

PERSONAL INFORMATION

Name and surname	Žiko Milanović
Date and place of birth	17.03.1994., Prijepolje
Scientific title	Research Associate
E-mail	ziko.milanovic@uni.kg.ac.rs ziko.milanovic@pmf.kg.ac.rs
Educational-scientific / educational-artistic field	Natural sciences
University, Faculty, Organizational unit	University of Kragujevac, Institute for Information Technologies
Research field and areas	Chemistry, Organic Chemistry

EDUCATION

BACHELOR

Year	2013 – 2017
Place	Novi Pazar
Institution	State University of Novi Pazar, Department of Chemical-Technological sciences
Average grade	9.69
Title of the thesis and date of defense	Antioxidant activity of trihydroxypyridine, July 7, 2017

MASTER STUDIES

Year	2017 – 2018
Place	Kragujevac
Institution	Faculty of Science, University of Kragujevac
Average grade	10.0
Title of the master thesis and date of defense	Comparison of the Antioxidant Activity of 2,4,6- Trihydroxypyridine and 1,3,5-Trihydroxybenzene – A Kinetic DFT Study, July 10, 2018.

DOCTORAL DISSERTATION

Year	2018 – 2023
Place	Kragujevac
Institution	Faculty of Science, University of Kragujevac
Average grade	10.0
Title of doctoral Dissertation and date of defense	Structural and antioxidant properties of newly synthesized phenol derivatives of 4,7-dihydroxycumarin, May 9, 2023.
Research area	Chemistry, Organic chemistry

PROFESSIONAL BIOGRAPHY – ELECTION IN RESEARCH OR SCIENTIFIC TITLE

Date	Institution	Scientific title
28.08.2023.	Institute for Information Technologies, University of Kragujevac	Research Associate
17.01.2021.	Institute for Information Technologies, University of Kragujevac	Research Assistant
16.01.2019.	Faculty of Science, University of Kragujevac	Junior research assistant

PROFESSIONAL BIOGRAPHY - TRAINING

Year	Institution	Duration
2021.	University of Applied Sciences, Merseburg, Germany	3 months
2022.	University of Applied Sciences, Merseburg, Germany	3 months

PARTICIPATION IN NATIONAL PROJECTS FINANCED BY MINISTRY OF EDUCATION/MINISTRY OF SCIENCE AND

TECHNOLOGICAL DEVELOPMENT/SCIENCE FUND OF THE REPUBLIC OF SERBIA:

- **2024–2025:** Bilateral Project SERBIA–SLOVAKIA: *Derivatives of phenolic compounds: experimental and theoretical investigation of their antioxidant effect and oxidation pathways*; collaboration between the University of Kragujevac – Project Leader: Dušica Simjonović, and the Department of Physical Chemistry, Faculty of Chemical and Food Technology, Slovak University of Technology, Slovakia – Project Leader: Erik Klein.
- **2023 – 2025:** Bilateral project SERBIA–SLOVENIA: *Development of a computational protocol to evaluate 4-hydroxycoumarin-neurotransmitter derivatives in the treatment of Alzheimer's disease*; cooperation between the University of Kragujevac - project manager Dejan Milenković and Nacional Institute of Chemistry, Slovenia – project manager Janez Konc.
- **2019:** National projects financed by the Ministry of the science of the Republic of Serbia: The national project of the Ministry of Education, Science, and Technological Development under the title “*Structure and Dynamics of the Molecular Systems in the ground and Excited Molecular States*” No. 172015.

PARTICIPATION IN INTERNATIONAL PROJECTS

- **2021 – 2022:** DAAD Internationalisation of universities of applied sciences (HAW/FH), “International HoME” (established between Merseburg University of Applied Sciences, the Department of Engineering, and Natural Sciences and the University of Kragujevac).
- **2020 – 2021:** DAAD Internationalisation of universities of applied sciences (HAW/FH), “International HoME” (established between Merseburg University of Applied Sciences, the Department of Engineering, and Natural Sciences, and the University of Kragujevac).
- **2020:** ERASMUS+ project KA103 STT - Learning Mobility of Individuals-Dipartimento DiChimica E Tecnologie Chimiche.

