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
ORCID	https://orcid.org/0000-0001-7232-2007
ResearchedID	https://www.webofscience.com/wos/author/rid/J-3813-2012

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

SCIENTIFIC RESEARCH PROJECTS

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

2021. Drug Attrition Oracle, AI4EU supported project, HORIZON 2020 ACTION; research associate, funded by the EU through the Horizon 2020 program.

HRZZ DOK-01-2018, "Career Development Project for Young Researchers - Training of New Doctors of Science", 2018-2021, „ https://pdb.irb.hr:8443/project/irb:006859, project leader, Financed by the Croatian Science Foundation and the European Social Fund.

Bioprospecting of Adriatic See, The Scientific Centre of Excellence (SCE) for Marine Bioprospecting – BioProCro (2017-2022), researcher, Financed by the Government of the Republic of Croatia and the EU through the European Fund for Regional Development - operational program "Competitiveness and Cohesion" (KK.01.1.1.01) http://bioproadriatic.hr/people.

Investigation of chemism and antioxidant activity of complexes of polyphenols with essential metals, CRO-SRB project (2016-2017), researcher

Developing methods for modeling properties of bioactive molecules and proteins (2012-2014), project leader, Financed by the Ministry of Science, Education and Sports of the Republic of Croatia
(Z-project MZOS-098-1770495-2919, https://www.bib.irb.hr/pregled/projekti/098-1770495-2919?page=6,

Investigation of relationships between structure and biological activity of polyphenols, CRO-SRB project (2011-2012), project leader from the Croatian side.

Developing methods for modeling properties of bioactive molecules and proteins (2007-2011), associate/researcher, researcher.

Development and application of models in chemistry and bioinformatics (2002-2006), researcher.

Toxicity and carcinogenicity of organic molecules on living organisms in the environment, HR-SLO project (2001-2003), project leader from the Croatian side

IQ QSAR program (2001-2003), project co-leader, PLIVA, Zagreb, transfer of knowledge to pharmaceutical industry Pliva d.d., Zagreb.

Predicting structure of proteins and bio-active molecules (1998-2001), supporting project for young scientists, project leader

Development and application of models in chemistry (1992-1996 and 1996-2002), researcher, http://zprojekti.mzos.hr/page.aspx?pid=6&lid=1 (00980606) http://bib.irb.hr/lista-radova?sif_teme=00980606&period=1996

Predicting structure and activity of membrane polypeptides (1991-1992), researcher

TEACHING ACTIVITIES AND TEACHING ACTIVITIES AND COURSES COURSES

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) (2009-)

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), (2008-2013.)

Bioinformatics (module within the course *Systemic biomedicine*, BUM101) at the postgraduate study of Biotechnology in medicine at the University of Rijeka, Croatia (2012-2020)

Member of five Committees for evaluation of PhD thesis and more submissions of dissertation topics at various Universities (Zagreb, Split, Rijeka, Osijek

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

2022 (May), Associate 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, 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, 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, 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 thesis, Zagreb, University of Zagreb, Faculty of Electrical Engineering and Computing (co-mentorship)

Mentoring two PhD students from Biophysics is ongoing, focusing on protein folding and aggregation modelling, as well as improved model validation protocols in protein folding rate modelling.

Co-leader (direct supervisor) of three BSc thesis all at the University of Zagreb, Zagreb:

(1) T. Piližota (2002, Faculty of Science of the Univesrity of Zagreb – Physics, Former group leader at the University of Edinburgh (https://edwebprofiles.ed.ac.uk/profile/teuta-pilizota), Scotland, UK, Now Professor at the University of Cambridge, UK (Cavendish Laboratory, Physics of Life), www.phy.cam.ac.uk/profile/prof-teuta-pilizota.

(2) P. Močilac (2002, Faculty of Pharmacy and Biochemistry of the Univesrity of Zagreb), now professor at the Lanzhou University, China, https://scholar.google.com/citations?user=f0WlZKAAAAAJ&hl=en

(3) D. Nasteski (2004, Faculty of Science of the University of Zagreb - Chemistry)

Guiding younger collaborators/researchers and encouraging their research creativity

Conducted (with professor Mile Šikić) B.Sc. students of the Faculty of Electrical Engineering and Computing (FER) of the University of Zagreb (I. Sović, I. Čanadi, M. Piškorec) in the work for the Rector's Award at the University of Zagreb. The students received the award (https://apps.unizg.hr/rektorova-nagrada/javno/stari-radovi/885/preuzmi), and later achieved excellent careers.

