BONO LUČIĆ - CURRICULUM VITAE

PERSONAL INFORMATION

Name and surname	**Bono Lučić**
Academic title	Ph. D., Chemistry
Year and institution of PhD obtained	1997, Faculty of Science, University of Zagreb, Zagreb, Croatia
Address	Bijenička c. 54, HR-10000, Zagreb, Croatia
Phone	++385-1-4571356
E-mail	lucic@irb.hr
Personal web page	https://www.irb.hr/eng/About-RBI/People/Bono-Lucic
Citizenship	Croatian
Date and place of birth	October 11, 1964, Turić, Bosnia and Herzegovina
Marital and family status	married; three children
CROSBI – list of publications	https://www.bib.irb.hr/pregled/znanstvenici/184293?autor=184293
PUBLONS – No. of reviews completed (registered)	https://publons.com/researcher/1202691/bono-lucic/
Google Scholar	https://scholar.google.com/citations?user=z8TnZFUAAAAJ&hl=en

WORK EXPERIENCE

Date (from – until)	*2009 - 2021*
Institution	*Ruđer Bošković Institute, Zagreb, Croatia*
Position	Senior research associate
Work field	*Development of algorithms, Chemoinformatics, Structural bioinformatics of proteins*
Date (from – until)	*2002 - 2009*
Institution	*Ruđer Bošković Institute, Zagreb, Croatia*
Position	Research associate
Work field	*Development of algorithms, Chemoinformatics, Structural bioinformatics of proteins*
Date (from – until)	*1997 - 2002*
Institution	*Ruđer Bošković Institute, Zagreb, Croatia*
Position	Scientific researcher (post-doctoral student), senior assistant
Work field	*Theoretical chemistry, chemoinformatics and molecular biophysics*
Date (from – until)	*1992 - 1997*
Position	Scientific researcher (PhD student), assistant
Institution	*Ruđer Bošković Institute, Zagreb, Croatia*
Work field	*Theoretical chemistry and chemoinformatics*
Date (from – until)	*1991 - 1992*
Institution	*Faculty of Science and Education, University of Split, Split, Croatia*
Position	*Scientific researcher*
Work field	*Molecular biophysics*

EDUCATION

Date, Place	*1995 - 1997, Zagreb*
Institution	Faculty of Science (Department of Chemistry), University of Zagreb, Croatia
Title of qualification awarded	Ph. D., Chemistry (theoretical chemistry)
Date, Place	*1991 - 1994, Zagreb*
Institution	Faculty of Science (Department of Physics), University of Zagreb, Croatia

Title of qualification awarded	Master of Science, Physics (molecular biophysics)
Date, Place	*1984 - 1989, Zagreb*
Institution	Faculty of Electrical Engineering and Computing (Department of Electronics), University of Zagreb, Croatia
Title of qualification awarded	Graduated Engineer of Electrical Engineering (microelectronics)
Date, Place	*1979 - 1983, Gradačac, Bosnia and Herzegovina*
Institution	High School (Gymnasium)

RESEARCH TOPICS

molecular modelling in chemistry and molecular biophysics // theoretical chemistry // cheminformatics // bioinformatics // structural bioinformatics of proteins // development of algorithms // model selection methods // development of model validation algorithms // development of methods for validation of classification models // development of molecular descriptors // structure-activity relationships of molecules // QSAR/QSPR (quantitative structure-activity/property relationship) // antioxidant activity modelling of molecules // modelling biological activity of polyphenols

RESEARCH AND OTHER PROJECTS

Development and application of improved chemoinformatics methods in the biosciences, CRO-GER project (DAAD) (2021-2022), **project leader** from the Croatian side, Ministry of Science Education and Sports of the Republic of Croatia and DAAD, Germany

HRZZ DOK-01-2018, "Career Development Project for Young Researchers - Training of New Doctors of Science", 2018, Croatian Science Foundation, Croatia, **project leader**

Bioprospecting of Adriatic See, Croatian Government and the European Union through the European Regional Development Fund - the Competitiveness and Cohesion Operational Programme (KK.01.1.1.01) – The Scientific Centre of Excellence for Marine Bioprospecting -BioProCro granted to Rozelinda Čož-Rakovac, (2017-2022), associate/researcher

