within the Faculty:

2019 - so far - member of the Commission for processing student surveys
2013, 2014, 2017 - member of the commission at the Sixth, Seventh and Tenth Student Mini-Congress, Faculty of Pharmacy, University ofBelgrade. Mentor of 15 student research papers.
2011 - proposer and lecturer on the course of the first category-continuous education: "Development of new drugs using theoretical andexperimental methods", Faculty of Pharmacy, University of Belgrade.
2009 - Organizer of the seminar entitled: "Research of new drugs - modern approaches" Faculty of Pharmacy, University of Belgrade.

Activities within wider Academic Community:

2019 - so far *Ambassador to the European Association for Cancer Research* www.eacr.org
2019 - so far representative of the Serbian Chemical Society in *EuChemS Division of Computational and Theoretical Chemistry* : https://www.euchems.eu/divisions/computational-chemistry-2/
2019 - so far Head of ITC CONFERENCE GRANTS applications in ERNEST HORISON 2020 / COST CA18133 Action.
2011-2015 - Head of Working Group-1 for Computational Chemistry of the international project FP7 / COST / CM1103 entitled: Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergicsystems of the brain, Action CM1103. http://www.cost.eu/COST_Actions/cmst/Actions/CM1103

Member of the Association: Serbian Society of Cancer Researchers, *Cheminformatics & QSAR Society and Cancer Epigenetics Society*
Since January 2011, he has been an associate, board member and head of working group-1 (WG-1) on the European project FP7 / COST(European Cooperation in the field of Scientific and Technical Research) entitled Structure-based drug design for diagnosis and treatment ofneurological 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

Conference organizer and member of the scientific committee:
The European Conference on Computational and Theoretical Chemistry (EuCo-CTC) of *EuChemS Division of Computational andTheoretical Chemistry*, online, 18-19 November 2021.
COST CM1406. WG1 Scientific Workshop - EPIGENETIC CHEMICAL PROBES. Belgrade, 16 January 2017
11 th Central European Symposium on Pharmaceutical Technology. September 22-24, 2016, Belgrade
COST CM1103 ESR Conference in Belgrade 6th-8th May 2015, Belgrade, Serbia.

Reviewer of papers for international journals: iScience, Journal of Medicinal Chemistry, QSAR & Combinatorial Science, European Journalof Medicinal Chemistry, Current Drug Metabolism, SAR and QSAR in Environmental Research, Bioorganic Medicinal Chemistry, Frontiersin Pharmacology, Frontiers in Chemistry ...
Reviewer of papers for national journals Archives of Pharmacy and Pharmaceutical Industry.
Reviewer of 3 national projects of UK, Poland and Croatia.
Previous examiner of 1 Doctoral dissertation at the 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).

Projects:
Bilateralni projekt, Hubert Curien Partnership Project for collaboration France-Serbia 2020-2022 (Program Pavle Savic 2020): Identificationof novel DOT1L and DNMT1 / 3A inhibitors, with Epigenetic Chemical Biology, Institute Pasteur, CNRS UMR3523, Paris 75015 France (Dr. Paola Arimondo research group).
Deutsche Forschungsgemeinschaft (DFG) project named: Control of epigenetic states through light-triggered protein-protein interactionmediators, 2020-2023 PI Asst. Prof. Olalla Vázquez, Fachbereich Chemie Philipps-Universität Marburg, Germany.
EU projects: Horison 2020 / COST action CA18133 (2019-2023): European Research Network on Signal Transduction. MC memberhttps://www.cost.eu/actions/CA18133/

EU project: Horison 2020 / COST action CA18240 (2019-2023): ADHEsion GPCR Network: Research and Implementation Set the path forfuture Exploration –MC Member, https://www.cost.eu/actions/CA18240/
Since 2020 , he has been the head of the research group for rational drug design within the institutional financing of scientific research workat the Faculty of Pharmacy, University of Belgrade.
Since 2010. (since May 2015 as a Scientific Adviser) on a scientific research project entitled: Synthesis, quantitative relationship betweenstructure and action, physico-chemical characterization and analysis of pharmacologically active substances, Ministry of Science of theRepublic of Serbia, led by prof. dr. Danica Agbaba, Department of Pharmaceutical Chemistry and Drug Analytics, Faculty of Pharmacy ,University of Belgrade (172033).
Since 2010. (since May 2015 as a Scientific Adviser) on a scientific research project entitled: Application of the EIIP / ISM bioinformaticsplatform in the discovery of new therapeutic targets and potential therapeutic molecules, the Ministry of Science of the Republic of Serbia,led by prof. dr. Veljko Veljković, Institute of Nuclear Sciences - Vinča, University of Belgrade (173001).
2017-2021 - Research Associate of the COST research project HORISON 2020 / COST Action CA16205: European Network onUnderstanding Gastrointestinal Absorption-related Processes: http://www.cost.eu/COST_Actions/ca/CA16205
2016-2020 - Associate on the European project HORISON 2020 / COST Action CA15135: Multi-target paradigm for innovative ligandidentification in the drug discovery process (MuTaLig). http://www.cost.eu/COST_Actions/ca/CA15135
2015-2019 - Associate and Board Member on the European project Horison 2020 / COST CM1406 Action: Epigenetic Chemical Biology(EPICHEM). http://www.cost.eu/COST_Actions/cmst/Actions/CM1406
2013-2017 - Associate and Board Member on the European project FP7 / COST / CM1207 entitled: GLISTEN: GPCR-Ligand Interactions,Structures, and Transmembrane Signaling: a European Research Network COSTAction.http://www.cost.eu/COST_Actions/cmst/Actions/CM1207
2011-2015 - Associate and member of the Steering Committee of the European COST project FP7 / COST / CM1103 entitled: Structure-baseddrug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systemsof the brain. http://www.cost.eu/COST_Actions/cmst/Actions/CM1103
2008-2011 - Member of the Steering Committee of the European FP7 / COST / CM0603 project entitled: Free Radicals in Chemical Biology(CHEMBIORADICAL).
2007-2010 - research associate on a research project entitled: "Synthesis, quantitative relationship between structure / properties andactivities, physico-chemical characterization and analysis of pharmacologically active substances." Ministry of Science of the Republic ofSerbia, led by prof. dr. Danica Agbaba, Department of Pharmaceutical Chemistry and Drug Analytics, Faculty of Pharmacy , University ofBelgrade (142071).
2008-2009 - research associate on the bilateral project Slovenia and the Republic of Serbia entitled: Determination of active ingredients indietary supplements.
2001-2005 - research associate on an international project: Synthesis, antioxidant and anticancer activities of mixed selenium-tocopherolantioxidants. under the leadership of prof. dr. Anastasios Keramidas at the Faculty of Chemistry, University of Nicosia, Cyprus.

