

CURRICULUM VITAE

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Expertise: discovery, design and development of compounds with biological activity; natural products; phytocompounds; medicinal chemistry; chemoinformatics; bioinformatics; working with large data sets and machine learning methods; molecular modeling; biochemistry; physical chemistry, analytical chemistry; ADME of chemicals, toxicology; nutraceuticals; functional food; work in the academic and private sector; experience with evaluations

Affiliation

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) **2023–2027** "Analyses of interactions between organophosphorus compounds and esterases and other targets for therapy in poisoning"

2) **2018-2023** "Enzymatic Synthesis of Fluorinated Chiral Building Blocks EnzyFluor" (IP-2018-01-4493)

3) **2014-2018** "Synthesis and cytostatic evaluations of novel nitrogen heterocycles library" (5596)

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)

2) **2009–2014** "Epigenetic and immunomodulatory changes in malignant head and neck tumors " (098–0982464–2511)

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

4) **1998–2001** "Isotopical labeling and molecular spectroscopies" (00980802)

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

6) **1996–1998** "Study of static and dynamical properties of molecules "

7) **1991–1995** "Development and application of models in chemistry "

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-)
- 2) "IGF2 and downstream signaling consequences in human lung cancers" (335-0000000-3532)
- 3) "Epidemiological features of systemic lupus erythematoses in Croatia " (108-1081874-2419).

Prizes

2022 - Recognition to the EnzyFluor project team (HrZZ IP-2018-01-4493) for the most demanding calculation using the Isabella cluster in 2021

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 pharmacokinetic behaviour of macrolides)

2008 GlaxoSmithKline Recognition/Bronze Award

(for participation in organization of in-house meeting of computational chemists (Europa) in UK)

Publications and meeting participation (<https://www.croris.hr/osobe/profil/6153>)

Book Editing

1. **Stepanić V**, Kučerová-Chlupáčová M. Redox Active Molecules in Cancer Treatments, I SBN 978-3-0365-6731-0 (hardback); ISBN 978-3-0365-6730-3 (PDF), <https://doi.org/10.3390/books978-3-0365-6730-3>
2. 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>

3. Book of Abstracts, 10th Joint Meeting on Medicinal Chemistry 2017 / Basarić N, Namjesnik D, Perković I, **Stepanić V** (Eds). Zagreb : Croatian Chemical Society, 2017

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. ISSN: 2459-9387

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. ISBN 978-953-154-282-1

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. ISBN 978-953-154-199-2

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)

More than 50 papers

In the last 5 years:

1. Pehar V, Kolić D, Zandona A, Šinko G, Katalinić M, **Stepanić V***, Kovarik Z*. Selected herbicides screened for toxicity and analysed as inhibitors of both cholinesterases. Chem Biol Interact. 2023 Jul 1;379:110506. doi: 10.1016/j.cbi.2023.110506

2. **Stepanić V***, Kučerová-Chlupáčová M, * Review and Chemoinformatic Analysis of Ferroptosis Modulators with a Focus on Natural Plant Products. *Molecules*, 2023, 28 (2), 475-505. doi:10.3390/molecules28020475
3. 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>
4. 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
5. 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>
6. 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>
7. 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.
8. 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>
9. 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

10. 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
11. 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
12. 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
13. **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.
14. 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.
15. **Stepanić V**,* Matić 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.
16. Matić 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.

Invited lectures in the last 5 years

1. **Stepanić V**, Use of Chemoinformatics in Toxicology, International Symposium on Environmental and Molecular Toxicology of Chemicals, Zagreb, December 7 2023.
2. **Stepanić V**, Brkljača Z, Majerić Elenkov M, Computational Insights into the Biocatalytic Activity of C-Type Halohydrin Dehalogenase HheC, Computational Chemistry Day 2023, September Zagreb, **2023**.
3. **Stepanić V**, Brkljača Z, Milčić N, Crnolatac I, Findrik Blažević Z, Majerić Elenkov M, Elucidation of DMSO effects on catalytic activity of halohydrin dehalogenase HheC by

molecular dynamics, Regional Biophysics Conference, Pečuh: Hungarian Biophysical Society, August 22-26, **2022**.