Investigation of chemism and antioxidant activity of complexes of polyphenols with essential metals, CRO-SRB project (2016-2017), Ministry of Science Education and Sports of the Republic of Croatia, researcher from the Croatian side

Developing methods for modeling properties of bioactive molecules and proteins (2012-2014), **project leader**, Ministry of Science, Education and Sports of the Republic of Croatia
(**Z-project** MZOS-098-1770495-2919, Project Performance Indicators: (**1**) **101** sci. papers published in journals, (**2**) **66** sci. papers in CC journals and **88** indexed in Scopus, (**3**) **17** sci. papers as chapters in books, (**4**) ranked among the first three Z-projects in Chemistry in Croatia according to CROSBI).

Investigation of relationships between structure and biological activity of polyphenols, CRO-SRB project (2011-2012), **project leader** from the Croatian side, Ministry of Science Education and Sports of the Republic of Croatia

Developing methods for modeling properties of bioactive molecules and proteins (2007-2011), associate/researcher, Ministry of Science Education and Sports of the Republic of Croatia, researcher

Development and application of models in chemistry and bioinformatics (2002-2006), associate/researcher, Ministry of Science Education and Sports of the Republic of Croatia

Toxicity and carcinogenicity of organic molecules on living organisms in the environment, HR-SLO project (2001-2003), **project leader** from the Croatian side, Ministry of Science Education and Sports of the Republic of Croatia

IQ QSAR program (2001-2004), **project co-leader**, PLIVA, Zagreb (budget: 265.000,00 HRK in year 2001), **transfer of knowledge to pharmaceutical industry Pliva**

Predicting structure of proteins and bio-active molecules (1998-2001), **project leader**, Ministry of Science

Education and Sports of the Republic of Croatia

Development and application of models in chemistry (1996-2002), associate/researcher, Ministry of Science Education and Sports of the Republic of Croatia

Development and application of models in chemistry (1992-1996), associate/researcher, Ministry of Science Education and Sports of the Republic of Croatia

Predicting structure and activity of membrane polypeptides (1991-1992), associate/researcher, Ministry of Science Education and Sports of the Republic of Croatia

TEACHING

Structural bioinformatics of proteins and bioactive molecules, PhD Study *Molecular Biosciences* (organized by: University of J. J. Strossmayer in Osijek, Ruđer Bošković Institute and University of Dubrovnik)

Models and methods in structural bioinformatics, PhD Study *Biophysics* organized by: University of Split, Ruđer Bošković Institute (Zagreb), Institute of Physics (Zagreb), and Mediterranean Institute for Life Sciences (Split)

Member of four Committees for evaluation of PhD thesis

2016. Assistant Professor (honorary position) at the J. J. Strossmayer University in Osijek, Osijek, Croatia

MENTORSHIP OF DEFENDED DOCTORAL AND MASTER DISSERTATIONS AND BSc THESES

M. Lovrić (June, 2021) Development and application of models for ecotoxicological risk assessment of bioactive chemical compounds (in Croatian: Razvoj i primjena modela za procjenu ekotoksikološkog rizika bioaktivnih kemijskih spojeva), PhD in Chemistry, Zagreb, University of Zagreb, Faculty of Science and Mathematics (Department of Chemistry), Croatia

V. Bojović (December, 2020) Novel parameters for estimating the complexity of classification variables and their application in modeling properties of molecules (in Croatian: Novi parametri za procjenu složenosti klasifikacijskih varijabli i njihova primjena u modeliranju svojstava molekula, PhD in Molecular biosciences, Osijek/Zagreb, University of Osijek, Croatia

J. Batista (January, 2018) Selection of representative set of membrane proteins of known structure: development of improved algorithms using the random model concept ((in Croatian: , Doctoral dissertation (in Biopohysics), PhD in biophysics, Split, University of Split, Faculty of Science and Mathematics, Croatia

D. Nadramija (April 26, 2010) Modeling of pharmacological properties of molecules by linear and nonlinear ensembles of multivariate regression models, PhD in Chemistry, Zagreb, University of Zagreb, Faculty of Science and Mathematics (Department of Chemistry), Croatia

L. Papeš Šokčević (October 26, 2011) Improved algorithm for selection and validation of best multivariate structure-property molecular models, Master of science dissertation, Zagreb, University of Zagreb, Faculty of Electrical Engineering and Computing (co-mentorship)

