Огляд цитування публікацій, які увійшли до роботи

№ п/п	Назва публікації	Кількість посилань згідно з базами даних		
		Web of Science	Scopus	Google Scholar
1	2	3	4	5
Колективні монографії				
1	Dataset Modelability by QSAR: Continuous Response Variable. *Practical Aspects of Computational Chemistry V* / A. Golbraikh et.al. Springer International Publishing, 2022. P. 233-253	-	-	1
2	Structural, Physicochemical and Stereochemical Interpretation of QSAR Models Based on Simplex Representation of Molecular Structure. *Advances in QSAR modeling: Applications in Pharmaceutical, Chemical, Food, Agricultural and Environmental Sciences* / P. Polischuk et. al. Ed. by K. Roy. Cham: Springer, 2017. P. 107–147	-	2	4
3	Application of Computational Techniques in Pharmacy and Medicine / Ed. by L. Gorb, V. Kuz'min, E. Muratov. Springer, Dordrecht, Hiedelberg, New York, London, 2014. 550 p	-	6	26
4	Quantitative Structure-Property Relationship Analysis of Drugs' Pharmacokinetics Withinthe Framework of Biopharmaceutics Classification System Using Simplex Representation of Molecular Structure. *Application of Computational Techniques in Pharmacy and Medicine* / N. Ya. Golovenko et. al. Ed. by L. Gorb, V. Kuz'min, E. Muratov. Springer, Dordrecht, Hiedelberg, New York, London, 2014. P. 461–499.	1	1	0
5	New advances in QSPR/QSAR analysis of nitrocompounds: solubility, lipophilicity and toxicity. *Practical aspects of computational chemistry II* / L. N. Ognichenko Ed. by J. Leszczynski, M. Shukla. Netherlands: Springer, 2012. P. 279–334	-	-	6

1	2	3	4	5
6	Progress in Prediction of Environmentally Important Phisicochemical Properties of Energetic Materials: Applications of Quantum-Chemical Calculations. *Practical aspects of computational chemistry II* / L. Gorb et. al. Ed. by J. Leszczynski, M. Shukla. London: Springer, 2012. P. 335–359.	-	-	7
7	Virtual Screening and Molecular Design Based on Hierarchical Qsar Technology. *Challenges and Advances in Computational Chemistry and Physics/* V.E. Kuz'min et. al. Dordrecht: Springer, 2010. P. 127–176.	27	24	36
8	Nyporko A. Yu. , Blume Ya. B. Spatial distribution of tubulin mutations conferring resistance to antimicrotubular compounds. *The Plant Cytoskeleton: a Key Tool for Agro-Biotechnology* Ed. by Ya. B. Blume, W. V. Baird, A. I. Yemets, D. Breviario. Dordrecht: Springer, 2008. P. 397–417	10	-	13
9	Michalkova A. , Gorb L. , Leszczynski J. Interactions of model organic species and explosives with clay minerals. *Energetic materials: Part 1. Decomposition, crystal and molecular properties* Ed.by P. A. Politzer and J. S. Murray. Elsevier Science, 2003. V. 12. P. 341–388.	-	1	1
10	Gorb L., Leszczynski J. Chemistry of the Liquid State: Current Trends in Quantum-Chemical Modeling. *Computational Chemistry: reviews of current trends* World Scientific, 1999. V. 3. P. 179–213.	-	-	2
Cmammi				
11	Sviatenko L. K. , Gorb L. , Leszczynski J. NTO degradation by direct photolysis: DFT study. *Structural Chemistry*. 2023. Vol. 34, No 1. P. 23–31. DOI: https://doi.org/10.1007/s11224-022-01923-1 (data of access 24.04.2024)	5	5	5

