Bakhtiyor Rasulev

List of Publications by Year
in descending order

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118 papers	3,642 citations	159358 30 h-index	143772 57 g-index
124 all docs	124 docs citations	124 times ranked	4079 citing authors

#	Article	IF	Citations
1	Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. Nature Nanotechnology, 2011, 6, 175-178.	15.6	654
2	Advancing risk assessment of engineered nanomaterials: Application of computational approaches. Advanced Drug Delivery Reviews, 2012, 64, 1663-1693.	6.6	186
3	Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. Nanoscale, 2015, 7, 2154-2198.	2.8	163
4	Zeta Potential for Metal Oxide Nanoparticles: A Predictive Model Developed by a Nano-Quantitative Structureâ€“Property Relationship Approach. Chemistry of Materials, 2015, 27, 2400-2407.	3.2	154
5	Towards understanding mechanisms governing cytotoxicity of metal oxides nanoparticles: Hints from nano-QSAR studies. Nanotoxicology, 2015, 9, 313-325.	1.6	147
6	Prediction of rate constants for radical degradation of aromatic pollutants in water matrix: A QSAR study. Chemosphere, 2009, 75, 1128-1134.	4.2	122
7	Immunotoxicity of nanoparticles: a computational study suggests that CNTs and C₆₀ fullerenes might be recognized as pathogens by Toll-like receptors. Nanoscale, 2014, 6, 3488-3495.	2.8	97
8	From basic physics to mechanisms of toxicity: the â€œliquid dropâ€•approach applied to develop predictive classification models for toxicity of metal oxide nanoparticles. Nanoscale, 2014, 6, 13986-13993.	2.8	92
9	A Quantitative Structure-Activity Relationship (QSAR) Study of the Antioxidant Activity of Flavonoids. QSAR and Combinatorial Science, 2005, 24, 1056-1065.	1.5	88
10	Structure-toxicity relationships of nitroaromatic compounds. Molecular Diversity, 2006, 10, 233-245.	2.1	79
11	Novel approach for efficient predictions properties of large pool of nanomaterials based on limited set of species: nano-read-across. Nanotechnology, 2015, 26, 015701.	1.3	61
12	Receptor- and ligand-based study of fullerene analogues: comprehensive computational approach including quantum-chemical, QSAR and molecular docking simulations. Organic and Biomolecular Chemistry, 2013, 11, 5798.	1.5	60
13	Extraordinarily Adaptive Properties of the Genetically Encoded Amino Acids. Scientific Reports, 2015, 5, 9414.	1.6	54
14	QSAR modeling of acute toxicity by balance of correlations. Bioorganic and Medicinal Chemistry, 2008, 16, 5999-6008.	1.4	53
15	Improved model for fullerene C60 solubility in organic solvents based on quantum-chemical and topological descriptors. Journal of Nanoparticle Research, 2011, 13, 3235-3247.	0.8	51
16	Nano-QSAR modeling for ecosafe design of heterogeneous TiO₂-based nano-photocatalysts. Environmental Science: Nano, 2018, 5, 1150-1160.	2.2	51
17	Refractive indices of diverse data set of polymers: A computational QSPR based study. Computational Materials Science, 2017, 137, 215-224.	1.4	45
18	How the toxicity of nanomaterials towards different species could be simultaneously evaluated: a novel multi-nano-read-across approach. Nanoscale, 2018, 10, 582-591.	2.8	45