Co-leader (direct supervisor) of three BSc thesis all at the University of Zagreb, Zagreb: (1) T. Piližota (2002, Faculty of Science – Physics, ORCID https://orcid.org/0000-0002-2156-0221), P. Močilac (2002, Faculty of Pharmacy and Biochemistry, ORCID https://orcid.org/0000-0002-0789-9528), D. Nasteski (2004, Faculty of Science - Chemistry)

ORGANIZATIONAL SKILLS AND COMPETENCES

Co-organizer of two home conferences of biophysicists (2003 and 2005)

Secretary and the member of AdvisoryBoard of Croatian Biphysics Society (2002-2009)

Co-editor of special issue of *Croatica Chemica Acta* journal dedicated to Professor Douglas Jay Klein (http://hrcak.srce.hr/index.php?show=toc&id_broj=9220&lang=en), Issue 4, Volume 86, 2013.

Co-editor of special issue of International Journal of Chemical Modeling dedicated to Professor Nenad Trinajstić, Issue 2-3, Volume 6, 2014.

Co-editor of special issue of *Croatica Chemica Acta* journal dedicated to Professor Nenad Trinajstić,

member of Croatian Academy of Sciences and Arts (https://hrcak.srce.hr/index.php?show=toc&id_broj=13598), Issue 4, Volume 89, 2016.

Editor of special issue "Chemoinformatics and Bioinformatics Tools in Structure-Activity Modelling in Molecular Sciences" of *International Journal of Molecular Sciences* (IJMS) indexed in CC (IF 5.923, Q1)

MEMBERSHIP IN SCIENCE ORGANIZATIONS AND BODIES

2000-present Croatian Society for Theoretical and Mathematical Biology, Zagreb

1993-present, Croatian Biophysical Society, Zagreb

1992-present, Croatian Chemical Society, Zagreb

COMMISSIONS, COMMITTEES, BOARDS AND WORK GROUPS

(2012-2019) Member of *IUPAC Committee on Publications and Cheminformatics Data Standards*, former name *Committee for Printed and Electronic Publications* (2012- 2014) as a representative of Croatian Chemical Society

(2015-2021) Member of Scientific Committee of International Scientific Conference MATH/CHEM/COMP 2015, 2016, 2017, 2018, 2019, 2020 and 2021.

Secretary of the Croatian Biophysical Society (2002-2009)

Member of the Steering Committee of the Croatian Biophysical Society (2002-2009)

Member of the Council of the PhD Study in Biophysics / University of Split, Croatia (2009-2018)

PAPERS

Co-author of **11** articles as chapters in books (in **8** as the first author)

Co-author of **74** scientific papers published in scientific journals (**60** in **CC**, **70 in WoS**)

More than **60** scientific contributions (posters or lectures) at international scientific conferences

CITATIONS OF PAPERS

(9/2021) - **2076** citations (**1944** without self-citations) in *Web of Science* (*WoS*)

(9/2021) **H-index** = **25**, average citations per article in *WoS* **29.24**

(9/2021) - **4** papers (the first author on two of them) cited more than 100 times in *WoS* (225, 148, 147 and 110 citations) and **8** papers (first author on three of them) cited more than 100 times in *Google Scholar*.

(9/2021) - **2984** citations in *Google Scholar* (**1279** citations since 2016)

OTHER RESEARCH ACTIVITIES

Member of Editorial Board of *Croatica Chemica Acta* (2000–) and Editor (2011-), journal indexed in CC

Member of Editorial Board of *Molecules* (2020–), journal indexed in CC (https://www.mdpi.com/journal/molecules/editors)

Member of Editorial Board of *International Journal of Quantitative Structure-Property Relationships (IJQSPR)* (2016–)

Member of Advisory Board of *Internet Electronic Journal of Molecular Design* (2004–2008)

Member of Editorial Board of Referees of the *ARKIVOC* journal (2002–)

Member of the Editorial Advisory Board of the Book "*Quantitative Structure-Activity Relationships in Drug Design, Predictive Toxicology, and Risk Assessment"*, IGI Global, 2015

COMPUTER SKILLS

Knowledge needed for work with many computer programs from different fields (on daily basis)

Programming skills

OTHER IMPORTANT SKILLS AND COMPETENCES

Reviewer for more than 75 scientific journals from *Current Contents* (mostly) and *Web of Science*.