MEMBERSHIP IN SCIENTIFIC AND PROFESSIONAL ASSOCIATIONS

- Serbian Chemical Society.
- Society of Physical Chemists of Serbia.
- Society of Biologists of Serbia.
- Serbian Society for Computational Mechanics.

ORGANIZATION OF NATIONAL/INTERNATIONAL SCIENTIFIC MEETINGS (CONFERENCES, CONGRESSES...)

- Member of the Scientific Committee of the *3rd International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2025.
- Member of the Organizing Committee of the *61st Conference of the Serbian Chemical Society*, Kragujevac, Serbia, 2025.
- Member of the organizing committee of the *2nd International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2021.
- Member of the organizing committee of the *1st International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2021.

LIST OF SCIENTIFIC PAPERS:

Monographs, Monographic studies, Thematic anthologies	Sum
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Papers published in scientific journals of international scientific importance	Sum
1. * <u>Žiko Milanović</u> , Dušan Dimić, Edina Avdović, Dušica Simijonović, Đuro Nakarada, Vladimir Jakovljević, Radiša Vojinović, Zoran Marković, Mechanism of antiradical activity of coumarin-trihydroxybenzohydrazide derivatives: a comprehensive kinetic dft study. <i>Antioxidants</i> , 13.2 (2024): 143. DOI: 10.3390/antiox13020143, ISSN: 2076-3921, IF ₂₀₂₂ =7.0, 6/60; M21a ; area: Chemistry, Medicinal). 2. *Jovana Dragojević, <u>Žiko Milanović</u> , Jovana Matić, Vera Divac, Marijan Kosanić, Dušan Milivojević, Miloš Petković, Fateh Veer	38

Singh, Marina Kostić, Dual Activity of Newly Synthesized Zn (II) and Cu (II) Schiff Base Complexes as a Potential Solution for Global Challenges in the Fight Against Priority Microorganisms. *Journal of Molecular Structure*, 2025, 142052. *Journal of Molecular Structure*, 2025, 1321, 140118. DOI: 10.1016/j.molstruc.2025.142052, ISSN: 0022-2860, IF₂₀₂₃ = 4.0; 65/161; **M22**; area: Chemistry, Physical).

3. *Saša Babić, Jovana Marjanović, Vera Divac, Olivera Klisurić, Dušan Milivojević, Jovana Bogojeski, Ivana Raković, Miulan Zarić, Mirjana Jovanović, Radica Živković Zarić, Slađana Veselinović, Branimi Radmanović, **Žiko Milanović**, Petar Čanović, Marina Kostić. Molecular docking study and in vitro evaluation of apoptotic effect of biogenic-amine-based N, O-Cu (II) complexes as potent antitumor agents. *Journal of Coordination Chemistry*, (2025): 1-20. DOI: 10.1080/00958972.2025.2477589, ISSN: 0095-8972, IF₂₀₂₃ = 2.2, 22/42; **M22**; area: Chemistry, Inorganic & Nuclear).
4. *Mia Stanković, Sanja Skaro Bogojevic, Jakob Kljun, Nevena Stevanović, **Žiko Milanović**, Jelena Lazic, Sandra Vojinovic, Iztok Turel, Miloš Đuran, Biljana Glišić, Silver (I) complexes with antifungal drug econazole: Structural characterization and antimicrobial activity study. *Journal of Molecular Structure*, 1321 (2025): 140118. DOI: 10.1016/j.molstruc.2024.140118, ISSN: 0022-2860, IF₂₀₂₃ = 4.0; 65/161; **M22**; area: Chemistry, Physical).
5. *Marko Antonijević, Edina Avdović, Dušica Simijonović, **Žiko Milanović**, Milan Žižić, Zoran Marković, Investigation of novel radical scavenging mechanisms in the alkaline environment: Green, sustainable and environmentally friendly antioxidative agent (s). *Science of The Total Environment*, 912 (2024): 169307. DOI: 10.1016/j.scitotenv.2023.169307, ISSN: 0048-9697, IF₂₀₂₂=9.8, 26/275; **M21a**; area: Environmental Sciences).
6. ***Žiko Milanović**, Urolithin D: A promising metabolite of ellagitannin in combatting oxidative stress. *Chemico-Biological Interactions*, 411 (2025): 111444. *Chemico-Biological Interactions*, 2024, 396, 111034. DOI: 10.1016/j.cbi.2025.111444, ISSN: 1477-9226, IF₂₀₂₃ = 4.7, 67/285; **M21**; area: Biochemistry & Molecular Biology).
7. *Ana Amić, Denisa Cagardová, **Žiko Milanović**. Theoretical Study of Antioxidant and Prooxidant Potency of Protocatechuic Aldehyde.

