

CURRICULUM VITAE

Name: Višnja Stepanić, born Šimek

Address: Laboratory for Machine Learning and Knowledge Representation, Division of Electronics, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb

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Employment

- **2009- present** Ruđer Bošković Institute, Researcher
- **2006– 2008** GlaxoSmithKline Research Centre Zagreb Ltd., Principle scientist
- **2002 – 2006** R & D, PLIVA Int., Researcher
- **1998 – 2002** Ruđer Bošković Institute, Department of Organic Chemistry and Biochemistry, Laboratory of Molecular spectroscopy, Research Assistant, Ph.D. Student
- **1994 – 1998** Ruđer Bošković Institute, Department of Physical Chemistry, Research Assistant, Group for Theoretical Chemistry, Master of phil. Student

Participation in projects / programs

EU Projects:

- 1) **2021** The AI4EU (The European AI on Demand Platform) Solutions Open Call 2021 for the challenge Modelling of drugs via deep learning neural network

Programs of Croatian science foundation:

- 1) **2018-2023** "Enzymatic Synthesis of Fluorinated Chiral Building Blocks EnzyFluor" (IP-2018-01-4493, PI: Maja Majerić Elenkov, PhD)

2) **2014-2018** "Synthesis and cytostatic evaluations of novel nitrogen heterocycles library" (5596; Leader: Prof. dr. sc. Silvana Raić-Malić)

Programs of Ministry of Science and Education of RH:

1) **2017-2022** The Scientific Centre of Excellence for Marine Bioprospecting –BioProCro (Competitiveness and Cohesion Operational Program, European Regional Development Fund KK.01.1.1.01, PI Rozelindra Čož – Rakovac, PhD)

2) **2009–2014** "Epigenetic and immunomodulatory changes in malignant head and neck tumors " (098–0982464–2511, PI Koraljka Gall Trošelj, MD, PhD)

3) **2012–2014** "Developing methods for modeling properties of bioactive molecules and proteins" (098-1770495-2919, PI Bono Lučić, PhD)

4) **1998–2001** "Isotopical labeling and molecular spectroscopies" (00980802, PI Goran Baranović, PhD)

5) **1998** "Theoretical study of protonated diimide cations" (Young investigator project, leader)

6) **1996–1998** "Study of static and dynamical properties of molecules " (00980605, PI Aleksandar Sabljic, PhD)

7) **1991–1995** "Development and application of models in chemistry " (PI academician Nenad Trinajstić)

Programs in the non-academic institutes Pliva d.o.o. and GlaxoSmithKline Research Centre Zagreb Ltd:

1) **2007- 2008** "Macrolides with anti-inflammatory activity", GSK Research Centre Zagreb Ltd.

2) **2006 – 2008** "Pharmacokinetic behaviour of macrolides", GSK Research Centre Zagreb Ltd.

3) **2006 – 2008** "Platform for generating macrolide hit molecules ", GSK Research Centre Zagreb Ltd.

4) **2006 – 2008** "Novel macrolide antibiotics", Research institute of Pliva d.o.o./ GSK Research Centre Zagreb Ltd.

5) **2004 – 2005** "New program generating platform ", Research institute of Pliva d.o.o.

6) **2002 – 2003** "Novel antibiotics targets ", R&D PLIVA Int.

Additionally, participation in realization of the following projects of Ministry of Science Education and Sports of the Republic of Croatia in period 2011 - 2014:

- 1) "Investigation of relationships between structure and biological activity of polyphenols", CRO-SRB project (2011-) (PI dr. sc. Bono Lučić)
- 2) "IGF2 and downstream signaling consequences in human lung cancers" (335-0000000-3532, PI dr. sc. S. Kraljević Pavelić)
- 3) "Epidemiological features of systemic lupus erythematoses in Croatia " (108-1081874-2419, PI Prof. dr. sc. Nada Mihelčić-Čikeš, MD).

Publications (<http://bib.irb.hr/lista-radova?autor=214770>)

Book Editing

1. Saso L, Gurer-Orhan H, **Stepanić V.** Modulators of Oxidative Stress: Chemical and Pharmacological Aspects, ISBN 978-3-03943-228-8 (Hbk); ISBN 978-3-03943-229-5 (PDF) <https://doi.org/10.3390/books978-3-03943-229-5> (registering DOI) (<https://www.mdpi.com/books/pdfview/book/3038>)
2. Book of Abstracts, 10th Joint Meeting on Medicinal Chemistry 2017 / Basarić, Nikola; Namjesnik, Danijel; Perković, Ivana; Stepanić, Višnja (Eds). Zagreb : Croatian Chemical Society, 2017.