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19	Multiplicative SMILES-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2008, 457, 332-336.	1.2	43
20	Room temperature synthesis of PbSe quantum dots in aqueous solution: stabilization by interactions with ligands. Nanoscale, 2012, 4, 1312.	2.8	39
21	In Silico Assessment of ADME Properties: Advances in Caco-2 Cell Monolayer Permeability Modeling. Current Topics in Medicinal Chemistry, 2019, 18, 2209-2229.	1.0	38
22	Additive SMILES based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2007, 444, 209-214.	1.2	37
23	Advantages and limitations of classic and 3D QSAR approaches in nano-QSAR studies based on biological activity of fullerene derivatives. Journal of Nanoparticle Research, 2016, 18, 256.	0.8	37
24	QSPR Modeling of the Refractive Index for Diverse Polymers Using 2D Descriptors. ACS Omega, 2018, 3, 13374-13386.	1.6	36
25	A chemoinformatics approach for the characterization of hybrid nanomaterials: safer and efficient design perspective. Nanoscale, 2019, 11, 11808-11818.	2.8	35
26	Predicting glass transition of amorphous polymers by application of cheminformatics and molecular dynamics simulations. Polymer, 2021, 218, 123495.	1.8	35
27	The way to cover prediction for cytotoxicity for all existing nano-sized metal oxides by using neural network method. Nanotoxicology, 2017, 11, 475-483.	1.6	34
28	Evaluating genotoxicity of metal oxide nanoparticles: Application of advanced supervised and unsupervised machine learning techniques. Ecotoxicology and Environmental Safety, 2019, 185, 109733.	2.9	34
29	Modeling of photooxidative degradation of aromatics in water matrix; combination of mechanistic and structural-relationship approach. Chemical Engineering Journal, 2014, 257, 229-241.	6.6	32
30	A QSAR Toxicity Study of a Series of Alkaloids with the Lycoctonine Skeleton. Molecules, 2004, 9, 1194-1207.	1.7	31
31	Molecular modelling and QSAR analysis of the estrogenic activity of terpenoids isolated fromFerulaplants. SAR and QSAR in Environmental Research, 2007, 18, 663-673.	1.0	31
32	QSAR Modeling of Acute Toxicity for Nitrobenzene Derivatives Towards Rats: Comparative Analysis by MLRA and Optimal Descriptors. QSAR and Combinatorial Science, 2007, 26, 686-693.	1.5	30
33	Coral: QSPR modeling of rate constants of reactions between organic aromatic pollutants and hydroxyl radical. Journal of Computational Chemistry, 2012, 33, 1902-1906.	1.5	30
34	Aconitum and Delphinium sp. alkaloids as antagonist modulators of voltage-gated Na+ channels. Computational Biology and Chemistry, 2008, 32, 88-101.	1.1	29
35	Aconitum and Delphinium alkaloids of curare-like activity. QSAR analysis and molecular docking of alkaloids into AChBP. European Journal of Medicinal Chemistry, 2010, 45, 3885-3894.	2.6	29
36	Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale, 2017, 9, 10263-10276.	2.8	29

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37	QSAR modeling of acute toxicity on mammals caused by aromatic compounds: the case study using oral LD50 for rats. Journal of Environmental Monitoring, 2010, 12, 1037.	2.1	28
38	Toxicity of aromatic pollutants and photooxidative intermediates in water: A QSAR study. Ecotoxicology and Environmental Safety, 2019, 169, 918-927.	2.9	28
39	QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by graph of atomic orbitals and SMILES. Structural Chemistry, 2012, 23, 1873-1878.	1.0	27
40	Polymer Coating Materials and Their Fouling Release Activity: A Cheminformatics Approach to Predict Properties. ACS Applied Materials & Interfaces, 2017, 9, 1781-1792.	4.0	27
41	Photofragmentation of the Gas-Phase Lanthanum Isopropylcyclopentadienyl Complex: Computational Modeling vs Experiment. Journal of Physical Chemistry A, 2015, 119, 10838-10848.	1.1	26
42	In vivo toxicity of nitroaromatics: A comprehensive quantitative structureâ€“activity relationship study. Environmental Toxicology and Chemistry, 2017, 36, 2227-2233.	2.2	26
43	Photoinduced Charge Transfer versus Fragmentation Pathways in Lanthanum Cyclopentadienyl Complexes. Journal of Chemical Theory and Computation, 2017, 13, 4281-4296.	2.3	26
44	A computational structureâ€“property relationship study of glass transition temperatures for a diverse set of polymers. Journal of Polymer Science, Part B: Polymer Physics, 2018, 56, 877-885.	2.4	25
45	Adaptive Properties of the Genetically Encoded Amino Acid Alphabet Are Inherited from Its Subsets. Scientific Reports, 2019, 9, 12468.	1.6	24
46	Key structural features promoting radical driven degradation of emerging contaminants in water. Environment International, 2019, 124, 38-48.	4.8	24
47	Aconitum and Delphinium alkaloids. Environmental Toxicology and Pharmacology, 2008, 25, 310-320.	2.0	23
48	Experimental and Simulation Studies on Nonwoven Polypropyleneâ€“Nitrile Rubber Blend: Recycling of Medical Face Masks to an Engineering Product. ACS Omega, 2022, 7, 4791-4803.	1.6	23
49	Genotoxicity induced by metal oxide nanoparticles: a weight of evidence study and effect of particle surface and electronic properties. Nanotoxicology, 2018, 12, 1113-1129.	1.6	22
50	Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 3185-3192.	2.1	21
51	Toxicity of pharmaceuticals in binary mixtures: Assessment by additive and non-additive toxicity models. Ecotoxicology and Environmental Safety, 2019, 185, 109696.	2.9	21
52	Choosing safe dispersing media for C60 fullerenes by using cytotoxicity tests on the bacterium Escherichia coli. Journal of Hazardous Materials, 2010, 176, 367-373.	6.5	19
53	Combined toxicities of binary mixtures of alachlor, chlorfenvinphos, diuron and isoproturon. Chemosphere, 2020, 240, 124973.	4.2	17
54	Modeling the Dispersibility of Single Walled Carbon Nanotubes in Organic Solvents by Quantitative Structure-Activity Relationship Approach. Nanomaterials, 2015, 5, 778-791.	1.9	16