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12	Sviatenko L.K., Gorb L., Leszczynski J. Role of Molecular Singlet Oxygen in Photochemical Degradation of NTO: DFT Study. *Journal of Physical Chemistry A*. 2023. Vol. 127, No 12. P. 2688–2696. DOI: https://doi.org/10.1021/acs.jpca.2c08225 (data of access 24.04.2024)	3	3	3
13	Aldo-keto reductase may contribute to glyphosate resistance in Lolium rigidum / F. Y. Zhou et al. *Pest Management Science*. 2023. Vol. 79, No 4. P. 1528–1537. DOI: https://doi.org/10.1002/ps.7325 (data of access 24.04.2024)	2	2	2
14	Influence of Chemical Structure of Molecules on Blood–Brain Barrier Permeability on the Pampa Model / G.P. Kosinska et al. *Theoretical and Experimental Chemistry*. 2022. Vol. 58, No 1. P. 29–33. DOI: https://doi.org/10.1007/s11237-022-09718-5 (data of access 24.04.2024)	0	1	0
15	A naturally evolved mutation (Ser59Gly) in glutamine synthetase confers glufosinate resistance in plants / C. Zhang et al. *Journal of experimental botany*. 2022. Vol. 73, No 7. P. 2251–2262. DOI: https://doi.org/10.1093/jxb/erac008 (data of access 24.04.2024)	16	16	19
16	Gorb L., Ilchenko M., Leszczynski J. Decomposition of 2,4,6,-trinitrotoluene (TNT) and 5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO) by $Fe_{13}O_{13}$ nanoparticle: density functional theory study. *Environmental science and pollution research*. 2022. Vol. 29, No 45. P. 68522–68531. DOI: https://doi.org/10.1007/s11356-022-20547-w (data of access 24.04.2024)	2	2	2
17	PreS/MD: Predictor of Sensitization Hazard for Chemical Substances Released From Medical Devices / V.M. Alves et al. *Toxicological Sciences*. 2022. Vol. 189. P. 250–259. DOI: https://doi.org/10.1093/toxsci/kfac078 (data of access 24.04.2024)	2	2	0

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18	Integrated approach to elucidate metal-implant related adverse outcome pathways // J.M.T. Beasley et al. *Regulatory Toxicology and Pharmacology*. 2022. Vol. 36. P. 105277. DOI: https://doi.org/10.1016/j.yrtph.2022.105277 (data of access 24.04.2024)	2	2	2
19	Sviatenko L.K., Gorb L., Leszczynski J. NTO Degradation by nitroreductaze: A DFT study. *Journal of Physical Chemistry B.* 2022. Vol. 126, No 32. P. 5991–6006. DOI: https://doi.org/10.1021/acs.jpcb.2c04153 (data of access 24.04.2024)	1	1	1
20	STopTox: an in Silico Alternative to Animal Testing for Acute Systemic and Topical Toxicity / J. Borba et al. *Environmental health perspectives*. 2022. Vol. 130, No 1(2?). P. 027012-1. DOI: https://doi.org/10.1289/EHP9341 (data of access 24.04.2024)	29	37	42
21	BeeToxAI: An Artificial Intelligence-Based Web App to Assess Acute Toxicity of Chemicals to Honey bees / J. T. Moreira-Filho et al. *Artificial Intelligence in the Life Sciences*. 2021. Vol. 1. P. 100013. DOI: https://doi.org/10.1016/j.ailsci.2021.100013 (data of access 24.04.2024)	-	13	20
22	Novel computational models offer alternatives to animal testing for assessing eye irritation and corrosion potential of chemicals / A. Silva et al. *Artificial Intelligence in the Life Sciences*. 2021. Vol. 1. P. 100028. DOI: https://doi.org/10.1016/j.ailsci.2021.100028 (data of access 24.04.2024)	-	11	12
23	An ABCC-type transporter endowing glyphosate resistance in plants / L. Pan et al. *Proceedings of the National Academy of Sciences of the United States of America*. 2021. Vol. 118, No 16. e2100136118. DOI: https://doi.org/10.1073/pnas.210013611 (data of access 24.04.2024)	79	84	101