International journal of molecular sciences, 26.1 (2025): 404. DOI: 10.3390/ijms26010404, ISSN: 1661-6596, IF₂₀₂₃ = 4.9, 63/285; **M21**; area: Biochemistry & Molecular Biology).

8. *Jovana Dragojević, **Žiko Milanović**, Jovana Matić, Vera Divac, Marijan Kosanić, Dušan Milivojević, Miloš Petković, Fateh Veer Singh, Marina Kostić, Dual Activity of Newly Synthesized Zn (II) and Cu (II) Schiff Base Complexes as a Potential Solution for Global Challenges in the Fight Against Priority Microorganisms. *Journal of Molecular Structure*, 2025, 142052. *Journal of Molecular Structure*, (2025): 142052. DOI: 10.1016/j.molstruc.2025.142052, ISSN: 0022-2860, IF₂₀₂₃ = 4.0; 65/161; **M22**; area: Chemistry, Physical).
9. * Mia Stanković, Sanja Skaro Bogojevic, Jakob Kljun, **Žiko Milanović**, Nevena Stevanović, Jelena Lazić, Iztok Turel, Miloš Đuran, Biljana Glišić, Silver (I) complexes with voriconazole as promising anti-Candida agents. *Journal of inorganic biochemistry*, 256 (2024): 112572. DOI: 10.1016/j.jinorgbio.2024.112572, ISSN: 0162-0134, IF₂₀₂₃ = 3.8, 9/42; **M21**; area: Chemistry, Inorganic & Nuclear).
- 10.*Lena Pantelić, Sanja Skaro Bogojevic, Tina Andrejević, Bojana Pantović, Violeta Marković, Darko Ašanin, **Žiko Milanović**, Tatjana Ilic Tomic, Jasmina Nikodinovic Runic, Biljana Glišić, Jelena Lazic, Copper (II) and Zinc (II) Complexes with Bacterial Prodigiosin Are Targeting Site III of Bovine Serum Albumin and Acting as DNA Minor Groove Binders. *International Journal of Molecular Sciences*, 25.15 (2024): 8395. DOI: 10.3390/ijms25158395, ISSN: 1661-6596, IF₂₀₂₃ = 4.9, 63/285; **M21**; area: Biochemistry & Molecular Biology).
- 11.*Marijana Kasalović, Sanja Jelača, **Žiko Milanović**, Danijela Maksimović-Ivanić, Sanja Mijatović, Jelena Lađarević, Bojan Božić, Zoran Marković, Duško Dunđerović, Tobias Ruffer, Robert Kretschmar, Goran Kaluđerović, Nebojša Pantelić, Novel triphenyltin (iv) compounds with carboxylato N-functionalized 2-quinolones as promising potential anticancer drug candidates: In vitro and in vivo evaluation. *Dalton Transactions*, 53.19 (2024): 8298-8314. DOI: 10.1039/D4DT00182F, ISSN: 0009-2797, IF₂₀₂₃ = 3.5, 12/42; **M21**; area: Chemistry, Inorganic & Nuclear).
- 12.***Žiko Milanović**, Zoran Marković, Ana Kesić, Snežana Jovanović Stević, Biljana Petrović, Edina Avdović, Influence of acid–base equilibrium on interactions of some monofunctional coumarin Pd (ii)