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55	Causal inference methods to assist in mechanistic interpretation of classification nano-SAR models. RSC Advances, 2015, 5, 77739-77745.	1.7	16
56	A Refractive Index Study of a Diverse Set of Polymeric Materials by QSPR with Quantum-Chemical and Additive Descriptors. Molecules, 2020, 25, 3772.	1.7	16
57	Metal Oxide Nanoparticles: Size-Dependence of Quantum-Mechanical Properties. Nanoscience and Nanotechnology - Asia, 2012, 1, 53-58.	0.3	15
58	Multiple Linear Regression Analysis and Optimal Descriptors: Predicting the Cholesteryl Ester Transfer Protein Inhibition Activity. QSAR and Combinatorial Science, 2008, 27, 595-606.	1.5	14
59	CORAL: Binary Classifications (Active/Inactive) for Liver-Related Adverse Effects of Drugs. Current Drug Safety, 2012, 7, 257-261.	0.3	14
60	Use of quantitative structureâ€“enantioselective retention relationship for the liquid chromatography chiral separation prediction of the series of pyrrolidinâ€2â€one compounds. Chirality, 2012, 24, 72-77.	1.3	14
61	Estimation of melting points of large set of persistent organic pollutants utilizing QSPR approach. Journal of Molecular Modeling, 2016, 22, 55.	0.8	14
62	Carbon Nanotubesâ€™ Effect on Mitochondrial Oxygen Flux Dynamics: Polarography Experimental Study and Machine Learning Models using Star Graph Trace Invariants of Raman Spectra. Nanomaterials, 2017, 7, 386.	1.9	14
63	QSAR Analysis of the Structureâ€”Toxicity Relationship of Aconitum and Delphinium Diterpene Alkaloids. Chemistry of Natural Compounds, 2005, 41, 213-219.	0.2	13
64	Structureâ€hepatoprotective activity relationship study of sesquiterpene lactones: A QSAR analysis. International Journal of Quantum Chemistry, 2009, 109, 17-27.	1.0	13
65	AconitumandDelphiniumDiterpenoid Alkaloids of Local Anesthetic Activity: Comparative QSAR Analysis Based on GA-MLRA/PLS and Optimal Descriptors Approach. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2014, 32, 213-238.	2.9	13
66	Estrogen activity of terpenoids from plants of the genus Ferula. Chemistry of Natural Compounds, 2008, 44, 572-577.	0.2	12
67	Metal Oxide Nanoparticles: Size-Dependence of Quantum-Mechanical Properties. Nanoscience and Nanotechnology - Asia, 2012, 1, 53-58.	0.3	12
68	Prediction of key structural features responsible for aromaticity of single-benzene ring pollutants and their photooxidative intermediates. Chemical Engineering Journal, 2015, 276, 261-273.	6.6	12
69	Application of ligand- and receptor-based approaches for prediction of the HIV-RT inhibitory activity of fullerene derivatives. Journal of Nanoparticle Research, 2016, 18, 1.	0.8	12
70	Combined computational and experimental study on the inclusion complexes of Î²-cyclodextrin with selected food phenolic compounds. Structural Chemistry, 2019, 30, 1395-1406.	1.0	12
71	Chapter 10. Nano-QSAR: Advances and Challenges. RSC Nanoscience and Nanotechnology, 2012, , 220-256.	0.2	11
72	Beyond model interpretability using <scp>LDA</scp> and decision trees for Î±â€amylase and Î±â€glucosidase inhibitor classification studies. Chemical Biology and Drug Design, 2019, 94, 1414-1421.	1.5	11