More details on the completed and registered reviews at the service PUBLONS (among all reviews I completed, 176 of them are verified at PUBLONS and 21 editorial records):
https://publons.com/author/1202691/bono-lucic#profile

Reviewer of scientific projects (from Croatia and from The Republic of Macedonia)

Reviewer of UKF scientific projects, Croatia, Zagreb

Reviewer of more than 10 IUPAC projects (2012-2019)

LIST OF PAPERS – Bono Lučić

A) Scientific papers published in the journals included in *Current Contents* and *Web of Science*

1. D. Juretić, B. Lučić, N. Trinajstić, Predicting Membrane Protein Secondary Structure - Preference Functions Method for Finding Optimal Conformational Parameters. *Croat. Chem. Acta* 66 (1993) 201-208.
2. D. Juretić, N. Trinajstić, B. Lučić, Protein Secondary Structure Conformations and Associated Hydrophobicity Scales. *J. Math. Chem.* 14 (1993) 35-45.
3. B. Lučić, S. Nikolić, N. Trinajstić, A Jurić, D. Juretić, A Novel QSPR Approach to Physicochemical Properties of the α-Amino Acids. *Croat. Chem. Acta* 68 (1995) 435-450.
4. B. Lučić, S. Nikolić, N. Trinajstić, A. Jurić, Z. Mihalić, A Structure-Property Study of the Solubility of Aliphatic Alcohols in Water. *Croat. Chem. Acta* 68 (1995) 417-434.
5. B. Lučić, S. Nikolić, N. Trinajstić, D. Juretić, The Structure-Property Models Can Be Improved Using the Orthogonalized Descriptors. *J. Chem. Inf. Comput. Sci.* 35 (1995) 532-538.
6. D. Juretić, B. Lučić, N. Trinajstić, Secondary Structure Prediction Quality for Naturally Occurring Amino Acids in Soluble Proteins. *J. Mol. Struct.-Teochem.* 338 (1995) 43-50.
7. D. Amić, D. Davidović-Amić, A. Jurić, B. Lučić, N. Trinajstić, Structure-Activity Correlation of Flavone Derivatives for Inhibition of cAMP Phosphodiesterase. *J. Chem. Inf. Comput. Sci*. 35 (1995) 1034-1038.
8. D. Amić, D. Davidović-Amić, D. Bešlo, B. Lučić, N. Trinajstić, The Use of the Ordered Orthogonalized Multivariate Linear Regression in a Structure-Activity Study of Coumarin and Flavonoid Derivatives as Inhibitors of Aldose Reductase. *J. Chem. Inf. Comput. Sci*. 37 (1997) 581-586.
9. N. Trinajstić, S. Nikolić, B. Lučić, D. Amić, The Detour-Matrix in Chemistry. *J. Chem. Inf. Comput. Sci*. 37 (1997) 631-638.
10. D. J. Klein, M. Randić, D. Babić, B. Lučić, S. Nikolić, N. Trinajstić, Hierarchical Orthogonalization of Descriptors. *Int. J. Quantum Chem*. 63 (1997) 215-222.
11. D. Amić, D. Davidović-Amić, D. Bešlo, B. Lučić, N. Trinajstić, A Simple QSAR Model for Trypsin Aminopeptidase Inhibitory Flavonoids. *Croat. Chem. Acta* 70 (1997) 905-911.
12. D. Juretić, D. Zucić, B. Lučić, N. Trinajstić, Preference Functions for Prediction of Membrane-Buried Helices in Integral Membrane Proteins. *Comput. Chem*. 22 (1998) 279-294.
13. D. Amić, D. Bešlo, B. Lučić, N. Trinajstić, The Vertex-Connectivity Index Revisited. *J. Chem. Inf. Comput. Sci*. 38: (1998) 819-822.
14. D. Amić, D. Davidović-Amić, D. Bešlo D, B. Lučić, N. Trinajstić, QSAR of Flavylium Salts as Inhibitors of Xanthine Oxidase. *J. Chem. Inf. Comput. Sci*. 38 (1998) 815-818.
15. B. Lučić, N. Trinajstić, Multivariate Regression Outperforms Several Robust Architectures of Neural Networks in QSAR Modeling. *J. Chem. Inf. Comput. Sci*. 39 (1999) 121-132.
16. B. Lučić, N. Trinajstić, S. Sild, M. Karelson, A. R. Katritzky, A New Efficient Approach for Variable Selection Based on Multiregression: Prediction of Gas Chromatographic Retention Times and Response Factors. *J. Chem. Inf. Comput. Sci*. 39 (1999) 610-621.
17. D. Amić, D. Davidović-Amić, D. Bešlo, B. Lučić, N. Trinajstić, Prediction of pK Values, Half-Lives, and Electronic Spectra of Flavylium Salts from Molecular Structure. *J. Chem. Inf. Comput. Sci*. 39 (1999) 967-973.