Journal special issue editing

Stepanić V, Kučerová-Chlupáčová M. Special Issue "Redox Active Molecules in Cancer Treatments" (2021), of Molecules (ISSN 1420-3049) belonging to the section "Medicinal Chemistry". https://www.mdpi.com/journal/molecules/special_issues/Redox_Active_Cancer

Book/Proceedings chapters

1. Pehar V, Oršolić D, **Stepanić V.*** Drug-likeness, herbicide-likeness and toxicity of herbicidal compounds – in silico analysis. Proceedings: 17th Ružička Days Today Science – Tomorrow Industry, Tomas S, Ačkar Đ. (Eds.). Osijek : Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek and Croatian Society of Chemical Engineers (CSCE), 2019. 112-123.
2. Parnham JM, **Stepanić V**, Tafferner N, Panek M, Verbanac D. Mild plant and dietary immunomodulators // Principles of Immunopharmacology / Parnham J. Michael ; Nijkamp P. Frans (Eds.). Basel: Birkhäuser Basel, 2018. str. 1-68.

3. **Stepanić V**, Novak Kujundžić R, Gall Trošelj K. Epigenome, Cancer Prevention and Flavonoids and Curcumin // Epigenetics and Epigenomics / Christopher J. Payne (Ed.). Rijeka: InTech, 2014. Pp. 173-209.
4. Verbanac D, Perić M, Čipčić-Paljetak H; Matijašić M, **Stepanić V**. Biologically active ingredients from food with anti-obesity properties // Obesity: Public Health Problem and Medical Challenge / Rukavina, Daniel (Ed). Rijeka : Hrvatska Akademija Znanosti i Umjetnosti, 2014. pp. 133-150.
5. Verbanac D, **Stepanić V***, Lučić B, Amić D, "The Must" of the Drug Discovery and Development is – Interdisciplinarity, / Bioinformatics and biological physics : proceedings of the scientific meeting / Paar, Vladimir (ur.). Zagreb, Hrvatska, 21.11.2012. : Croatian Academy of Sciences and Arts, 2013. pp. 179-189.

Original scientific and review articles with international peer-review (IF at publishing time; IF current; journal rank at publishing time; number of citations in Web of Science)

1. Dokli I, Brkljača Z, Švaco P, Tang L, **Stepanić V,*** Majerić Elenkov M.* Biocatalytic approach to chiral fluoroaromatic scaffolds, *Org. Biomol. Chem.*, 2022,20, 9734-9741. <https://doi.org/10.1039/D2OB01955H>
2. Milčić N, **Stepanić V**, Crnolatac I, Findrik Blažević Z, Brkljača Z, Majerić Elenkov M. Inhibitory Effect of DMSO on Halohydrin Dehalogenase: Experimental and Computational Insights into the Influence of an Organic Co-solvent on the Structural and Catalytic Properties of a Biocatalyst. *Chemistry- A European Journal*. 2022;28(56):e202201923. doi: 10.1002/chem.202201923, with front cover doi.org/10.1002/chem.202202869
3. Antonijević MR, Simijonović DM, Avdović EH, Ćirić A, Petrović ZD, Marković JD, **Stepanić V**, Marković ZS. Green One-Pot Synthesis of Coumarin-Hydroxybenzohydrazide Hybrids and Their Antioxidant Potency. *Antioxidants* 2021; 10(7):1106. <https://doi.org/10.3390/antiox10071106>
4. Oršolić D, Pehar V, Šmuc T, **Stepanić V,*** Comprehensive machine learning based study of the chemical space of herbicides, *Scientific reports* 11 (1), 1-12, doi: <https://doi.org/10.1038/s41598-021-90690-w>
5. Cichońska A, Ravikumar B, Allaway RJ, Wan F, Park S, Isayev O, Li S, Mason M, Lamb A, Tanoli Z, Jeon M, Kim S, Popova M, Capuzzi S, Zeng J, Dang K, Koytiger G, Kang J, Wells CI, Willson TM; IDG-DREAM Drug-Kinase Binding Prediction Challenge Consortium (Oršolić D,