complexes with biologically relevant nucleophiles-comprehensive kinetic study. *Dalton Transactions*, 53.19 (2024): 8275-8288. DOI: 10.1039/D4DT00789A, ISSN: 0009-2797, IF₂₀₂₃ = 3.5, 12/42; **M21**; area: Chemistry, Inorganic & Nuclear).

13. ***Žiko Milanović**, Exploring enzyme inhibition and comprehensive mechanisms of antioxidant/prooxidative activity of natural furanocoumarin derivatives: A comparative kinetic DFT study. *Chemico-Biological Interactions*, 396 (2024): 111034. DOI: 10.1016/j.cbi.2024.111034, ISSN: 1477-9226, IF₂₀₂₃ = 4.7, 67/285; **M21**; area: Biochemistry & Molecular Biology).
14. ***Žiko Milanović**, Comprehensive kinetic investigation of antiradical activity of urolithins and their potential inhibitory effect on Xanthine Dehydrogenase. *Journal of Molecular Liquids*, 408 (2024): 125330. DOI: 10.1016/j.molliq.2024.125330, ISSN: 0167-7322, IF₂₀₂₃ = 5.3, 5/35; **M21**; area: Physics, Atomic, Molecular & Chemical).
15. ***Žiko Milanović**, Marko Antonijević, Edina Avdović, Vladimir Simić, Miljan Milošević, Zana Dolićanin, Miloš Kojić, Zoran Marković, In silico evaluation of pharmacokinetic parameters, delivery, distribution and anticoagulative effects of new 4,7-dihydroxycoumarin derivative. *Journal of Biomolecular Structure and Dynamics*, 42.16 (2024): 8343-8358. DOI: 10.1080/07391102.2023.2245071, ISSN: 0739-1102, IF₂₀₂₂ = 4.4, 15/70; **M21**; area: Biophysics).
16. *Edina Avdović, **Žiko Milanović**, Dušica Simijonović, Marko Antonijević, Milena Milutinović, Danijela Nikodijević, Nenad Filipović, Zoran Marković, Radiša Vojinović, An effective, green synthesis procedure for obtaining coumarin-hydroxybenzohydrazide derivatives and assessment of their antioxidant activity and redox status. *Antioxidants*, 12.12 (2023): 2070. DOI: 10.3390/antiox12122070, ISSN: 2076-3921, IF₂₀₂₂=7.0, 6/60; **M21a**; area: Chemistry, Medicinal).
17. ****Žiko Milanović**, Svetlana Jeremić, Marko Antonijević, Dušan Dimić, Đuro Nakarada, Edina Avdović, Zoran Marković, The inhibitory potential of 4, 7-dihydroxycoumarin derivatives on ROS-producing enzymes and direct HOO•/o2•-radical scavenging activity—a comprehensive kinetic DFT study. *Free radical research*, 58.8-9 (2024): 493-508. DOI: 10.1080/10715762.2024.2400674,

ISSN: 1071-5762, IF₂₀₂₃ = 3.6, 119/285; **M22**; area: Biochemistry & Molecular Biology).