Led in the student research work B.Sc. student of the Faculty of Electrical Engineering and Computing (University of Zagreb) M. Flajšlik (https://scholar.google.com/citations?hl=en&user=lHOn84AAAAAJ&view_op=list_works&sortby=pubdat).

ORGANIZATIONAL SKILLS AND COMPETENCES

Co-organizer of two home conferences of biophysicists (2003 and 2005) as part of which an exceptionally well-attended round table was organized on the Popularization of biophysics among students and in connection with the economy.

President (2022-2025) of the Croatian Biophysical Society, and Secretary (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 issues "Chemoinformatics and Bioinformatics Tools in Structure-Activity Modeling in Molecular Sciences 1., 2. and 3." of International Journal of Molecular Sciences (IJMS) indexed in CC (IF 4.9, Q1 JCR, Q1 SJR)

Co-editor of the special issue "QSAR and QSPR: Recent Developments and Applications III, IV and V" of the journal Molecules indexed in the CC database (IF 4.6, Q2 JCR, Q1 SJR,)

MEMBERSHIP IN SCIENCE ORGANIZATIONS AND BODIES

1993-present, Croatian Biophysical Society, Zagreb

1992-present, Croatian Chemical Society, Zagreb

2000-present Croatian Society for Theoretical and Mathematical Biology, 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, 2021, 2022, 2023, 2024, 2025, 2026.

(2026) Member of Scientific Committee of 5th International Physics Conference in Bosnia and Herzegovina PHYCONBA 2026

Member of the Steering (2002-2009) and Advisory (2018-2022) Committee of the Croatian Biophysical Society

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

Member of several commissions for elections to scientific and professional positions at IRB, PMF, University of Osijek, Polytechnic in Bjelovar.

PAPERS

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

Co-author of **85** scientific papers published in scientific journals (**65** in **CC**, **>70 in WoS**)

More than **100** scientific contributions (posters or lectures) at international scientific conferences

More than **10** invited lectures at international scientific conferences in the last 10 years

CITATIONS OF PAPERS

(4/ 2026) - >**3100** citations (**2930** without self-citations) in *Web of Science* (*WoS*)

(4/ 2026) **H-index** = **31**, average citations per article in *WoS* **38.03**

(4/ 2026) - **12** papers cited more than 100 times in *Google Scholar*.

(4/2021) – more than **4600** citations in *Google Scholar* (**1700** citations since 2021), H-index = 36

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

(2022 –) member of the Editorial Board of the international scientific (CC) journal Discrete Mathematical Chemistry, https://dmc-journal.eu/index.php/dmc/about/editorialTeam

Member of the HRČAK Council since 2015, and I am currently a member of the fourth convocation (the mandate of the convocation lasts two years) https://hrcak.srce.hr/savjet-hrcka, and the work is defined by https://hrcak.srce.hr/docs /Pravilnik-Hrcak-20210705.pdf.

COMPUTER SKILLS

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

Programming skills

REVIEWING ACTIVITIES AND OTHER COMPETENCES

Reviewer for more than 80 scientific journals from *Current Contents* (mostly) and *Web of Science* such as Acta Chimica Slovenica, ARKIVOC, Bioorganic Medicinal Chemistry, Bioorganic Medicinal Chemistry Letters, Chemical Communications, *Chemical Reviews*, Chemical Biology & Drug Design, Chemosphere, Computers & Chemistry (now Computational Biology and Chemistry), Croatica Chemica Acta, International Journal of Molecular Sciences, Journal of Chemical Information and Modeling (and for J. of Chem. Inf. Comput. Sci.), Journal of Chemometrics, Journal of Chromatography A, Journal of Computational Chemistry, Journal of Environmental Monitoring, Journal of Molecular Graphics and Modelling, Molecular Diversity, Molecules, Organic & Biomolecular Chemistry, Journal of Physical Chemistry, Journal of Agricultural and Food Chemistry, Dalton Transactions, SAR and QSAR in Environmental Research, Molecular Informatics, Polymer, Royal Society of Chemistry Advances, Science of the Total Environment, Scientific Reports, etc.
The list/details of submitted/performed reviews since the launch of the PUBLONS service can be found at: https://publons.com/author/1202691/bono-lucic#profile (> **227** reviews and many editor records since 2009).