- Lučić B, **Stepanić V**, Šmuc T), Oprea TI, Schlessinger A, Drewry DH, Stolovitzky G, Wennerberg K, Guinney J, Aittokallio T. Crowdsourced mapping of unexplored target space of kinase inhibitors. *Nat Commun.* 2021 Jun 3;12(1):3307. doi: 10.1038/s41467-021-23165-1.
6. Tascioglu Aliyev A, Panieri E, **Stepanić V**, Gurer-Orhan H, Saso L, Involvement of NRF2 in Breast Cancer and Possible Therapeutical Role of Polyphenols and Melatonin. *Molecules* 2021, 26, 1853. <https://doi.org/10.3390/molecules26071853>
7. Gelemanović A, Vidović T, **Stepanić V**, Trajković K, Identification of 37 Heterogeneous Drug Candidates for Treatment of COVID-19 via a Rational Transcriptomics-Based Drug Repurposing Approach, *Pharmaceuticals* 2021;14:87. doi: doi.org/10.3390/ph14020087
8. Amić A, Marković Z, Dimitrić Marković JM, Milenković D, **Stepanić V**. Antioxidative potential of ferulic acid phenoxy radical. *Phytochemistry.* 2020; 170: 112218. doi:10.1016/j.phytochem.2019.112218
9. Macan Meščić A, Harej A, Cazin I, Klobučar M, **Stepanić V**, Pavelić K, Pavelić Kraljević S, Schols D, Snoeck R, Andrei G, Raić-Malić S. Antitumor and antiviral activities of 4-substituted 1,2,3-triazolyl-2,3-dibenzyl-L-ascorbic acid derivatives. *Eur. J. Med. Chem.* 2019;184:111739. doi:10.1016/j.ejmech.2019.111739
10. Harej A, Macan Meščić A, **Stepanić V**, Klobučar M, Pavelić K, Pavelić Kraljević S, Raić-Malić S. The Antioxidant and Antiproliferative Activities of 1,2,3-Triazolyl-L-Ascorbic Acid Derivatives. *Int. J. Mol. Sci.* 20(19) (2019) 4735. doi:10.3390/ijms20194735
11. **Stepanić V**,* Matijašić M, Horvat T, Verbanac D, Kučerová-Chlupáčová M, Saso L, Žarković N.* Antioxidant Activities of Alkyl Substituted Pyrazine Derivatives of Chalcones—In Vitro and In Silico Study. *Antioxidants.* 8(4) (2019) E90.
12. Kujundžić Novak R, **Stepanić V**, Milković L, Čipak Gašparović A, Tomljanović M, Gall Trošelj K. Curcumin and its potential for systemic targeting of inflamm-aging and metabolic reprogramming in cancer. *Int J Mol Sci.* 20(5) (2019) E1180.
13. **Stepanić V**,* Matic S, Amić A, Lučić B, Milenković D, Marković Z. Effects of conjugation metabolism on radical scavenging and transport properties of quercetin – *In silico* study, *J. Mol. Graph. Model.* 86 (2019) 278-285.
14. Matic S, Jadrijević-Mladar Takač M, Barbarić M, Lučić B, Gall Trošelj K, **Stepanić V**.* The Influence of In Vivo Metabolic Modifications on ADMET Properties of Green Tea Catechins-In Silico Analysis. *J. Pharm. Sci.* 107(11) (2018) 2957-2964.