4. **Stepanić V**, Technology driven drug discovery, 1st European Congress of Biomedical and Veterinary Engineering - BIOMEDVETMECH, Zagreb, Croatia, October 20-22, **2022**
5. **Stepanić V**, Oršolić D, Šmuc T, Machine learning in chemical compound space, Mini symposium of Croatia Chemical Society, Rijeka, Croatia, July **2022**.
6. **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
7. **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
8. **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**.
9. **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.
10. **Stepanić V**, Malignant Tumors in medicinal chemistry, Regular seminar of Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, April **2019**., Zagreb.
11. **Stepanić V**, Physicochemical properties and ADME profile of molecules – *in vitro* and *in silico* approaches, Annual meeting of Croatian Biophysical Society, February **2019**, Zagreb.

Teaching in Higher Education in the last 5 years

2016- present participation in course "Design of novel drugs", of graduate study on Faculty of Pharmacy and Biochemistry, University of Zagreb.

Supervision

Dilber Ivana, The use of the AI tool AlphaFold 2 for protein structure modeling, Master's thesis, Stepanić Višnja, Nela Malatesti (Supervisors), Department of Biotechnology, University of Rijeka, 2023.

Pehar Vesna, Toxicity of selected herbicides analysed by in silico methods and by bioassays, Doctoral Thesis, Kovarik Zrinka, Stepanić, Višnja (Supervisors), Faculty of sciences, University of Zagreb, 2023.

Jagar Fran, Study of interactions between Olive compounds and tyrosine kinase HGFR/c-Met using molecular docking, Master's thesis, Stepanić Višnja, Barbarić Monika (Supervisors), Faculty of Pharmacy and Biochemistry, University of Zagreb, 2023.

Workshops in the last 5 years

2023 - an organizer and lecturer of the workshop for the researchers and students " How to design and apply a proof-of-concept (PoC) proposal?" together with Croatian association for cancer research (HDIR), 25/5/2023

2023 - an organizer and lecturer of the workshop for the researchers and students " Why take the path of innovation and commercialisation?" together with Croatian association for cancer research (HDIR), 27/3/2023

2014 – present an organizer and lecturer of the workshop for the researchers and students from academic and non-academic environments, "Introduction into Molecular Modelling" together with Croatian association for cancer research (HDIR)

Conference/Meeting organization in the last 5 years

1. Member of organizing committee of annual Mini symposium of Section of medicinal and pharmaceutical chemistry of Croatian Chemical Society
2. Member of organizing committee of annual meeting Computational Chemistry Day (CCD) of Section of theoretical and computation chemistry of Croatian Chemical Society
3. Member of International organizing committee. The 12th Joint Meeting of Medicinal Chemistry (on-line), Bratislava, Slovakia, 2022.
4. Member of International organizing committee. The 11th Joint Meeting of Medicinal Chemistry, Prague, Czech Republic, 2019.

5. Member of International scientific committee and Local organizing committee. The 10th Joint Meeting of Medicinal Chemistry, Dubrovnik, Croatia, June 25-28, 2017.

Memberships

- Croatian chemical society (a member of Council for Section of Medicinal and Pharmaceutical Chemistry)
- Croatian biophysical society (a member of the Steering board)
- Croatian society for biochemistry and molecular biology
- Croatian association for cancer research and EACR
- Member of WG3 of COST Action CA21134 - Towards zero Pesticide Agriculture : European Network for sustainability (TOP-AGRI-Network)
- MC Substitute at COST Action CA16205 European Network on Understanding Gastrointestinal Absorption-related Processes 2017-2021
- MC member of COST Action BM1203 EU-ROS 2012-2016
- MC member of COST Action CM1106 Chemical Approaches to Targeting Drug Resistance in Cancer Stem Cells 2012-2016

Education

2001 Ph. D. Degree, Faculty of Science University of Zagreb, Field of theoretical and computational chemistry

1997 M. Sc. Degree, Faculty of Science, University of Zagreb

1993 B. Sc. degree, Department of Physical Chemistry, Faculty of Science, University of Zagreb

1988 High school, School for pharmaceutical technicians, Zagreb