18. A. R. Katritzky, K. Chen, Z. L. Wang, M. Karelson, B. Lučić, N. Trinajstić, T. Suzuki, G. Schüürmann, Prediction of Liquid Viscosity for Organic Compounds by a Quantitative Structure-Property Relationship. *J. Phys. Org. Chem.* 13 (2000) 80-86.

19. S. C. Basak, B. D. Gute, B. Lučić, S. Nikolić, N. Trinajstić, A Comparative QSAR Study of Benzamidines Complement-Inhibitory Activity and Benzene Derivatives Acute Toxicity. *Comput. Chem*. 24 (2000) 181-191.

20. B. Lučić, D. Amić, N. Trinajstić, Nonlinear Multivariate Regression Outperforms Several Concisely Designed Neural Networks on Three QSPR Data Sets. *J. Chem. Inf. Comput. Sci*. 40 (2000) 403-413.

21. D. Amić, B. Lučić, S. Nikolić, N. Trinajstić, Predicting Inhibition of Microsomal p-Hydroxylation of Aniline by Aliphatic Alcohols: A QSAR Approach Based on the Weighted Path Numbers. *Croat. Chem. Acta* 74 (2001) 237-220.

22. B. Lučić, I. Lukovits, S. Nikolić, N. Trinajstić, Distance-Related Indexes in the Quantitative Structure-Property Relationship Modeling. *J. Chem. Inf. Comput. Sci*. 41 (2001) 527-535.

23. D. Amić, S. C. Basak, B. Lučić, S. Nikolić, N. Trinajstić, Structure-Water Solubility Modeling of Aliphatic Alcohols Using the Weighted Path Numbers. *SAR QSAR Environ. Res.* 13 (2002) 281-295.

24. B. Lučić, I. Bašic, N. Nadramija, A. Miličević, N. Trinajstić, T. Suzuki, R. Petrukhin, M. Karelson, A. R. Katritzky, Correlation of Liquid Viscosity with Molecular Structure for Organic Compounds Using Different Variable Selection Methods. *Arkivoc* 4 (2002) 45-59.

25. B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, Harary Index - Twelve Years Later. *Croat. Chem. Acta* 75 (2002) 847-868.

26. B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, On Variable Wiener Index. *Indian J. Chem. Sect A-Inorg. Bio-Inorg. Phys. Theor. Anal. Chem*. 42 (2003) 1279-1282.

27. B. Lučić, N. Nadramija, I. Bašic, N. Trinajstić, Toward Generating Simpler QSAR Models: Nonlinear Multivariate Regression Versus Several Neural Network Ensembles and Some Related Methods. *J. Chem. Inf. Comput. Sci*. 43 (2003) 1094-1102.

28. T. Piližota, B. Lučić, N. Trinajstić, Use of Variable Selection in Modeling the Secondary Structural Content of Proteins from Their Composition of Amino Acid Residues. *J. Chem. Inf. Comput. Sci*. 44 (2004) 113-121.

29. F. Supek, T. Šmuc, B. Lučić, A Prototype Structure-Activity Relationship Model Based on National Cancer Institute Cell Line Screening Data. *Period. Biol*. 107 (2005) 451-455.

30. D. Amić, D. Davidović-Amić, D. Bešlo, V. Rastija, B. Lučić, N. Trinajstić, SAR and QSAR of Antioxidant Activity of Flavonoids. *Curr. Med. Chem.* 14 (2007) 827-845.