15. Perin N, Starčević K, Perić M, Čipčić Paljetak H, Matijašić M, **Stepanić V**, Verbanac D, Karminski-Zamola G, Hranjec M. Synthesis and SAR study of novel amidino 2-substituted benzimidazoles as potential antibacterial agents. *Croat. Chem. Acta.* 90 (2017) DOI: 10.5562/cca3147
16. Perković I, **Stepanić V**, Gabelica Marković V. The 10th Joint Meeting on Medicinal Chemistry (JMMC2017) Held in Dubrovnik, Croatia, *ChemMedChem*, 13(1) (2018) 116-119.
17. Egea J, Fabregat I, Frapart YM, Ghezzi P, Görlach A, Kietzmann T, Kubaichuk K, Knaus UG, Lopez MG, Olaso-Gonzalez G, Petry A, Schulz R, Vina J, Winyard P, Abbas K, Ademowo OS, Afonso CB, Andreadou I, Antelmann H, Antunes F, Aslan M, Bachschmid MM, Barbosa RM, Belousov V, Berndt C, Bernlohr D, Bertrán E, Bindoli A, Bottari SP, Brito PM, Carrara G, Casas AI, Chatzi A, Chondrogianni N, Conrad M, Cooke MS, Costa JG, Cuadrado A, My-Chan Dang P, De Smet B, Debeleć-Butuner B, Dias IHK, Dunn JD, Edson AJ, El Assar M, El-Benna J, Ferdinandy P, Fernandes AS, Fladmark KE, Förstermann U, Giniatullin R, Giricz Z, Görbe A, Griffiths H, Hampl V, Hanf A, Herget J, Hernansanz-Agustín P, Hillion M, Huang J, Ilikay S, Jansen-Dürr P, Jaquet V, Joles JA, Kalyanaraman B, Kaminsky D, Karbaschi M, Kleanthous M, Klotz LO, Korac B, Korkmaz KS, Koziel R, Kračun D, Krause KH, Křen V, Krieg T, Laranjinha J, Lazou A, Li H, Martínez-Ruiz A, Matsui R, McBean GJ, Meredith SP, Messens J, Miguel V, Mikhed Y, Milisav I, Milković L, Miranda-Vizuete A, Mojović M, Monsalve M, Mouthuy PA, Mulvey J, Münzel T, Muzykantov V, Nguyen ITN, Oelze M, Oliveira NG, Palmeira CM, Papaevgeniou N, Pavićević A, Pedre B, Peyrot F, Phylactides M, Pircalabioru GG, Pitt AR, Poulsen HE, Prieto I, Rigobello MP, Robledinos-Antón N, Rodríguez-Mañas L, Rolo AP, Rousset F, Ruskovska T, Saraiva N, Sasson S, Schröder K, Semen K, Seredenina T, Shakirzyanova A, Smith GL, Soldati T, Sousa BC, Spickett CM, Stancic A, Stasia MJ, Steinbrenner H, **Stepanić V**, Steven S, Tokatlidis K, Tuncay E, Turan B, Ursini F, Vacek J, Vajnerova O, Valentová K, Van Breusegem F, Varisli L, Veal EA, Yalçın AS, Yelisyeyeva O, Žarković N, Zatloukalová M, Zielonka J, Touyz RM, Papapetropoulos A, Grune T, Lamas S, Schmidt HHHW, Di Lisa F, Daiber A. European contribution to the study of ROS: A summary of the findings and prospects for the future from the COST action BM1203 (EU-ROS). // *Redox Biol.* 13 (2017) 94-162.
18. Amić A, Lučić B, **Stepanić V**, Marković Z, Marković S, Dimitrić Marković JM, Amić D. Free radical scavenging potency of quercetin catecholic colonic metabolites: Thermodynamics of 2H⁺/2e⁻ processes. *Food Chem.* 218 (2017) 144-151.

19. Kraljević Gazivoda T, Harej A, Sedić M, Kraljević Pavelić S, **Stepanić V**, Drenjančević D, Talapko J, Raić-Malić S. Synthesis, in vitro anticancer and antibacterial activities and in silico studies of new 4-substituted 1,2,3-triazole-coumarin hybrids. *Eur. J. Med. Chem.* 124 (2016) 794-808.
20. Amić A, Marković Z, Dimitrić Marković J, Lučić B, **Stepanić V**, Amić D. The $2\text{H}^+/2\text{e}^-$ free radical scavenging mechanisms of uric acid: thermodynamics of N-H bond cleavage. *Comp. Theor. Chem.* 1077 (2016) 2-10.
21. Verbanac D, Malik R, Chand M, Kushwaha K, Vashist M, Matijašić M, **Stepanić V**, Perić M, Čipčić Paljetak H, Saso L, Jain Subhash C. Synthesis and evaluation of antibacterial and antioxidant activity of novel 2-phenyl-quinoline analogs derivatized at position 4 with aromatically substituted 4H-1, 2, 4-triazoles. *J. Enzyme Inhib. Med. Chem.* 31 (S2) (2016) 104-110.
22. **Stepanić V**, Čipak Gašparović A, Gall Trošelj K, Amić D, Žarković N. Selected attributes of polyphenols in targeting oxidative stress in cancer. *Curr. Top. Med. Chem.* 15(5) (2015) 496-509.
23. Stolić I, Čipčić Paljetak H, Perić M, Matijašić M, **Stepanić V**, Verbanac D, Bajić M. Synthesis and structure–activity relationship of amidine derivatives of 3, 4-ethylenedioxythiophene as novel antibacterial agents. *Eur. J. Med. Chem.* 90 (2015) 68-81.
24. Đorović J, Dimitrić Marković J, **Stepanić V**, Begović N, Amić D, Marković Z. Influence of different free radicals on scavenging potency of gallic acid. *J. Mol. Model.* 20 (7) (2014) 2345-1-2345-9.
25. Gazivoda Kraljević T, Ilić N, **Stepanić V**, Sappe L, Petranović J, Kraljević Pavelić S, Raić-Malić S. Synthesis and in vitro antiproliferative evaluation of novel N-alkylated 6-isobutyl- and propyl pyrimidine derivatives. *Bioorg Med Chem Lett.* 24 (13) (2014) 2913-2917.
26. Amić A, Marković Z, Dimitrić Marković J, **Stepanić V**, Lučić B, Amić D. Towards an improved prediction of the free radical scavenging potency of flavonoids: The significance of double PCET mechanisms. *Food chem.* 152 (2014) 578-585.
27. Lučić B, **Stepanić V**, Plavšić D, Amić A, Amić D. Correlation between ^{13}C NMR chemical shifts and antiradical activity of flavonoids. *Monats Chem.* 145(3) (2014) 457-463.
28. Amić D, **Stepanić V**, Lučić B, Marković Z, Dimitrić Marković J. PM6 study of free radical scavenging mechanisms of flavonoids: why does O–H bond dissociation enthalpy effectively represent free radical scavenging activity? *J. Mol. Model.* 19 (2013) 2593-2603.