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73	Reactive Molecular Dynamics Study of Hygrothermal Degradation of Crosslinked Epoxy Polymers. ACS Applied Polymer Materials, 2022, 4, 4411-4423.	2.0	11
74	A Comprehensive Cheminformatics Analysis of Structural Features Affecting the Binding Activity of Fullerene Derivatives. Nanomaterials, 2020, 10, 90.	1.9	10
75	Predicting Metabolic Reaction Networks with Perturbation-Theory Machine Learning (PTML) Models. Current Topics in Medicinal Chemistry, 2021, 21, 819-827.	1.0	10
76	QSPR/QSAR Analyses by Means of the CORAL Software. Advances in Chemical and Materials Engineering Book Series, 2015, , 560-585.	0.2	10
77	Soysome: A Surfactant-Free, Fully Biobased, Self-Assembled Platform for Nanoscale Drug Delivery Applications. ACS Applied Bio Materials, 2018, 1, 1830-1841.	2.3	9
78	Computational Proteinâ€“Ligand Docking and Experimental Study of Bioplastic Films from Soybean Protein, Zein, and Natural Modifiers. ACS Sustainable Chemistry and Engineering, 2021, 9, 10740-10748.	3.2	9
79	How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases. Computational and Structural Biotechnology Journal, 2022, 20, 913-924.	1.9	9
80	Amino substituted nitrogen heterocycle ureas as kinase insert domain containing receptor (KDR) inhibitors: Performance of structureâ€“activity relationship approaches. Journal of Food and Drug Analysis, 2015, 23, 168-175.	0.9	7
81	Iridoid glucosides and triterpene acids from Phlomis linearifolia, growing in Uzbekistan and its hepatoprotective activity. Natural Product Research, 2021, 35, 2449-2453.	1.0	7
82	QSAR/QSPR in Polymers. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 80-88.	1.1	7
83	Detection of macromolecular inversionâ€“induced structural changes in osteosarcoma cells by FTIR microspectroscopy. Analytical and Bioanalytical Chemistry, 2020, 412, 7253-7262.	1.9	7
84	Structureâ€“Activity Relationship Investigations Of Leishmanicidal Nâ€Benzylcytisine Derivatives. Chemical Biology and Drug Design, 2011, 78, 183-189.	1.5	6
85	Exploring Simple, Interpretable, and Predictive QSPR Model of Fullerene C60 Solubility in Organic Solvents. Journal of Nanotoxicology and Nanomedicine, 2017, 2, 28-43.	0.7	6
86	Recent Developments in 3D QSAR and Molecular Docking Studies of Organic and Nanostructures. , 2017, , 2133-2161.		5
87	Preparation and Characterization of Inclusion Complexes of Î²-Cyclodextrin and Phenolics from Wheat Bran by Combination of Experimental and Computational Techniques. Molecules, 2020, 25, 4275.	1.7	5
88	Towards rational nanomaterial design by predicting drugâ€“nanoparticle system interaction vs. bacterial metabolic networks. Environmental Science: Nano, 2022, 9, 1391-1413.	2.2	5
89	Synergistic Behavior of Plant Proteins and Biobased Latexes in Bioplastic Food Packaging Materials: Experimental and Machine Learning Study. ACS Applied Materials & Interfaces, 2022, 14, 8384-8393.	4.0	4
90	Synthesis, Tautomeric States and Crystal Structure of (Z)-Ethyl 2-Cyano-2-(3H-Quinazoline-4-ylidene) Acetate and (Z)-Ethyl 2-Cyano-2-(2-Methyl-3H-Quinazoline-4-ylidene) Acetate. Molecules, 2005, 10, 1209-1217.	1.7	3