1	2	3	4	5
24	Catalytic role of solvated electron in the spontaneous degradation of insensitive munition compounds: computational chemistry investigation / L. K. Sviatenko et al. *Structural Chemistry*. 2021. Vol. 32, No. 2. P. 521–527. DOI: https://doi.org/10.1007/s11224-020-01710-w (data of access 24.04.2024)	2	3	3
25	Gelmboldt V., Ognichenko L., Shyshkin I., Kuz'min V. QSPR models for water solubility of ammonium hexafluorosilicates: analysis of the effects of hydrogen bonds. *Structural Chemistry*. 2021. Vol. 32, No 1. P. 309–319. DOI: https://doi.org/10.1007/s11224-020-01652-3 (data of access 24.04.2024)	7	7	11
26	Chemical safety assessment of transformation products of landfill leachate formed during the Fenton process / L. de Morais E Silva et al. *Journal of Hazardous Materials*. 2021. Vol. 419. P. 126438. DOI: https://doi.org/10.1016/j.jhazmat.2021.126438 (data of access 24.04.2024)	5	7	9
27	Computer-assisted discovery of compounds with insecticidal activity against Musca domestica and Mythimna separate / G. C. Soares Rodrigues et al. *Food and Chemical Toxicology*. 2021. Vol. 147. P. 111899. DOI: https://doi.org/10.1016/j.fct.2020.111899 (data of access 24.04.2024)	7	10	10
28	CATMoS: Collaborative acute toxicity modeling suite / K. Mansouri et al. *Environmental health perspectives*. 2021. Vol. 129, No 4. P. 047013. DOI: https://doi.org/10.1289/EHP8495 (data of access 24.04.2024)	63	63	83
29	Simplex representation of molecular structure as universal QSAR/QSPR tool / V. Kuz'min et al. *Structural Chemistry*. 2021. Vol. 32. P. 1365–1392. DOI: https://doi.org/10.1007/s11224-021-01793-z (data of access 24.04.2024)	9	12	23

1	2	3	4	5
30	Curated Data In — Trustworthy In Silico Models Out: The Impact of Data Quality on the Reliability of Artificial Intelligence Models as Alternatives to Animal Testing / V. M. Alves et al. *Alternatives to Laboratory Animals*. 2021. Vol. 49, No 3. P. 73–82. DOI: https://doi.org/10.1177/02611929211029635 (data of access 24.04.2024)	16	21	29
31	Large-scale modeling of multispecies acute toxicity end points using consensus of multitask deep learning methods / S. Jain et al. *Journal of Chemical Information and Modeling*. 2021. Vol. 61, No 2. P. 653–663. DOI: https://doi.org/10.1021/acs.jcim.0c01164 (data of access 24.04.2024)	27	30	41
32	Quantitative Structure-Activity Relationship Modeling and Docking of Monoterpenes with Insecticidal Activity Against Reticulitermes chinensis Snyder and Drosophila melanogaster / G. Soares Rodrigues et al. *Journal of Agricultural and Food Chemistry*. 2020. Vol. 68, No 16. P. 4687–4698. DOI: https://doi.org/10.1021/acs.jafc.0c00272 (data of access 24.04.2024)	14	15	17
33	SCAM detective: accurate predictor of small, colloidally aggregating molecules / V. M. Alves et al. *Journal of Chemical Information and Modeling*. 2020. Vol. 60, No 8. P. 4056–4063. DOI: https://doi.org/10.1021/acs.jcim.0c00415 (data of access 24.04.2024)	16	20	28
34	QSAR Without Borders / E. Muratov et al. *Chemical Society Reviews.* 2020. Vol. 49, No 11. P. 3525–3564. DOI: https://doi.org/10.1039/D0CS00098A (data of access 24.04.2024)	363	412	589
35	Compara: Collaborative modeling project for androgen receptor activity / K. Mansouri et al. *Environmental health perspectives.* 2020. Vol. 128, No 2. P. 027002. DOI: https://doi.org/10.1289/EHP5580 (data of access 24.04.2024)	106	116	137