29. **Stepanić V**, Gall Trošelj K, Lučić B, Marković Z, Amić D.* Bond dissociation free energy as general parameter for flavonoid radical scavenging activity. *Food Chem.* 141 (2013) 1562-1570.
30. Šaban N, **Stepanić V**, Vučinić S, Horvatić A, Cindrić M, Perković I, Zorc B, Oršolić N, Mintas M, Pavelić K, Pavelić SK. Antitumor mechanisms of amino Acid hydroxyurea derivatives in the metastatic colon cancer model. *Int. J. Mol. Sci.* 14(12) (2013) 23654-23671.
31. Munić Kos V, Koštrun S, Fajdetić A, Bosnar M, Kelnerić Ž, **Stepanić V**, Eraković Haber V. Structure-property relationship for cellular accumulation of macrolones in human polymorphonuclear leukocytes (PMNs). *Eur. J. Pharm. Sci.* 49 (2013) 206-219.
32. Ilijaš M, Malnar I, Gabelica Marković V, **Stepanić V***. Study of lipophilicity and membrane partition of 4-hydroxycoumarins by HPLC and PCA. *J. Pharm. Biomed. Anal.* 76 (2013) 104-111.
33. Marković Z, Milenković D, Đorović J, Dimitrić Marković JM, **Stepanić V**, Lučić B, Amić D. Free radical scavenging activity of morin 2'-O(-) phenoxide anion. *Food Chem.* 135 (2012) 2070-2077.
34. Marković Z, Milenković D, Đorović J, Dimitrić Marković JM, **Stepanić V**, Lučić B, Amić D. PM6 and DFT study of free radical scavenging activity of morin. *Food Chem.* 134 (2012) 1754-1760.
35. Racané L, Kraljević Pavelić S, Ratkaj I, **Stepanić V**, Pavelić K, Tralić-Kulenović V, Karminski-Zamola G. Synthesis and antiproliferative evaluation of some new amidino-substituted bis-benzothiazolyl-pyridines and pyrazine. *Eur. J. Med. Chem.* 55 (2012) 108-116.
36. Rubelj I, **Stepanić V**, Jelić D, Vidaček NŠ, Kalajžić AĆ, Ivanković M, Nujić K, Matijašić M, Verbanac D. Tebrophen--an old polyphenol drug with anticancer potential. *Molecules.* 17 (2012) 7864-7886.
37. Verbanac D, Jain SC, Jain N, Chand M, Čipčić Paljetak H, Matijašić M, Perić M, **Stepanić V**, Saso L. An efficient and convenient microwave-assisted chemical synthesis of (thio)xanthenes with additional in vitro and in silico characterization. *Bioorg. Med. Chem.* 20 (2012) 3180-3185.
38. **Stepanić V***, Žiher D, Gabelica–Marković V, Jelić D, Nunhuck S, Valko K, Koštrun S. Physicochemical profile of macrolides and their comparison with small molecules. *Eur. J. Med. Chem.* 47 (2012) 462–472.
39. Jelić D, Nujić K, **Stepanić V**, Kovačević K, Verbanac D. 6–Imino–2–thioxo–pyrimidinones as a new class of dipeptidyl peptidase IV inhibitors. *Med. Chem. Res.* 20 (3) (2011) 339–345

