Nemanja Djokovic, PhD

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Date and place of birth: 11th of November, 1992, Čačak, Serbia

Scientific interests
- Development and application of biomolecular simulations, cheminformatics, and bioinformatics methods and protocols in computer-aided drug design. Synthesis, characterization, and biological evaluation of new classes of antineoplastics.

Bibliographical data
- Co-author of 17 papers and one chapter in an internationally recognized monograph (First author on 5 publications, corresponding author on 2 publications). Full list available here or here. 187 total citations (without self-citations), h-index: 7 (Scopus, 10.03.2024.) Cumulative impact factor (IF): 120.523

Education
- 2023. Ph.D., University of Belgrade, Faculty of Pharmacy – Thesis title: *Molecular dynamics simulations, design, synthesis and in vitro evaluation of inhibitors of epigenetic proteins as potential antineoplastic drugs* (Mentor: Prof. dr Katarina Nikolic)
- 2016. B.Sc., University of Belgrade, Faculty of Pharmacy (Avrg. Ach 9.73/10.00) – Thesis title: *Application of the 3D-QSAR and virtual screening methods in the design of novel antidepressants with dual activity on serotonin transporter and histamine H3 receptor*

Employment
- April 2024 – current: Research Associate at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.
- March 2024 – current: Teaching Assistant with PhD at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.
- June 2022 – March 2024: Teaching Assistant at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.
- May 2021 – June 2022: Research Assistant at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.
- October 2017 – April 2021: Junior Research Assistant at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.
- March 2017: Teaching Associate at the Department of Analytical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.
- October 2016 – March 2017: Teaching Associate at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Belgrade, Serbia.

Participation in domestic and foreign projects
- 2017 – 2019: Synthesis, Quantitative relationships between structure and effects, physico-chemical characterization and analysis of pharmacologically active substances, Project number 172033, funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia
- 2019 – present: Institutional financing of national projects by Serbian Ministry of Education, Science and Technological Development through Grant Agreement with University of Belgrade-Faculty of Pharmacy No: 451-03-65/2024-03/ 200161. Member of KN research group.

- 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).
- 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.
- EU projects: 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
- EU projects: COST action CA18133 (2019-2023): European Research Network on Signal Transduction (ERNEST). https://www.cost.eu/actions/CA18133/#tabs|Name:overview
- EU projects: Horison 2020/COST CM1406 action (2015-2019): Epigenetic Chemical Biology (EPICHEM) http://www.cost.eu/COST_Actions/cmst/Actions/CM1406

Training
- Short Term Scientific Mission (COST CM1406) at University of Eastern Finland, Kuopio, Finland (Dr Maija Lahtella-Kakkonen, School of Pharmacy); Title: Ligand and structure based design of sirtuin 2 inhibitors; Subject: Training in application of advanced molecular modelling techniques in the design of sirtuin 2 inhibitors. May-June 2017.
- Short Term Scientific Mission (COST CM1406) at University of Eastern Finland, Kuopio, Finland (Dr Maija Lahtella-Kakkonen, School of Pharmacy); Title: Drug design of sirtuin 2 inhibitors; Subject: Training in techniques for in vitro evaluation of sirtuin 2 inhibitors. February 2019.
- Training school From Molecule to Medicine (COST CM1406), Faculty of Pharmacy, University of Ljubljana, Ljubljana, Slovenia. 18-20 March 2019.
- DesignIT-to-LEAD2019 training school in computational medicinal chemistry jointly organized by Rome Center for Molecular Design and Faculty of Science, University of Kragujevac, Kragujevac, Serbia (host). 10-11 July 2019.
- COST CA18240 Training School (online) – Experimental models in Adhesion GPCR Research. Mediterranean Institute for Life Sciences – MedILS, Split, Croatia. 5-6 October 2020.

Academic awards and distinctions
- Faculty of Pharmacy, University of Belgrade: 2023 – Recognition for exceptional contribution to the scientific research.
- Faculty of Pharmacy, University of Belgrade: 2023 – Annual award for the best research results of PhD students.
- Faculty of Pharmacy, University of Belgrade: 2022 – Recognition for exceptional contribution to the scientific research.
- Faculty of Pharmacy, University of Belgrade: 2021 – Recognition for exceptional contribution to the scientific research.
- Faculty of Pharmacy, University of Belgrade: 2018 – Annual award for the best research results of PhD students.
- Scholarships of Foundation for Young Talents – Dositeja – 2015/2016.
- Annual award for the best students of Integrated Academic Studies of Pharmacy (Faculty of Pharmacy, University of Belgrade): years 2012 and 2013. The Scholarship of the Ministry of Education of Republic of Serbia for undergraduate students (2001-2004)

Activities within wider Academic Community
- Member of The Serbian Association for Cancer Research
- Member of The European Association for Cancer Research
- Member of the organizing committee "WG1 Scientific Workshop - EPIGENETIC CHEMICAL PROBES", which took place on 16.01. 2017 in Belgrade as part of the project COST CM1406 – Epigenetic Chemical Biology (EPICHEMBIO).
- Reviewer for international scientific journals: iScience; ACS medicinal chemistry letters ; RSC Advances; Chemistry & biodiversity; ChemMedChem; Computational Biology and Chemistry; Journal of Biomolecular Structure & Dynamics; Journal of Chemical Information and Modeling; PLOS Computational Biology.

Teaching activities

- October 2016 – current: Involvement in teaching activities for the courses *Pharmaceutical Chemistry I, II and III* (Integrated Academic Studies).
- March 2017: Involvement in teaching activity for the course *Analytical Chemistry I* (Integrated Academic Studies).
- Fall semester 2023: Course „Advanced data analysis in pharmaceutical research and development" as a part of Advanced Data Analysis – Master Programme at University of Belgrade.
- Tutor on two training courses on cheminformatics and bioinformatics for PhD students and early-stage researchers (September 2022 - Bioinformatics approaches in adhesion GPCR research, organized jointly by 'Adher´n Rise' (CA18240) and IMGGI, Belgrade, Serbia; December 2023 – Resources and software for computational chemistry and its application in biomedicine, organized jointly by Vinča Institute of Nuclear Sciences and INEP, Belgrade, Serbia)
- Co-supervisor of 3 master theses at the Faculty of Pharmacy, University of Belgrade and member of the committee for 8 defended graduated thesis at the Faculty of Pharmacy, University of Belgrade
- Supervisor of 4 student scientific research papers presented at student congresses organized by the Center for Scientific Research of Students of the Faculty of Pharmacy

Computational and laboratory skills

- **Expertise in leading molecular modeling packages and platforms:** Gromacs, Amber, PLUMED, ffTK, ORCA, Gaussian, Avogadro, Schrödinger suite, Molecular Discovery Suite, Cambridge Crystallographic Data Centre CCDC suite, Modeller, Pymol, VMD, UCSF Chimera, UCSF DOCK, AutoDock and AutoDock Vina, ADMET predictor and ACD/Labs Percepta, ChemAxon, RDKit.
- **Programming skills:** Extensive working knowledge of Python programming (experience with libraries relevant for the project: NumPy, SciPy, Scikit-learn, Keras and Tensorflow, PyTorch, XGBoost, Pandas, Matplotlib), Unix Shell scripting and experience with HPC working environment.
- **Laboratory skills:** Organic synthesis, UV/VIS spectroscopy, IR-spectroscopy, NMR spectroscopy, Fluorometric *in vitro* enzymatic assays.