1	2	3	4	5
36	Adsorption of nitrogen-containing compounds on hydroxylated α-quartz surfaces / O. Tsendra et al. *RSC ADVANCES*. 2019. Vol. 9, No 62. P. 36066–36074. DOI: https://doi.org/10.1039/C9RA07130J (data of access 24.04.2024)	2	2	1
37	Aldo-keto Reductase Metabolizes Glyphosate and Confers Glyphosate Resistance in Echinochloa colona / L. Pan et al. *Plant Physiology*. 2019. Vol. 181, No 4. P. 1519–1534. DOI: https://doi.org/10.1104/pp.19.00979 (data of access 24.04.2024)	-	94	118
38	Oy Vey! A Comment on "Machine Learning of Toxicological Big Data Enables Read-Across Structure Activity Relationships Outperforming Animal Test Reproducibility / V. M. Alves et al. *Toxicological sciences*. 2019. Vol. 167, No 1. P. 3–4. 227-238? DOI: https://doi.org/10.1093/toxsci/kfy286 (data of access 24.04.2024)	17	20	30
39	Role of singlet oxygen in the degradation of selected insensitive munitions compounds: A comprehensive, quantum chemical investigation / L. K. Sviatenko et al. *Journal of Physical Chemistry A*. 2019. Vol. 123, No 35. P. 7597–7608. DOI: https://doi.org/10.1021/acs.jpca.9b01772 (data of access 24.04.2024)	5	5	6
40	A density functional theory investigation of degradation of Nitroguanidine in the photoactivated triplet state / L.K. Sviatenko et al. *Journal of molecular modeling*. 2019. Vol. 25, No 12. P. 372 DOI: https://doi.org/10.1007/s00894-019-4252-8 (data of access 24.04.2024)	0	1	0
41	Predicting Adverse Drug Effects from Literature- and Database-Mined Assertions / M. K. La et al. *Drug Safety*. 2018. Vol. 41, No 11. P. 1059–1072. DOI: https://doi.org/10.1007/s4026 (data of access 24.04.2024)	1	1	3

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42	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structure-Activity Relationships / Y. S. Low et al. *Journal of Chemical Information and Modeling.* 2018. Vol. 58, No 11. P. 2203–2213. DOI: https://doi.org/10.1021/acs.jcim.8b00450 (data of access 24.04.2024)	4	5	8
43	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment / V. M. Alves et al. *ACS Sustainable Chemistry & Engineering*. 2018. Vol. 6, No 3. P. 2845–2859. DOI: https://doi.org/10.1021/acssuschemeng.7b04220 (data of access 24.04.2024)	31	30	37
44	Multi-Descriptor Read Across (MuDRA): A Simple and Transparent Approach for Developing Accurate Quantitative Structure–Activity Relationship Models / V. M. Alves et al. *Journal of chemical information and modeling.* 2018. Vol. 58, No 6. P. 1214–1223. DOI: https://doi.org/10.1021/acs.jcim.8b00124 (data of access 24.04.2024)	35	36	49
45	Chemotext: A Publicly-Accessible, Integrated Cheminformatics Portal / S. J. Capuzzi et al. *Journal of chemical information and modeling*. 2018. Vol. 58, No 2. P. 212–218. DOI: https://doi.org/10.1021/acs.jcim.7b00589 (data of access 24.04.2024)	30	35	46
46	Development of Web and Mobile Applications for Chemical Toxicity Prediction / V. M. Alves et al. *Journal of the Brazilian Chemical Society.* 2018. Vol. 29. P. 982–988. DOI: https://doi.org/10.21577/0103-5053.20180013 (data of access 24.04.2024)	8	10	18
47	Glyphosate Resistance in Tridax procumbens via a Novel EPSPS Thr-102-Ser Substitution / J. Li et al. *Journal of Agricultural and Food Chemistry*. 2018. Vol. 66, No 30. P. 7880–7888. DOI: https://doi.org/10.1021/acs.jafc.8b01651 (data of access 24.04.2024)	-	40	51