40. **Stepanić V**, Koštrun S, Malnar I, Hlevnjak M, Butković K, Čaleta I, Dukši M, Kragol G, Makaruha-Stegić O, Mikac L, Ralić J, Tatić I, Tavčar B, Valko K, Zulfikari S, Munić V*, Modeling cellular pharmacokinetics of 14- and 15-membered macrolides with physicochemical properties. *J. Med. Chem.* 54 (3) (2011) 719–733
41. Verbanac D, Jelić D, **Stepanić V**, Tatić I, Žiher D, Koštrun S. Combined in silico and in vitro Approach to Drug Screening. *Croat. Chem. Acta* 78 (2005) 133–139.
42. **Stepanić V**, Baranović G, Smrečki V, Structure and vibrational spectra of conjugated acids of trans- and cis-azobenzene, *J. Mol. Struct.* 569 (1–3) (2001) 89–109.
43. **Stepanić V**, Baranović G, Ground and excited states of isodiazene – an ab initio study, *Chem. Phys.* 254 (2000) 151 – 168.
44. **Šimek V***, Živković T P, Ground-state properties of benzenoid hydrocarbons by simple bond orbital resonance theory approach, *J. Math. Chem.* 24 (1998) 155–168.
45. **Šimek V**, Živković T P, Analysis of MO ground states of benzenoid hydrocarbons in terms of BORT resonance structures, *Croat. Chem. Acta* 70 (1997) 757–775.

Secondary

1. Verbanac D, **Stepanić V**. Novel perspective in drug development– novel formulations and combinations. *Farmaceutski tehničar - informative journal of croatian pharmaceutical technicians.* 63 (2013) 7-12.
2. **Stepanić V**, Došlić N. Theoretical approaches to chemical reactivity: 1. Dynamical approach. *Kemija u industriji.* 49 (2000) ; 467–476.
3. **Stepanić V**, Sekušak S. Theoretical approaches to chemical reactivity: 1. Statical approach. *Kemija u industriji.* 49 (2000) , 12; 519–525.

Invited lectures

1. **Stepanić V**, Technology driven drug discovery, 1st European Congress of Biomedical and Veterinary Engineering - BIOMEDVETMECH, Zagreb, Croatia, 20-22. October 2022
2. **Stepanić V**, Oršolić D, Šmuc T, Machine learning in chemical compound space, Mini symposium of Croatia Chemical Society, Rijeka, Croatia, July 2022.
3. **Stepanić V**, Machine Learning in Chemistry, XIV Meeting of Young Chemical Engineers : Book of Abstracts / Žižek, Krunoslav ; Katančić, Zvonimir ; Kovačić, Marin (ur.). Zagreb: Croatian Society of Chemical Engineers, 2022. p. 32

4. **Stepanić V**, (Re)purposing starts virtually by predictive machine-learning models, 27th Croatian Meeting of Chemists and Chemical Engineers, October **2021**, Veli Lošinj, Croatia, Book of Abstracts / Marković, Dean ; Meštrović, Ernest ; Namjesnik, Danijel ; Tomašić, Vesna (ur.). p.16
5. **Stepanić V**, Development of phytotoxic natural molecules as complementary herbicidal agents is supported by machine learning study, Book of Abstracts of 1st international conference "Food & Climate Change" / Šamec, Dunja ; Šarkanj, Bojan ; Sviličić Petrić, Ines (ur.). Koprivnica, October 2021. p. 39-39.
6. **Stepanić V**, By polyphenols against cancer?, Symposium "The First 10 Years of HDIR", Croatian Society for Cancer Research, Ruđer Bošković Institute, June 4, **2019**, Book of abstracts, P. Ozretić Ed., Zagreb, p.5.
7. **Stepanić V**, Malignant Tumors in medicinal chemistry, Regular seminar of Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, April **2019**., Zagreb.
8. **Stepanić V**, Physicochemical properties and ADME profile of molecules – *in vitro* and *in silico* approaches, Annual meeting of Croatian Biophysical Society, February **2019**, Zagreb.
9. **Stepanić V**, Meščić A; Harej A; Kraljević Pavelić S; Raić-Malić S. Design of novel hybrid compounds of vitamin C and 1,2,3-triazole with anticancer properties – impact of physicochemical profile on biological activity. HDIR-4: "From Bench to Clinic". Fourth Meeting of the Croatian Association for Cancer Research with International Participation. November 3-4, **2016**, Zagreb.
10. **Stepanić V**, Matić S, Amić D, Lučić B, Milenković D, Marković Z. *In silico* portrayal of quercetin metabolites. ROS in drug discovery: from target identification to redox-based therapeutics. Working Groups Meeting. COST Action BM1203, EU-ROS. April 11-13, **2016**, Lisbon
11. **Stepanić V**, Predicting redox bioactivities of natural and synthetical compounds, 4. Meeting of Section for medicinal and pharmaceutical chemistry of Croatian Chemical Society. PMF, Zagreb, **2015**.
12. **Stepanić V**, Selected attributes of polyphenols in targeting oxidative stress in cancer. 1st International Munich ROS Meeting of COST Action BM1203, German Heart Center Munich, **2015**.
13. Amić D, **Stepanić V**, Lučić B, Marković Z, Dimitrić Marković J. Why does O–H bond dissociation enthalpy effectively represent free radical scavenging activity of flavonoids?