- 18.*Milica Međedović, Dušan Ćoćić, Aleksandar Mijatović, Vladimir Simić, **Žiko Milanović**, Marijana Kosanić, Nevena Petrović, Snežana Sretenović, Ana Rilak Simović, In silico and in vitro biological evaluation: distribution of Ru (III) Schiff base complexes through the pancreatic 3D model and immersed blood vessel network. *Journal of Coordination Chemistry*, 77.7-8 (2024): 766-785. DOI: 10.1080/00958972.2024.2303736, ISSN: 0095-8972, IF₂₀₂₃ = 2.2, 22/42; **M22**; area: Chemistry, Inorganic & Nuclear).
- 19.***Žiko Milanović**, Structural properties of newly 4,7-dihydroxycoumarin derivatives as potential inhibitors of XIIa, Xa, IIa factors of coagulation. *Journal of Molecular Structure*, 1298 (2024): 137049. DOI: 10.1016/j.molstruc.2023.137049, ISSN: 0022-2860, IF₂₀₂₃ = 4.0; 65/161; **M22**; area: Chemistry, Physical).
- 20.*Marko Antonijević, Edina Avdović, Dušica Simijonović, **Žiko Milanović**, Olivera Klisurić, Marta Erminia Alberto, Nino Russo, Zoran Marković, Comprehensive Experimental and Computational Analysis of the Structural and HSA Binding Properties of Newly Synthesized Coumarin – Trimethoxybenzohydrazide Derivative. *Polycyclic Aromatic Compounds*, 44.10 (2024): 7006-7030. DOI: 10.1080/10406638.2024.2339846, ISSN: 1040-6638, IF₂₀₂₃ = 6.208, 19/52; **M22**; area: Chemistry, Organic).
- 21.*Dušica Simijonović, Dejan Milenković, Edina Avdović, **Žiko Milanović**, Marko Antonijević, Ana Amić, Zana Dolićanin, Zoran Marković, Coumarin N-Acylhydrazone Derivatives: Green Synthesis and Antioxidant Potential – Experimental and Theoretical Study. *Antioxidants*, 12.10 (2023): 1858. DOI: 10.3390/antiox12101858, ISSN: 2076-3921, IF₂₀₂₂=7.0, 6/60; **M21a**; area: Chemistry, Medicinal).
- 22.***Žiko Milanović**, Dušan Dimić, Marko Antonijević, Milan Žižić, Dejan Milenković, Edina Avdović, Zoran Marković. Influence of acid-base equilibria on the rate of the chemical reaction in the advanced oxidation processes: Coumarin derivatives and hydroxyl radical. *Chemical Engineering Journal*, 453 (2023): 139648. DOI: 10.1016/j.cej.2022.139648, ISSN: 1385-8947, IF₂₀₂₁=16.744, 4/143; **M21a**; area: Engineering, Chemical.

23. *Milica Međedović, Aleksandar Mijatović, Rada Baošić, Dejan Lazić, **Žiko Milanović**, Zoran Marković, Jelena Milovnović, Dragana Arsenijević, Bojana Stojanović, Miloš Arsenijević, Marija Milovanović, Biljana Petrović, Ana Rilak Simović, Synthesis, characterization, biomolecular interactions, molecular docking, and in vitro and in vivo anticancer activities of novel ruthenium (III) Schiff base complexes. *Journal of Inorganic Biochemistry*, 248 (2023): 112363. DOI: 10.1016/j.jinorgbio.2023.112363, ISSN: 0162-0134, IF₂₀₂₂ = 3.9, 8/42; **M21**; area: Chemistry, Inorganic & Nuclear).
24. **Žiko Milanović**, Dušan Dimić, Erik Klein, Monika Biela, Vladimír Lukeš, Milan Žižić, Edina Avdović, Drago Bešlo, Radiša Vojinović, Jasmina Dimitrić Marković, Zoran Marković, Degradation Mechanisms of 4,7-dihydroxycoumarin derivatives in Advanced Oxidation Processes: Experimental and Kinetic DFT study. *International journal of environmental research and public health*, 20.3 (2023): 2046. DOI: 10.3390/ijerph20032046, ISSN: 1661-7827, IF₂₀₂₁ = 4.614, 81/302; **M21**; area: Public, Environmental & Occupational Health).
25. Marko Antonijević, Edina Avdović, Dušica Simijonović, **Žiko Milanović**, Ana Amić, Zoran Marković, Radical Scavenging Activity and Pharmacokinetic Properties of Coumarin-Hydroxybenzohydrazide Hybrids. *International journal of molecular sciences*, 23.1 (2022): 490. DOI: 10.3390/ijms23010490, ISSN: 1422-0067, IF₂₀₂₁ = 6.208, 50/180; **M21**; area: Chemistry, Multidisciplinary).
26. Filip Stašević, **Žiko Milanović**, Jelena Tošović, Jelena Đurđević Nikolić, Svetlana Marković, What Happens When Two Radicals Meet? A Practical Approach to Free Radical Reaction Mechanisms. *Journal of Chemical Education*, 99.10 (2022): 3522-3529. DOI: 10.1021/acs.jchemed.2c00622, IF₂₀₂₁=3.208; 95/180; **M22**; area: Chemistry, Multidisciplinary).
27. Edina Avdović, **Žiko Milanović**, Krešimir Molčanov, Sunčica Roca, S., Dražen Vikić-Topić, Eimina Mrkalić, Ratimir Jelić, Zoran Marković, Z. S. (2022). Synthesis, characterization and investigating the binding mechanism of novel coumarin derivatives with human serum albumin: Spectroscopic and computational approach. *Journal of Molecular Structure*, 1254 (2022): 132366. DOI:

10.1016/j.molstruc.2022.132366, ISSN: 0022-2860, IF₂₀₂₁ = 3.841; 83/165; **M22**; area: Chemistry, Physical).

28. Ana Amić, Jasmina Dimitrić Marković, Zoran Marković, Dejan Milenković, **Žiko Milanović**, Marko Antonijević, Denisa Mastilák Cagardová, Jaime Rodríguez-Guerra Pedregal, Theoretical Study of Radical Inactivation, LOX Inhibition, and Iron Chelation: The Role of Ferulic Acid in Skin Protection against UVA Induced Oxidative Stress. *Antioxidants*, 10.8 (2021): 1303. DOI: 10.3390/antiox10081303, ISSN: 2076-3921, IF₂₀₂₁=7.675, 4/63; **M21a**; area: Chemistry, Medicinal).
29. **Žiko Milanović**, Dušan Dimić, Milan Žižić, Zoran Marković, Edina Avdović, Mechanism of antiradical activity of newly synthesized 4,7-dihydroxycoumarinderivatives-experimental and kinetic DFT study, *International Journal of Molecular Science*, 22.24 (2021): 13273. DOI: 10.3390/ijms222413273, ISSN: 1422-0067, IF₂₀₂₁ = 6.208, 50/180; **M21**; area: Chemistry, Multidisciplinary).
30. **Žiko B. Milanović**, Zoran S. Marković, Dušan S. Dimić, Olivera R. Klisurić, Ivana D. Radojević, Dragana S. Šeklić, Marko N. Živanović, Jasmina Dimitrić Marković, Milanka Radulović, Edina H. Avdović, Synthesis, structural characterization, biological activity and molecular docking study of 4,7-dihydroxycoumarin modified by aminophenol derivatives. *Comptes Rendus. Chimie*, 24.2 (2021): 215-232. DOI: 10.5802/crchim.68, ISSN: 1631-0748, IF₂₀₂₀ = 3.117; 88/178; **M22**; area: Chemistry, Multidisciplinary).
31. Edina Avdović, Dušan Dimić, Marek Fronc, Jozef Kozisek, Erik Klein, **Žiko Milanović**, Ana Kesić, Zoran Marković, Structural and theoretical analysis, molecular docking/dynamics investigation of 3-(1-m-chloridoethylidene)-chromane-2,4-dione: the role of chlorine atom. *Journal of Molecular Structure*, 1231 (2021): 129962. DOI: 10.1016/j.molstruc.2021.129962, ISSN: 2046-2069, ISSN: 2046-2069, IF₂₀₂₁ = 3.841; 83/165; **M22**; област: Chemistry, Multidisciplinary).
32. **Žiko Milanović**, Marko Antonijević, Ana Amić, Edina Avdović, Dušan Dimić, Dejan Milenković, Zoran Marković, Inhibitory activity of quercetin, its metabolite, and standard antiviral drugs towards enzymes essential for SARS-CoV-2: the role of acid-base equilibria. *RSC Advances*, 11.5 (2021): 2838-2847. DOI: 10.1039/d0ra09632f, ISSN:

2046-2069, ISSN: 2046-2069, IF₂₀₂₁ = 4.036; 75/180; **M22**; област: Chemistry, Multidisciplinary).

33. **Žiko Milanović**, Jelena Tošović, Svetlana Marković, Zoran Marković, Comparison of the scavenging capacities of phloroglucinol and 2,4,6-trihydroxypyridine towards HO[•] radical: a computational study. *RSC Advances*, 10.71 (2020): 43262-43272. DOI: 10.1039/d0ra08377a, ISSN: 2046-2069, IF₂₀₂₀ = 3.361; 81/178; **M22**; област: Chemistry, Multidisciplinary).
34. **Žiko Milanović**, Dušan Dimić, Edina Avdović, Dejan Milenković, Jasmina Dimitrić Marković, Olivera Klisurić, Srećko Trifunović, Zoran Marković, Synthesis and comprehensive spectroscopic (X-ray, NMR, FTIR, UV-Vis), quantum chemical and molecular docking investigation of 3-acetyl-4 hydroxy 2-oxo-2H-chromen-7-yl acetate. *Journal of Molecular Structure*, 1225 (2021): 129256. DOI: 10.1016/j.molstruc.2020.129256, ISSN: 0022-2860, IF₂₀₂₁ = 3.841; 83/165; **M22**; area: Chemistry, Physical).
35. Dejan Milenković, Edina Avdović, Dušan Dimić, S. Sudha, D. Ramarajan, **Žiko Milanović**, Srećko Trifunović, Zoran Marković, Vibrational and Hirshfeld surface analyses, quantum chemical calculations, and molecular docking studies of coumarin derivative 3-(1-m-toluidinoethylidene)-chromane-2,4-dione and its corresponding palladium(II) complex. *Journal of Molecular Structure*, 1209 (2020): 127935. DOI: 10.1016/j.molstruc.2020.127935, ISSN: 0022-2860, IF₂₀₂₀ = 3.196; 92/159; **M22**; area: Chemistry, Physical).
36. Edina Avdović, **Žiko Milanović**, Marko Živanović, Dragana Šeklić, Ivana Radojević, Ljiljana Čomić, Srećko Trifunović, Ana Amić, Zoran Marković, Synthesis, spectroscopic characterization, biological activity, DFT and molecular docking study of novel 4-hydroxycoumarine derivatives and corresponding palladium (II) complexes. *Inorganica Chimica Acta*, 504 (2020): 119465. DOI: 10.1016/j.ica.2020.119465, ISSN: 0020-1693, IF₂₀₂₀ = 2.545; 19/45; **M22**; област: Chemistry, Inorganic & Nuclear).
37. Dušan Dimić, **Žiko Milanović**, Goran Jovanović, Dragana Sretenović, Dejan Milenković, Zoran Marković, Jasmina Dimitrić Marković, Comparative Antiradical Activity and Molecular

Docking/Dynamics Analysis of Octopamine and Norepinephrine: the Role of OH Groups. *Computational Biology and Chemistry*, 84 (2020): 107170. DOI: 10.1016/j.compbiolchem.2019.107170, ISSN: 1476-9271, IF₂₀₂₀ = 2.877, 59/112; **M22**; area: Computer Science, Interdisciplinary Applications).