1	2	3	4	5
48	Novel α-tubulin mutations conferring resistance to dinitroaniline herbicides in Lolium rigidum / Z. Chu et al. *Frontiers in Plant Science*. 2018. Vol. 9. P. 97. DOI: https://doi.org/10.3389/fpls.2018.00097 (data of access 24.04.2024)	39	41	53
49	A. Conditional Toxicity Value (CTV) Predictor: An In Silico Approach for Generating Quantitative Risk Estimates for Chemicals / J. A. Wignall et al. *Environmental health perspectives*. 2018. Vol. 126, No 5. P. 057008. DOI: https://doi.org/10.1289/EHP2998 (data of access 24.04.2024)	51	54	66
50	Chemical toxicity prediction for major classes of industrial chemicals: Is it possible to develop universal models covering cosmetics, drugs, and pesticides? / V. M. Alves et al. *Food and Chemical Toxicology*. 2018. Vol. 112. Pa. 526–534. DOI: https://doi.org/10.1016/j.fct.2017.04.008 (data of access 24.04.2024)	45	53	66
51	A quantum chemical based toxicity study of estimated reduction potential and hydrophobicity in series of nitroaromatic compounds / A. Gooch et al. *SAR and QSAR in Environmental Research*. 2017. Vol. 28, No 2. P. 133–150. DOI: https://doi.org/10.1080/1062936X.2017.1286687 (data of access 24.04.2024)	13	12	14
52	In vivo toxicity of nitroaromatics: A comprehensive quantitative structure–activity relationship study / A. Gooch et al. *Environmental toxicology and chemistry*. 2017. Vol. 36, No 8. P. 2227–2233. DOI: https://doi.org/10.1002/etc.3761 (data of access 24.04.2024)	23	25	34
53	Pred-Skin: A Fast and Reliable Web Application to Assess SkinSensitization Effect of Chemicals / R. C. Braga et al. *Journal of chemical information and modeling*. 2017. Vol. 57, No 5. P. 1013–1017. DOI: https://doi.org/10.1021/acs.jcim.7b00194 (data of access 24.04.2024)	54	62	80

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54	Capuzzi S. J., Muratov E. N., Tropsha A. Phantom PAINS: Problems with the Utility of Alerts for Pan-Assay Interference CompoundS. *Journal of chemical information and modeling*. 2017. Vol. 57, No 3. P. 417–427. DOI: https://doi.org/10.1021/acs.jcim.6b00465 (data of access 24.04.2024)	175	186	229
55	Chembench: A Publicly-Accessible, Integrated Cheminformatics Portal / S. J. Capuzzi et al. *Journal of chemical information and modeling*. 2017. Vol. 57, No 2. P. 105–108. DOI: https://doi.org/10.1021/acs.jcim.6b00462 (data of access 24.04.2024)	42	46	60
56	In silicokinetics of alkaline hydrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX): M06-2X investigation / L. K. Sviatenko et al. *Environmental Science: Processes & Impacts*. 2017. Vol. 19, No 3. P. 388–394. DOI: https://doi.org/10.1039/C6EM00565A (data of access 24.04.2024)	16	15	19
57	Structure and redox properties of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) adsorbed on a silica surface. A DFT M05 computational study / L. K. Sviatenko et al. *Journal of Chemistry and Technologies*. 2017. Vol. 25, No 1. P. 1–8. DOI: https://doi.org/10.15421/081701 (data of access 24.04.2024)	1	-	1
58	Activity prediction and identification of mis-annotated chemical compounds using extreme descriptors / P. Borysov et al. *Journal of Chemometrics*. 2016. Vol. 30, No 3. P. 99–108. DOI: https://doi.org/10.1002/cem.2776 (data of access 24.04.2024)	3	4	6
59	Novel Enhanced Applications of QSPR Models: Temperature Dependence of Aqueous Solubility / K. Klimenko et al. *Journal of Computational Chemistry*. 2016. Vol. 37, No 22. P. 2045–2051. DOI: https://doi.org/10.1002/jcc.24424 (data of access 24.04.2024)	12	13	20