31. D. Janežič, B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, D. Vukičević, Hosoya Matrices as the Numerical Realization of Graphical Matrices and Derived Structural Descriptors. *Croat. Chem. Acta*. 80 (2007) 271-276.

32. D. Amić, B. Lučić, G. Kovačević, N. Trinajstić, Bond Dissociation Enthalpies Calculated by the PM3 Method Confirm Activity Cliffs in Radical Scavenging of Flavonoids. *Mol. Divers*. 13 (2009) 27-36.

33. B. Lučić, N. Trinajstić, B. Zhou, Comparison Between the Sum-connectivity Index and Product-connectivity Index for Benzenoid Hydrocarbons. *Chem. Phys. Lett*. 475 (2009) 146–148.

34. D. Amić, B. Lučić, Reliability of Bond Dissociation Enthalpy Calculated by the PM6 Method and Experimental TEAC Values in Antiradical QSAR of Flavonoids. *Bioorg. Med. Chem*. 18 (2010) 28–35.

35. K. Tanabe, B. Lučić, D. Amić, T. Kurita, M. Kaihara, N. Onodera, T. Suzuki, Prediction of Carcinogenicity for Diverse Chemicals Based on Substructure Grouping and SVM Modeling. *Mol. Divers*. 14 (2010) 789–802.

36. D. Vukičević, N. Trinajstić, S. Nikolić, B. Lučić, B. Zhou, Master Connectivity Index and Master Connectivity Polynomial. *Curr. Comput.-Aided Drug Des*. 6 (2010) 235-239.

37. D. Juretić, D. Vukičević, D. Petrov, M. Novković, V. Bojović, B. Lučić, N. Ilić, A. Tossi. Knowledge-Based Computational Methods for Identifying or Designing Novel, Non-Homologous Antimicrobial Peptides. *Eur. Biophys. J*. 40 (2011) 371–385.

38. Z. Marković, D. Milenković, J. Đorović, J. Dimitrić Marković, V. Stepanić, B. Lučić, D. Amić. PM6 and DFT Study of Free Radical Scavenging Activity of Morin. *Food Chem*. 134 (2012) 1754-1760.