Reviewer of scientific projects (from Croatia, Macedonia, Bosnia and Herzegovina and Serbia)

Reviewer of UKF (Unity through knowledge Fund, http://www.ukf.hr/) scientific projects, Croatia, Zagreb

Reviewer of more than 15 IUPAC projects (2012-2019)

Reviewer of several EU scientific projects MSCA-DN (Marie Skłodowska-Curie Actions-Doctoral Networks) in several years

POSITIONS ON SOME RANKINGS OF SCIENTISTS FROM CROATIA

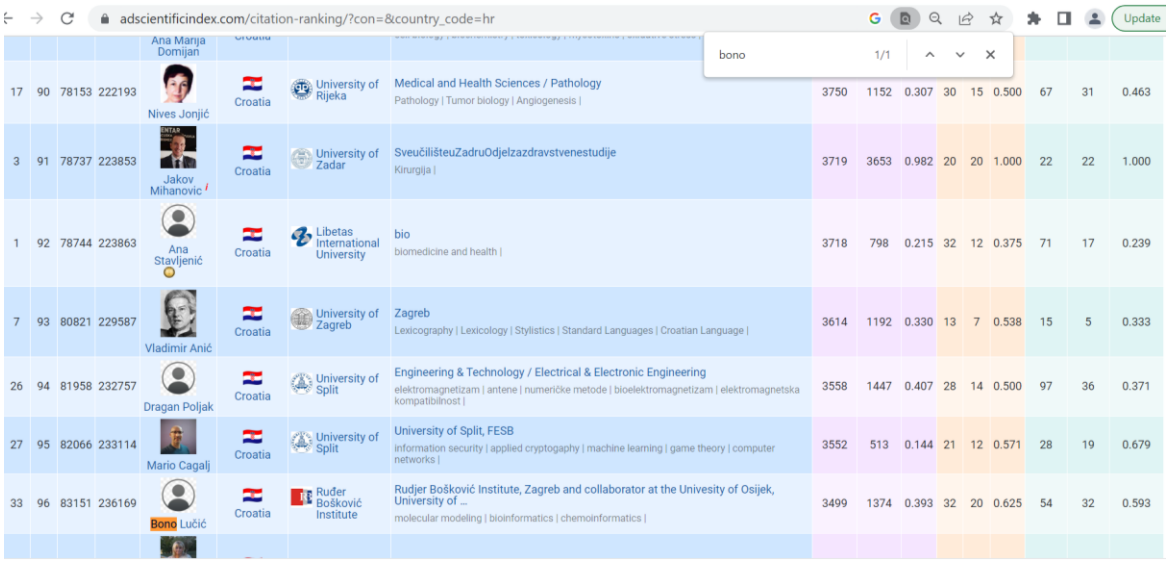
1) **According to the AD Scientific Index, ranked among the first 100 (69) of 2,000 Croatian scientists** according to total measured contributions based on data from the Google Scholar profile (6/2023)