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60	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization / V. Alves et al. *Green Chemistry*. 2016. Vol. 18, No 24. P. 6501–6515.18. DOI: https://doi.org/10.1039/C6GC01836J (data of access 24.04.2024)	40	45	51
61	Structural and physico-chemical interpretation (SPCI) of QSAR models and its comparison with MMP analysis / P. Polishchuk et al. *Journal of Chemical Information and Modeling*. 2016. Vol. 56, No 8. P. 1455–1469. DOI: https://doi.org/10.1021/acs.jcim.6b00371 (data of access 24.04.2024)	30	33	54
62	QSAR Modeling and Prediction of Drug-Drug Interactions / A. V. Zakharov et al. *Molecular Pharmaceutics*. 2016. Vol. 13, No 2. P. 545–556. DOI: https://doi.org/10.1021/acs.molpharmaceut.5b00762 (data of access 24.04.2024)	51	55	72
63	Alarms About Structural Alerts / V. Alves et al. *Green Chemistry*. 2016. Vol. 18, No 16. P. 4348–4360. DOI: https://doi.org/10.1039/C6GC01492E (data of access 24.04.2024)	84	95	131
64	Fourches D., Muratov E. N., Tropsha A. Trust, But Verify II: A Practical Guide to Chemogenomics Data Curation. *Journal of chemical information and modeling*. 2016. Vol. 56, No7. P. 1243–1252. DOI: https://doi.org/10.1021/acs.jcim.6b00129 (data of access 24.04.2024)	183	204	270
65	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project / K. Mansouri et al. *Environmental health perspectives.* 2016. Vol. 124, No 7. P. 1023–1033. DOI: https://doi.org/10.1289/ehp.1510267 (data of access 24.04.2024)	218	252	311
66	Modelling of compound combination effects and applications to efficacy and toxicity: state-of-the-art, challenges and perspectives / K. Bulusu et al. *Drug Discovery Today*. 2016. Vol. 21, No 2. P. 225–238. DOI: https://doi.org/10.1016/j.drudis.2015.09.003 (data of access 24.04.2024)	117	129	192

1	2	3	4	5
67	Adsorption of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) on a soil organic matter. A DFT M05 computational study / L. K. Sviatenko et al. *Chemosphere*. 2016. Vol. 148. P. 294–299. DOI: https://doi.org/10.1016/j.chemosphere.2016.01.011 (data of access 24.04.2024)	7	8	13
68	Computational assessment of environmental hazards of nitroaromatic compounds: influence of the type and position of aromatic ring substituents on toxicity / O. V. Tinkov et al. *Structural Chemistry*. 2016. Vol. 27, No 1. P. 191–198. DOI: https://doi.org/10.1007/s11224-015-0715-4 (data of access 24.04.2024)	12	12	13
69	In silico alkaline hydrolysis of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: Density functional theory investigation / L. K. Sviatenko et al. *Environmental Science & Technology*. 2016. Vol. 50, No 18. P. 10039–10046. DOI: https://doi.org/10.1021/acs.est.5b06130 (data of access 24.04.2024)	11	11	16
70	Radical decomposition of 2,4-dinitrotoluene (DNT) at conditions of advanced oxidation. Computational study / L. K. Sviatenko et al. *Journal of Chemistry and Technologies*. 2016. Vol. 24, No 2. P. 56–61. DOI: https://doi.org/10.15421/081608 (data of access 24.04.2024)	1	-	1
71	Two-electron reduction of nitroaromatic compounds by flavin mononucleotide. DFT computational study / L. K. Sviatenko et al. *Journal of Chemistry and Technologies*. 2016. Vol. 24, No 1. P. 1–6. DOI: https://doi.org/10.15421/081601 (data of access 24.04.2024)	3	-	4
72	Theoretical study on alkaline hydrolysis of trinitrotoluene: later steps / L. K. Sviatenko et al. *Journal of Chemistry and Technologies*. 2015. Vol. 23, No 1. P. 1–7. DOI: https://doi.org/10.15421/081501 (data of access 24.04.2024)	1	-	3