39. Z. Marković, D. Milenković, J. Đorović, J. Dimitrić Marković, V. Stepanić, B. Lučić, D. Amić. Free Radical Scavenging Activity of Morin 2'-O− Phenoxide Anion. *Food Chem*. 135 (2012) 2070-2077.
40. J. Dimitrić Marković, Z. Marković, J. Krstić, D. Milenković, B. Lučić, D. Amić. Interpretation of the IR and Raman Spectra of Morin by Density Functional Theory and Comparative Analysis. *Vib. Spectrosc*. 64 (2013) 1-9.
41. Z. Marković, D. Milenković, J. Đorović, J. Dimitrić Marković, B. Lučić, D. Amić. A DFT and PM6 Study of Free Radical Scavenging Activity of Ellagic Acid. *Monatsh. Chem*. 144 (2013) 803-812.
42. D. Amić, V. Stepanić, B. Lučić, Z. Marković, J. Dimitrić Marković. 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.
43. V. Stepanić, K. Gall Trošelj, B. Lučić, Z. Marković, D. Amić. Bond Dissociation Free Energy as General Parameter for Flavonoid Radical Scavenging Activity. *Food Chem*. 141 (2013) 1562-1570.
44. K. Tanabe, T. Kurita, K. Nishida, B. Lučić, D. Amić, T. Suzuki. Improvement of Carcinogenicity Prediction Performances Based on Sensitivity Analysis in Variable Selection of SVM Models. *SAR QSAR Environ.Res*. 24 (2013) 565-580.
45. B. Lučić, I. Sović, J. Batista, K. Skala, D. Plavšić, D. Vikić-Topić, D. Bešlo, S. Nikolić, N. Trinajstić, The Additive Variant of the Randić Connectivity Index. *Curr. Comput.-Aided Drug Des*. 9 (2013) 184-194.
46. B. Lučić, V. Stepanić, D. Plavšić, A. Amić, D. Amić. Correlation between ^{13}C NMR chemical shifts and antiradical activity of flavonoids. *Monatsh. Chem*. 145 (2014) 457-463.
47. J. Dimitrić Marković, D. Amić, B. Lučić, Z. Marković. Oxidation of kaempferol and its iron(III) complex by DPPH radical: spectroscopic and theoretical study. *Monatsh. Chem*. 145 (2014) 557-563.
48. A. Amić, Z. Marković, J. Dimitrić Marković, V. Stepanić, B. Lučić, D. Amić. Towards an improved prediction of the free radical scavenging potency of flavonoids: The significance of double PCET mechanisms. *Food Chem*. 152 (2014) 578-585.
49. M. Filipović, Z. Marković, J. Đorović, J. Dimitrić Marković, B. Lučić, D. Amić. QSAR of the free radical scavenging potency of selected hydroxybenzoic acids and simple phenolics. *C. R. Chim*. 18 (2015) 492-498.
50. A. Amić, Z. Marković, J. Dimitrić Marković, B. Lučić, V. Stepanić, D. Amić. The 2H+/2e− free radical scavenging mechanisms of uric acid: thermodynamics of N-H bond cleavage. *Comput. Theor. Chem*. 1077 (2016) 2-10.
51. A. Amić, Z. Marković, J. Dimitrić Marković, S. Jeremić, B. Lučić, D. Amić, Free radical scavenging and COX-2 inhibition by simple colon metabolites of polyphenols: A theoretical approach. *Comput. Biol. Chem*. 65 (2016) 45-53.
52. A. Amić, B. Lučić, Z. Marković, D. Amić, Carboxyl Group as a Radical Scavenging Moiety: Thermodynamics of 2H+/2e– Processes of Phloretic Acid. *Croatica chemica acta*. 89 (2016) 517-525.
53. J. Batista, D. Vikić-Topić, B. Lučić, The difference between the accuracy of real and the corresponding random model is a useful parameter for validation of two-state classification model quality. *Croatica chemica acta*. 89 (2016) 527-534.
54. A. Amić, B. Lučić, V. Stepanić, Z. Marković, S. Marković, J. Dimitrić Marković, D. Amić. Free radical scavenging potency of quercetin catecholic colonic metabolites: thermodynamics of 2H+/2e- processes. *Food Chem*. 218 (2017) 144-151.
55. S. Matić, M. Jadrijević-Mladar Takač, M. Barbarić, B. Lučić, K. Gall Trošelj, V. Stepanić, The Influence of In Vivo Metabolic Modifications on ADMET Properties of Green Tea Catechins-In Silico Analysis // *Journal of pharmaceutical sciences*, 107 (2018), 11; 2957-2964, doi:10.1016/j.xphs.2018.07.026
56. A. Amić, Z. Marković, J. Dimitrić Marković, D. Milenković, B. Lučić,The role of guaiacyl moiety in free radical scavenging by 3, 5-dihydroxy-4-methoxybenzyl alcohol: Thermodynamics of 3H+/3e- mechanisms // *Molecular physics*, 117 (2019), 2; 207-217, doi:10.1080/00268976.2018.1508777
57. V. Stepanić, S. Matić, A. Amić, B. Lučić, D. Milenković, Z. Marković, Effects of conjugation metabolism on radical scavenging and transport properties of quercetin – In silico study. *J, Mol. Graphics & Modelling*, 86 (2019), 278-285, https://doi.org/10.1016/j.jmgm.2018.10.023

58. B. Lučić, J. Batista, V. Bojović, M. Lovrić, A. Sović Kržić, D. Bešlo, D. Nadramija, D. Vikić-Topić, Estimation of Random Accuracy and its Use in Validation of Predictive Quality of Classification Models within Predictive Challenges // *Croatica Chemica Acta*, 92 (2019), 379-391. https://doi.org/10.5562/cca3551
59. M. Lovrić, O. Malev, G. Klobučar, R. Kern, J.J. Liu, B. Lučić, Predictive Capability of QSAR Models Based on the CompTox Zebrafish Embryo Assays: An Imbalanced Classification Problem, *Molecules*. 26 (2021) 1617. https://doi.org/10.3390/molecules26061617
60. M. Lovrić, K. Pavlović, P. Žuvela, A. Spataru, B. Lučić, R. Kern, M.W. Wong, Machine learning in prediction of intrinsic aqueous solubility of drug-like compounds: Generalization, complexity, or predictive ability?, *Journal of Chemometrics*, (2021), e3349. https://doi.org/10.1002/cem.3349
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