PROCEEDINGS IConSSM **2011** Proceedings of the 4th International Congress of Serbian Society of Mechanics-2013.

14. Verbanac D, Čipčić–Paljetak H, Perić M, Matijašić M, **Stepanić V**, Screening natural antioxidants for their activities – from in silico analysis to in vitro probing // 10th Indo–Italian Workshop on Chemistry and Biology of Antioxidants. Rome, Italy, **2011**. 46–46

15. Verbanac D, **Stepanić V**, Jelić D, New Project Generation Platform Combining In silico and In vitro Approaches, 10. Congress of the Croatian Society of Biochemistry and Molecular Biology – HDBMB2010, Opatija, **2010**.

16. Verbanac D, Jelić D, Koštrun S, **Stepanić V**, Žiher D. Quo Vadis Drug Discovery. The 19th International Course and Conference on the interfaces among Mathematics, Chemistry and Computer Sciences, Dubrovnik, Croatia, **2004**.

17. **Stepanić V**, ^{13}C and ^{15}N NMR spectra of trans–azobenzene and other aza bases in very acidic solutions. XVIII Croatian Meeting of Chemists and Chemical Engineers, Zagreb, Croatia, **2003**.

18. **Šimek V**, The Nobel Prize in Chemistry 1999: Ahmed H. Zewail "for his studies of the transition states of chemical reactions using femtosecond spectroscopy", Regular seminar of Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, **1999**.

Prizes

- **2008** GlaxoSmithKline Exceptional Science Award (individual)
(for application of physicochemical properties on chemical class of macrolides and their global popularization in GSK)
- **2008** GlaxoSmithKline Recognition/Bronze Award
(for contribution to understanding of pharmacokinetical behaviour of macrolides)
- **2008** GlaxoSmithKline Recognition/Bronze Award
(for participation in organization of in-house meeting of computational chemists (Europa) in UK)

Meeting organization:

1. Member of International organizing committee. The 12th Joint Meeting of Medicinal Chemistry (on-line), Bratislava, Slovakia, 2022.

2. Member of International organizing committee. The 11th Joint Meeting of Medicinal Chemistry, Prague, Czech Republic, 2019.
3. Member of International scientific committee and Local organizing committee. The 10th Joint Meeting of Medicinal Chemistry, Dubrovnik, June 25-28, 2017.
4. Member of a national organizing committee. HDIR-4: "From Bench to Clinic". Fourth Meeting of the Croatian Association for Cancer Research with International Participation. November 3-4, 2016, Zagreb.
5. Member of an organizing team. GSK meeting of computational chemists Europe, Stevenage, UK, 2008.
6. Member of an organizing team. The second conference of PMI project leaders (PMI, Zagreb), Hotel Sheraton Zagreb 11-12 December 2008.

Teaching

- **2014 – present** a main organizer and lecturer of the workshop for the researchers and students "Introduction into Molecular Modelling" together with Croatian association for cancer research
- **2016- present** participation in course "Design of novel drugs", of graduate study on Faculty of Pharmacy and Biochemistry, University of Zagreb.
- **2011–2018** participation in course "Biologically active compounds in food", of graduate study Medical studies in Croatian on School of medicine, University of Zagreb
- **2013 – 2018** participation in course "P4 in medicine: Predictive, preventive, personalized and participatory medicine ", of graduate study Medical studies in Croatian on School of medicine, University of Zagreb
- **2012-2014** participation in course "IME6852Z Instrumental methods", of Specialist study of environmental health engineering on University of applied health studies, Zagreb
- **1998–2001** participation in courses "Molecular spectroscopy" and "Chemical kinetics" of graduate study on Faculty of natural sciences, University of Zagreb