1	2	3	4	5
73	Sviatenko L. K., Gorb L., Okovytyy S. Structure and redox properties of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) adsorbed on a silica surface. M05 computational study. *JOURNAL of chemistry and technologies*. 2015. Vol. 23, No 2. P. 1–9. DOI: https://doi.org/10.15421/081511 (data of access 24.04.2024)	1	-	3
74	Structure and redox properties of 5-amino-3-nitro-1H-1,2,4-triazole (ANTA) adsorbed on a silica surface: A DFT M05 computational study / L. K. Sviatenko et al. *Journal of Physical Chemistry A.* 2015. Vol. 119, No 29. P. 8139–8145. DOI: https://doi.org/10.1021/acs.jpca.5b03393 (data of access 24.04.2024)	15	13	15
75	Are the reduction and oxidation properties of nitrocompounds dissolved in water different from those produced when adsorbed on a silica surface? An DFT M05-2X computational study / L. K. Sviatenko et al. *Journal of Computational Chemistry*. 2015. Vol. 36, No 14. P. 1029–1035. DOI: https://doi.org/10.1002/jcc.23878 (data of access 24.04.2024)	12	10	15
76	Alkaline hydrolysis of hexahydro-1,3,5-trinitro-1,3,5-triazine: M06-2X investigation / L. K. Sviatenko et al. *Chemosphere.* 2015. Vol. 134. P. 31–38. DOI: https://doi.org/10.1016/j.chemosphere.2015.03.064 (data of access 24.04.2024)	10	9	15
77	Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds / V. Alves et al. *Toxicology and Applied Pharmacology.* 2015. Vol. 284, No 2. P. 262–272. DOI: https://doi.org/10.1016/j.taap.2014.12.014 (data of access 24.04.2024)	56	63	85
78	Pred-hERG: A Novel web-Accessible Computational Tool for Predicting Cardiac Toxicity / R. Braga et al. *Molecular Informatics*. 2015. Vol. 34, No 10. P. 698–701. DOI: https://doi.org/10.1002/minf.201500040 (data of access 24.04.2024)	127	146	172

1	2	3	4	5
79	Fourches D., Muratov E., Tropsha A. Curation of chemogenomics data. *Nature chemical Biology*. 2015. Vol. 11, No 8. P. 535. DOI: https://doi.org/10.1038/nchembio.1881 (data of access 24.04.2024)	136	152	196
80	Predicting chemically-induced skin reactions. Part II: QSAR models of skin permeability and the relationships between skin permeability and skin sensitization / V. Alves et al. *Toxicology and Applied Pharmacology*. 2015. Vol. 284, No 2. P. 273–280. DOI: https://doi.org/10.1016/j.taap.2014.12.013 (data of access 24.04.2024)	47	57	68
81	In silico kinetics and mechanism of an interaction of cis-2-butene-1,4-dial with 2'-deoxycytidine / L. K. Sviatenko et al. *Chemical Research in Toxicology*. 2014. Vol. 27, No 6. P. 981–989. DOI: https://doi.org/10.1021/tx5000427 (data of access 24.04.2024)	2	2	5
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98	Does Rational Selection of Training and Test Sets Improve the Outcome of QSAR Modeling? / T. M. Martin et al. *Journal of chemical information and modeling.* 2012. Vol. 52, No 10. P. 2570–2578. DOI: https://doi.org/10.1021/ci300338w (data of access 24.04.2024)	202	223	303
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122	Kuz'min V. E., Artemenko A. G., Muratov E. N. Hierarchical QSAR technology based on the Simplex representation of molecular structure. *Journal of Computer - aided Molecular design.* 2008. Vol. 22, No 6. P. 403–421. DOI: https://doi.org/10.1007/s10822-008-9179-6 (data of access 24.04.2024)	114	119	188
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Загальна кількість цитувань		**6519**	**7352**	**9839**
h-індекс		**41**	**43**	**49**