38. D. Ramarajan, **Žiko Milanović**, Dejan Milenković, Zoran Marković, K. Tamilarasan, E. Kavitha, S. Sudha, Vibrational spectroscopic studies (FT-IR and FT-Raman) and molecular dynamics analysis of industry inspired 3-amino-4-hydroxybenzene sulfonic acid. *Journal of Molecular Structure*, 1205 (2020): 127579. DOI: 10.1016/j.molstruc.2019.127579, ISSN: 0022-2860, IF₂₀₂₀ = 3.196; 92/159; **M22**; area: Chemistry, Physical).

Proceedings of international scientific conferences

**Sum
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1. *Vladimir Simić, Miljan Milošević, **Žiko Milanović**, Miloš Kojić, Numerical modeling of new 4,7-dihydroxycoumarin derivative diffusion within finite element liver model, *2nd International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2023, p. 347-350. ISBN: 978-86-82172-02-4. DOI: 10.46793/ICCBi23.347S.
2. ***Žiko Milanović**, Marko Antonijević, Dušica Simijonović, Jelena Đorović Jovanović, Marijana Stanojević Pirković, Investigating the potential inhibitory effect of the megaphone (molecule) on nasopharyngeal cancer growth factor receptors, *2nd International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2023, p. 682-685. ISBN: 978-86-82172-02-4. DOI: 10.46793/ICCBi23.682M.
3. *Dušica Simijonović, Edina Avdović, **Žiko Milanović**, Dejan Milenković, Zoran Marković, Green synthesis of chromeno-pyrimidine derivatives – Part I, *2nd International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2023, p. 686-689. ISBN: 978-86-82172-02-4. DOI: 10.46793/ICCBi23.686S.
4. *Edina Avdović, Dušica Simijonović, **Žiko Milanović**, Sandra Jovičić Milić, Sunčica Roca; Dražen Vikić Topić, Chromeno-pyrimidine-type compounds (part II): in vitro evaluation of antioxidant potential, *2nd International Conference on Chemo and BioInformatics*, Kragujevac, Serbia, 2023, p. 690-693. ISBN: 978-86-82172-02-4. DOI: 10.46793/ICCBi23.690A.

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- Dimensions: 511 citations; h-index: 13.

BRIEF DESCRIPTION OF RESEARCH IN THE PREVIOUS PERIOD

The synthesis, characterization, and evaluation of the biological activity of various coumarin derivatives have been the focus of recent research. In order to assess the structural properties and possible reactivity and stability of the chemical, the newly synthesized derivatives performed NBO and QTAIM research. Additionally, research during the previous time period included sophisticated computer methods and tools for molecular docking and molecular dynamics with the goal of evaluating inhibitory activity and rational drug design. By using the software, it was possible to predict how newly synthesized derivatives (potential drugs) will bind to their protein targets.

BRIEF DESCRIPTION OF PLANNED RESEARCH IN THE NEXT PERIOD

The upcoming research will encompass both theoretical and experimental analysis of the kinetics and mechanisms of various organic and inorganic reactions, with a particular emphasis on elucidating the antioxidant and antiradical mechanisms of diverse compounds, especially those of polyphenolic nature. The theoretical approach will involve the application of advanced computational chemistry methods, including DFT calculations, molecular docking, and molecular dynamics, aimed at understanding the interactions between the investigated compounds and biologically relevant targets, as well as at designing novel, potentially effective molecules with possible applications in the pharmaceutical and other industries. The experimental part of the research will include the use of modern

spectroscopic techniques and standard in vitro assays for the evaluation of antioxidant activity, thereby enabling the validation of theoretical predictions. In addition to the core research activities, continuous efforts will be dedicated to the preparation and publication of scientific papers in SCI-listed journals, participation in national and international research projects, as well as the popularization of science through public lectures, the writing of popular science books, and the mentoring of young researchers. Through this interdisciplinary and integrative approach, the research aims to contribute to the development of new models for evaluating the reactivity, stability, and biological activity of compounds, providing a solid foundation for the rational design of novel molecules with favorable pharmacological and industrial properties.