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91	Antiparasitic activity of certain isoquinoline alkaloids and their hypothetical complexes with oligonucleotides. Chemistry of Natural Compounds, 2008, 44, 341-345.	0.2	3
92	Classification nano-SAR modeling of metal oxides nanoparticles genotoxicity based on comet assay data. Toxicology Letters, 2016, 258, S271.	0.4	3
93	Modeling of Glass Transition Temperatures for Polymeric Coating Materials: Application of QSPR Mixtureâ€based Approach. Molecular Informatics, 2019, 38, e1800150.	1.4	3
94	Hot Carrier Dynamics at Ligated Silicon(111) Surfaces: A Computational Study. Journal of Physical Chemistry Letters, 2021, 12, 7504-7511.	2.1	3
95	Synthesis of 6-N-R-Tetrazolo[1,5-c]quinazolin-5(6H)-ones and Their Anticancer Activity. Acta Chimica Slovenica, 2016, 63, 638-645.	0.2	3
96	Machine Learning Study of Metabolic NetworksvsChEMBL Data of Antibacterial Compounds. Molecular Pharmaceutics, 2022, 19, 2151-2163.	2.3	3
97	Advances in In Silico Research on Nerve Agents. , 2014, , 283-322.		2
98	Comparison of the molecular descriptors efficiency in modeling the structure-activity relationship. , 2019, , .		2
99	Structure-Hepatoprotective Activity Relationship Study of Iridoids. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 108-118.	1.1	2
100	Structures and Stabilities: Quantum-Chemical Study of Aun (n = 2-2016) Nanoclusters by Extended Huckel and DFT Approaches. Nanoscience and Nanotechnology - Asia, 2012, 2, 2-10.	0.3	2
101	Molecular Dynamics Study of the Photodegradation of Polymeric Chains. Journal of Physical Chemistry Letters, 2022, 13, 4374-4380.	2.1	2
102	Structures and Stabilities: Quantum-Chemical Study of Aun (n = 2-2016) Nanoclusters by Extended Huckel and DFT Approaches. Nanoscience and Nanotechnology - Asia, 2012, 2, 2-10.	0.3	1
103	USEDAT: USA-Europe Data Analysis Training Worldwide Program, 2019 ed.. , 0, , .		1
104	Recent Developments in 3D QSAR and Molecular Docking Studies of Organic and Nanostructures. , 2016, , 1-29.		1
105	Chemometric modeling of refractive index of polymers using 2D descriptors: A QSPR approach. , 0, , .		1
106	Ecotoxicological QSAR Modeling of Nanomaterials: Methods in 3D-QSARs and Combined Docking Studies for Carbon Nanostructures. Methods in Pharmacology and Toxicology, 2020, , 215-233.	0.1	1
107	Nanoparticles. , 0, , 92-110.		1
108	Investigation of the spatial structure of the sesquiterpene lactone hanphyllin by1H NMR spectroscopy using the shift reagent Eu(FOD)3. Chemistry of Natural Compounds, 1995, 31, 196-199.	0.2	0

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109	AOP degradation of emerging contaminants in water: Prediction of second order kinetics by QSPR modeling. AIP Conference Proceedings, 2018, , .	0.3	0
110	Modeling of Photooxidative Degradation of Aromatics in Water Matrix: A Quantitative Structureâ^'Property Relationship Approach. ACS Symposium Series, 2019, , 257-292.	0.5	0
111	Determining the Activity of Fullerene Nanoparticles Using QSAR Models. Advances in Intelligent Systems and Computing, 2021, , 81-95.	0.5	0
112	Protein-ligand docking as a tool to predict properties and performance of plant-protein based bioplastics films. , 0, , .		0
113	Reliable but Timesaving: In Search of an Efficient Quantum-chemical Method for the Description of Functional Fullerenes. Current Topics in Medicinal Chemistry, 2015, 15, 1845-1858.	1.0	0
114	QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955.		0
115	Nanoparticles mutagenicity: search for matches and potential limitations of Comet assay and Ames test. , 0, , .		0
116	MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK), 2016, 2nd edition.. , 0, , .		0
117	Nanoparticles. , 0, , 1071-1089.		0
118	Mathematical modeling of refractive index based on machine learning (kNN-QSPR) method. , 2020, , .		0