AD Scientific Index - 2023 Croatia Top 2.000 Scientists								H INDEX			i10 INDEX			CITATION		
University	Country	Region	World	Name	Country	University	Subject	Total	Last 6 year	Last 6 year / total	Total	Last 6 year	Last 6 year / total	Total	Last 6 year	Last 6 year / total
26	65	62700	172189	Maja Mustapic	Croatia	Ruđer Bošković Institute	Staff Scientist, National Institute on Aging Extracellular vesicles | Neuroscience | Neurodegeneration |	33	24	0.727	56	45	0.804	3939	3007	0.763
4	66	63547	174417	Branko Grisogono	Croatia	University of Zagreb	Engineering & Technology / Earth Sciences boundary-layers | atmospheric buoyancy waves | coastal & mountain meteorology |	33	18	0.545	62	38	0.613	3414	1261	0.369
27	67	63787	175022	Robert Vianello	Croatia	Ruđer Bošković Institute	Senior Scientist and Group Leader at Ruđjer Boskovic Institute computational chemistry and biochemistry | enzymology | reactivity | drug design | functional materials |	33	22	0.667	87	61	0.701	3232	1845	0.571
1	68	66583	182851	Ana Stavljenić	Croatia	Libetas International University	bio biomedicine and health |	32	12	0.375	71	17	0.239	3718	798	0.215
28	69	66967	183900	Bono Lučić	Croatia	Ruđer Bošković Institute	Ruđjer Bošković Institute, Zagreb and collaborator at the Univesity of Osijek, University of ... molecular modeling | bioinformatics | chemoinformatics |	32	20	0.625	54	32	0.593	3499	1374	0.393
29	70	67419	185030	Saša Ceci	Croatia	Ruđer Bošković Institute	Natural Sciences / Physics Physics | Hadron physics | Particle physics |	32	30	0.938	46	39	0.848	3266	2991	0.916
11	71	67790	185951	Vera Vlahović Palčevski	Croatia	University of Rijeka	MedicinskifakultetSveučilištauRijeciKliničkibolničkicentarRijeka klinička farmakologija |	32	25	0.781	53	36	0.679	3050	1551	0.509
12	72	69734	191232	Sandra Kraljević Pavelić	Croatia	University of Rijeka	Natural Sciences / Molecular Biology & Genetics Proteomics | molecular mechanisms of disease | cancer therapy |	31	25	0.806	104	83	0.798	4231	2688	0.635
5	73	69762	191299	Mirko Orlic	Croatia	University of Zagreb	Engineering & Technology / Earth Sciences geophysics | physical oceanography |	31	20	0.645	80	41	0.513	4212	1430	0.340
21	74	70320	192812	Ilja Doršner	Croatia	University of Split	Natural Sciences / Physics High Energy Physics |	31	20	0.645	43	26	0.605	3789	1937	0.511
30	75	71053	194782	Marijan Gotic	Croatia	Ruđer Bošković Institute	znanstveni savjetnik, Institut "Ruđer Bošković", Zagreb, Hrvatska Sinteza i karakterizacija nanostrukturnih materijala |	31	21	0.677	56	41	0.732	3394	1325	0.390
31	76	71506	195987	Krunoslav Užarević	Croatia	Ruđer Bošković Institute	Ruđer Bošković Institute Green Chemistry | Mechanochemistry | Materials | MOF | Solid-State Science |	31	26	0.839	58	45	0.776	3171	2432	0.767
32	77	72276	197966	Tvrtko Smital	Croatia	Ruđer Bošković Institute	Natural Sciences / Biological Science biology | environmental toxicology |	31	18	0.581	52	35	0.673	2733	965	0.353
13	78	73098	200307	Biserka Mulac	Croatia	University of	SveučilišteuRijeciMedicinskifakultet	30	15	0.500	45	23	0.511	5751	1391	0.242

2) **According to the AD Scientific Index, ranked 97 out of 2000 Croatian scientists in terms of productivity** according to data from the Google Scholar profile (6/2023)

11	93	77405	209580	Jakob Pamić	Croatia	University of Zagreb	Engineering & Technology / Earth Sciences Geology | Historical Geology | Ophiolites | Magmatism | Pannonian Basin |	56	18	0.321	27	12	0.444	2798	661	0.236
39	94	77838	210666	Stjepko Fazinic	Croatia	Ruđer Bošković Institute	Ruđer Bošković Institute	56	24	0.429	23	14	0.609	1870	845	0.452
14	95	78067	211430	Astrid Krmpotić	Croatia	University of Rijeka	Medical and Health Sciences / Virology viral immunology |	55	50	0.909	36	25	0.694	4668	1545	0.331
22	96	79332	214681	Zoran Dogas	Croatia	University of Split	Medical and Health Sciences / Neuroscience Neuroscience | Control of breathing | Sleep medicine | Sleep disordered breathing | Obstructive sleep apnea |	55	34	0.618	25	20	0.800	2340	1310	0.560
40	97	80165	216868	Bono Lučić	Croatia	Ruđer Bošković Institute	Ruđjer Bošković Institute, Zagreb and collaborator at the Univesity of Osijek, University of ... molecular modeling | bioinformatics | chemoinformatics |	54	32	0.593	32	20	0.625	3499	1374	0.393
41	98	80442	217557	Sanja Kapitanovic	Croatia	Ruđer Bošković Institute	Natural Sciences / Molecular Biology & Genetics cancer genetics | personalized medicine |	54	20	0.370	30	13	0.433	2804	769	0.274

3) **According to the AD Scientific Index, he is ranked 96 out of 2,000 Croatian scientists by citations** based on data from the Google Scholar profile (6/2023)



LIST OF PAPERS – Bono Lučić (4/ 2026)

Scientific papers in *Web of Science* (*Current Contents*) journals.

1. Juretić, D.; Trinajstić, N.; Lučić, B. Protein Secondary Structure Conformations and Associated Hydrophobicity Scale. *J. Math. Chem.* **1993**, *14*, 35–45. doi:10.1007/BF01164453.

2. Juretić, D.; Lučić, B.; Trinajstić, N. Predicting Membrane Protein Secondary Structure: Preference Functions Method for Finding Optimal Conformational Parameters. *Croat. Chem. Acta* **1993**, *66*, 201–208.