Selected publications:

1. I. Asanovic, E. Strandback, A. Kroupova, Dj. Pasajlic, A. Meinhart, P. Tsung-Pin, N. Djokovic, D. Anrather, T. Schuetz, MJ 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 proteinresponse. *Molecular Cell* 2021, 81 (12), P2520-2532.E16, https://doi.org/10.1016/j.molcel.2021.04.007

2. S. Rodriguez-Arévalo, A. Bagán, Christian G. Ferré, F. Vasilopoulou, M. Pallàs, I. Brocos-Mosquera, LF Callado, M. Isabel Loza, AL Martínez, J.Brea, B. Pérez, E. Molins, S. De Jonghe, D. Daelemans, M. Radan, T. Djikic, K. Nikolic, EH Hernández, MJ García-Fuster, JA 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 .

3. N. Djokovic, D. Ruzic, T. Djikic, S. Cvijic, J. Ignjatovic, S. Ibric, K. Baralic, A. Buha Djordjevic, M. Curcic, D. Djukic-Cosic, K. Nikolic. AnIntegrative in Silico Drug Repurposing Approach for Identification of Potential Inhibitors of SARS-CoV-2 Main Protease. *Molecular Informatics*2021, 40, 2000187. https://doi.org/10.1002/minf.202000187

4. S. Abás, S. Rodríguez-Arévalo, A. Bagán, C. Griñán-Ferré, F. Vasilopoulou, I. Brocos-Mosquera, C. Muguruza, B. Pérez, E. Molins, F. JavierLuque, P. Pérez -Lozano, S. de Jonghe, D. Daelemans, L. Naesens, J. Brea, M. Isabel Loza, E. Hernández-Hernández, JA García-Sevilla, M. JuliaGarcía-Fuster, M. Radan, T. Djikic , K. Nikolic, M. Pallàs, LF Callado, C. Escolano. Bicyclic α - Iminophosphonates as High Affinity ImidazolineI2 Receptor Ligands for Alzheimer's Disease. *Journal of Medicinal Chemistry* 2020, 63, 7, 3610–3633.https://doi.org/10.1021/acs.jmedchem.9b02080

5. T. Djikic, J. Vucicevic, J. Laurila, M. Radi, N. Veljkovic, H. Xhaard, K. Nikolic. Deciphering Imidazoline Off - Targets by Fishing in the Class Aof GPCR field. *Molecular Informatics* 2020, 39, 1900165. https://doi.org/10.1002/minf.201900165

6. LA Alves Avelar, D. Ruzic, N. Djokovic, T. Kurz, K. Nikolic. Structure-based design of selective histone deacetylase 6 zinc binding groups.*Journal of Biomolecular Structure and Dynamics* 2020, 38, 11, 3166-3177. https://doi.org/10.1080/07391102.2019.1652687

7. D. Ruzic, M. Petkovic, D. Agbaba, A Ganesan, K. Nikolic. Combined Ligand and Fragment-based Drug Design of Selective Histone Deacetylase-6 Inhibitors. *Molecular Informatics* 2019, 38 (5), 1800083. https://doi.org/10.1002/minf.201800083

8. S. Bouchet, C. Linot, D. Ruzic, D. Agbaba, B. Fouchaq, J. Roche, K. Nikolic, C. Blanquart, P. Bertrand. Extending Cross Metathesis To IdentifySelective HDAC Inhibitors: Synthesis, Biological Activities, and Modeling. *ACS Medicinal Chemistry Letters* 2019, 10, 863−868.https://doi.org/10.1021/acsmedchemlett.8b00440

9. L. Albert, A. Peñalver, N. Djokovic, L. Werel, M. Hoffarth, D. Ruzic, J. Xu, LO Essen, K. Nikolic, Y. Dou, O. Vázquez. Modulating Protein-Protein Interactions with Visible-Light Responsive Peptide Backbone Photoswitches. *ChemBioChem* 2019, 20 (11), 1417-1429.https://doi.org/10.1002/cbic.201800737