Supervision and Mentoring

Informal supervising and coaching

Reviewing

ACS Omega, African Journal of Biotechnology, Anti-Cancer Agents in medicinal Chemistry, Antioxidants, Arabian Journal of Chemistry, Biochemistry & Analytical Biochemistry: Current Research, Briefings in Bioinformatics, Cell Proliferation, Oxidative Medicine and Cellular Longevity, Computational and Structural Biotechnology Journal, Croatica Chemica Acta, European Journal of Medicinal Chemistry, European Journal of Pharmacology, Food Chemistry, Food Technology and Biotechnology, Foods, Frontiers in Pharmacology, Free Radical Research, Frontiers, Future Journal of Pharmaceutical Sciences, Future medicinal chemistry, Heliyon, International Journal of Environmental Research and Public Health, International Journal of Food Properties, Journal of Medicinal Plants Research, Journal of the Chemical Society of Pakistan, Journal of computational chemistry, Journal of Separation Science, Kemija u industriji, Marine Drugs, Medicinal Chemistry, Molecular Biology Reports, Molecules, Natural Product Communications, Phytotherapy Research, Pharmaceuticals, PLoS One, Scientific Reports, Sensors

- a reviewer of the manual for students Barbarić Monika "Design of new drugs (Part 1)", Faculty of Pharmacy and Biochemistry of the University of Zagreb, Zagreb, 2017. (ISBN 978-953-6256-89-1)

Popularization of Science

- **2018-2019** – a supervisor at the BASF Chemgeneration – Reaching Zero experimentation workshop at the Ruđer Bošković Institute
- **2017-2019** – an educator at the ESF project "Affirmative and innovative approaches for education of talented primary school pupils and development of interdisciplinary multiannual program for the talents in STEM fields Ja raSTEM!" (Beneficiary: Primary school Lauder-Hugo Kon)
- **2016 -2019** – a mentor of the workshop "Discovering medicines with the aid of computers" with Marko Tomin, BSc, and prof. Sanja Tomić, provided to the project Exploring Worlds of Science and Innovation' organized by the foundation Wissen am Werk (ZZND) and the Rudjer Boskovic Institute
- **2019**- Participation on the Open Day of IRB ODI2019, as a lecturer, with the lecture "The Bright and the Dark Side of Drugs".

- **2013**- Participation in Open Days of IRB 2013, as a guide coordinator.

Memberships

- Croatian chemical society (a member of Council for Medicinal Chemistry)
- Croatian society for biochemistry and molecular biology
- Croatian biophysical society
- Croatian association for cancer research and EACR
- Croatian pharmacological society
- MC Substitute at COST Action CA16205 European Network on Understanding Gastrointestinal Absorption-related Processes till 2022
- MC member of COST Action BM1203 EU-ROS till 2017
- MC member of COST Action CM1106 Chemical Approaches to Targeting Drug Resistance in Cancer Stem Cells till 2015

Education

- **2001** Ph. D. Degree, Faculty of Science University of Zagreb, Supervisor: Dr. sc. G. Baranović, Prof. T. Cvitaš
- **1997** M. Sc. Degree, Faculty of Science, University of Zagreb, Supervisor: Prof. T. Živković
- **1993** B. Sc. degree, Department of Physical Chemistry, Faculty of Science, University of Zagreb
- **1988** High school, School for pharmaceutical technicians, Zagreb

Other education

- **2022** MedILS Summer School in Bioinformatics, The Mediterranean Institute for Life Sciences (MedILS), Split, Croatia
- **2018** Adverse outcome pathways (AOP): The how and why of development & application (Lectures: D. Martinović-Weigelt & K. R. Illig), Department of Biology, Faculty of Science, University of Zagreb, Croatia
- **2016** Introduction into R – applications in basic statistical and graphical data analysis (S720), University Computing Centre SRCE, University of Zagreb, Croatia

- **2009** Introduction to statistics by the program JMP (SAS), University Computing Centre SRCE, University of Zagreb, Croatia
- **2009** SAS - basics and program language, University Computing Centre SRCE, University of Zagreb, Croatia
- **2009** Introduction to entrepreneurship environment, VG Poduzetnički centar d.o.o., Velika Gorica, Croatia
- **2008** Communication efficiency, Creativa d.o.o., Zagreb, Croatia
- **2006** SIMCA-P Umetrics, Multivariate analysis for Metabonomics, Windsor, UK
- **2003** Fourth European Workshop in Drug Design (4EWDD), Siena, Italy
- **2003** Team building, Pliva, Zagreb, Croatia
- **2003** Writing & Report Writing, Pliva, Zagreb, Croatia
- **2003** Time & Meeting Management, Pliva, Zagreb, Croatia
- **2003** Presentation skills & Negotiation Skills, Pliva, Zagreb, Croatia
- **1998** EPA Summer School '98, The Netherlands
- **1997** Training Course on “Molecular Modeling and Computer Assisted Combinatorial Chemistry”, ICS-UNIDO, Trieste, Italy