3. Lučić, B.; Nikolić, S.; Trinajstić, N.; Juretić, D. The Structure-Property Models Can Be Improved Using the Orthogonalized Descriptors. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 532–538. doi:10.1021/ci00025a022.

4. Juretić, D.; Lučić, B.; Trinajstić, N. Secondary Structure Prediction Quality for Naturally Occurring Amino Acids in Soluble Proteins. *J. Mol. Struct. THEOCHEM* **1995**, *338*, 43–50. doi:10.1016/0166-1280(94)04047-V.

5. Amić, D.; Davidović-Amić, D.; Bešlo, D.; Lučić, B.; Trinajstić, N. Structure-activity correlation of flavone derivatives for inhibition of cAMP phosphodiesterase. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 1034–1038. doi:10.1021/ci00028a013.

6. Lučić, B.; Nikolić, S.; Trinajstić, N.; Jurić, A.; Mihalić, Z. A Structure-Property Study of the Solubility of Aliphatic-Alcohols in Water. *Croat. Chem. Acta* **1995**, *68*, 417–434.

7. Lučić, B.; Nikolić, S.; Trinajstić, N.; Juretić, D.; Jurić, A. Novel QSPR Approach to Physicochemical Properties of the Alpha-Amino-Acids. *Croat. Chem. Acta* **1995**, *68*, 435–450.

8. Trinajstić, N.; Nikolić, S.; Lučić, B.; Amić, D. On QSAR Modeling. *Acta Pharm.* **1996**, *45*, 24–263.

9. Klein, D.J.; Randić, M.; Babić, D.; Lučić, B.; Nikolić, S.; Trinajstić, N. Hierarchical Orthogonalization of Descriptors. *Int. J. Quantum Chem.* **1997**, *63*, 215–222. doi: 10.1002/(SICI)1097-461X(1997)63:1<215::AID-QUA22>3.0.CO;2-9.

10. Amić, D.; Davidović-Amić, D.; Bešlo, D.; Lučić, B.; Trinajstić, N. A simple QSAR model for trypsin aminopeptidase inhibitory flavonoids. *Croat. Chem. Acta* **1997**, *70*, 905–911.

11. Trinajstić, N.; Nikolić, S.; Lučić, B.; Amić, D.; Mihalić, Z. The detour matrix in chemistry. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 631–638. doi:10.1021/ci960149n.

12. Amić, D.; Davidović-Amić, D.; Bešlo, D.; Trinajstić, N.; Lučić, B. 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.* **1997**, *37*, 581–586. doi:10.1021/ci960158w.

13. Juretić, D.; Zucić, D.; Lučić, B.; Trinajstić, N. Preference Functions for Prediction of Membrane-buried Helices in Integral Membrane Proteins. *Comput. Chem.* **1998**, *22*, 279–294.

14. Amić, D.; Davidović-Amić, D.; Bešlo, D.; Lučić, B.; Trinajstić, N. QSAR of flavylium salts as inhibitors of xanthine oxidase. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 815–818.

15. Amić, D.; Bešlo, D.; Lučić, B.; Nikolić, S.; Trinajstić, N. The vertex-connectivity index revisited. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 819–822.

16. Amić, D.; Davidović-Amić, D.; Bešlo, D.; Lučić, B.; Trinajstić, N. Prediction of pK Values, half-lives and electronic spectra of flavylium salts from molecular structure. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 967–973.

17. Lučić, B.; Trinajstić, N.; Sild, S.; Karelson, M.; Katritzky, A.R. A new efficient approach for variable selection based on multiregression: prediction of gas chromatographic retention time and response factors. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 610–621.

18. Lučić, B.; Trinajstić, N. Multivariate regression outperforms several robust architectures of neural networks in QSAR modeling. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 121–132. doi:10.1021/ci980090f.

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

20. Basak, S.C.; Gute, B.D.; Lučić, B.; Nikolić, S.; Trinajstić, N. A comparative QSAR study of benzamidines complement-inhibitory activity and benzene derivatives acute toxicity. *Comput. Chem.* **2000**, *24*, 181–191.

21. Katritzky, A.R.; Chen, K.; Wang, Y.; Karelson, M.; Lučić, B.; Trinajstić, N.; Suzuki, T.; Schüürmann, G. Prediction of liquid viscosity for organic compounds by a quantative structure-property relationship. *J. Phys. Org. Chem.* **2000**, *13*, 80–86.

22. Lučić, B.; Lukovits, I.; Nikolić, S.; Trinajstić, N. Distance-related indexes in the quantitative structure-property relationship modeling. *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 527–535.

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