# 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 | 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 |
| 2 | Towards rational nanomaterial design by predicting drugâ€“nanoparticle system interaction vs. bacterial metabolic networks. Environmental Science: Nano, 2022, 9, 1391-1413. | 2.2 | 5 |
| 3 | 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 |
| 4 | 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 |
| 5 | Molecular Dynamics Study of the Photodegradation of Polymeric Chains. Journal of Physical Chemistry Letters, 2022, 13, 4374-4380. | 2.1 | 2 |
| 6 | Reactive Molecular Dynamics Study of Hygrothermal Degradation of Crosslinked Epoxy Polymers. ACS Applied Polymer Materials, 2022, 4, 4411-4423. | 2.0 | 11 |
| 7 | Machine Learning Study of Metabolic NetworksvsChEMBL Data of Antibacterial Compounds. Molecular Pharmaceutics, 2022, 19, 2151-2163. | 2.3 | 3 |
| 8 | 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 |
| 9 | Determining the Activity of Fullerene Nanoparticles Using QSAR Models. Advances in Intelligent Systems and Computing, 2021, , 81-95. | 0.5 | 0 |
| 10 | Predicting glass transition of amorphous polymers by application of cheminformatics and molecular dynamics simulations. Polymer, 2021, 218, 123495. | 1.8 | 35 |
| 11 | Predicting Metabolic Reaction Networks with Perturbation-Theory Machine Learning (PTML) Models. Current Topics in Medicinal Chemistry, 2021, 21, 819-827. | 1.0 | 10 |
| 12 | 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 |
| 13 | Hot Carrier Dynamics at Ligated Silicon(111) Surfaces: A Computational Study. Journal of Physical Chemistry Letters, 2021, 12, 7504-7511. | 2.1 | 3 |
| 14 | Combined toxicities of binary mixtures of alachlor, chlorfenvinphos, diuron and isoproturon. Chemosphere, 2020, 240, 124973. | 4.2 | 17 |
| 15 | QSAR/QSPR in Polymers. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 80-88. | 1.1 | 7 |
| 16 | A Comprehensive Cheminformatics Analysis of Structural Features Affecting the Binding Activity of Fullerene Derivatives. Nanomaterials, 2020, 10, 90. | 1.9 | 10 |
| 17 | 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 |
| 18 | Detection of macromolecular inversionâ€“induced structural changes in osteosarcoma cells by FTIR microspectroscopy. Analytical and Bioanalytical Chemistry, 2020, 412, 7253-7262. | 1.9 | 7 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | Structure-Hepatoprotective Activity Relationship Study of Iridoids. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 108-118. | 1.1 | 2 |
| 21 | 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 |
| 22 | Mathematical modeling of refractive index based on machine learning (kNN-QSPR) method. , 2020, , . | | 0 |
| 23 | Adaptive Properties of the Genetically Encoded Amino Acid Alphabet Are Inherited from Its Subsets. Scientific Reports, 2019, 9, 12468. | 1.6 | 24 |
| 24 | Toxicity of pharmaceuticals in binary mixtures: Assessment by additive and non-additive toxicity models. Ecotoxicology and Environmental Safety, 2019, 185, 109696. | 2.9 | 21 |
| 25 | 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 |
| 26 | Key structural features promoting radical driven degradation of emerging contaminants in water. Environment International, 2019, 124, 38-48. | 4.8 | 24 |
| 27 | 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 |
| 28 | A chemoinformatics approach for the characterization of hybrid nanomaterials: safer and efficient design perspective. Nanoscale, 2019, 11, 11808-11818. | 2.8 | 35 |
| 29 | 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 |
| 30 | Modeling of Glass Transition Temperatures for Polymeric Coating Materials: Application of QSPR Mixtureâ€based Approach. Molecular Informatics, 2019, 38, e1800150. | 1.4 | 3 |
| 31 | Comparison of the molecular descriptors efficiency in modeling the structure-activity relationship. , 2019, , . | | 2 |
| 32 | Modeling of Photooxidative Degradation of Aromatics in Water Matrix: A Quantitative Structureâ^'Property Relationship Approach. ACS Symposium Series, 2019, , 257-292. | 0.5 | 0 |
| 33 | Toxicity of aromatic pollutants and photooxidative intermediates in water: A QSAR study. Ecotoxicology and Environmental Safety, 2019, 169, 918-927. | 2.9 | 28 |
| 34 | 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 |
| 35 | Nano-QSAR modeling for ecosafe design of heterogeneous TiO<sub>2</sub>-based nano-photocatalysts. Environmental Science: Nano, 2018, 5, 1150-1160. | 2.2 | 51 |
| 36 | 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 |

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|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | AOP degradation of emerging contaminants in water: Prediction of second order kinetics by QSPR modeling. AIP Conference Proceedings, 2018, , . | 0.3 | 0 |
| 40 | QSPR Modeling of the Refractive Index for Diverse Polymers Using 2D Descriptors. ACS Omega, 2018, 3, 13374-13386. | 1.6 | 36 |
| 41 | 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 |
| 42 | Recent Developments in 3D QSAR and Molecular Docking Studies of Organic and Nanostructures. , 2017, , 2133-2161. | | 5 |
| 43 | In vivo toxicity of nitroaromatics: A comprehensive quantitative structureâ€“activity relationship study. Environmental Toxicology and Chemistry, 2017, 36, 2227-2233. | 2.2 | 26 |
| 44 | Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 3185-3192. | 2.1 | 21 |
| 45 | Refractive indices of diverse data set of polymers: A computational QSPR based study. Computational Materials Science, 2017, 137, 215-224. | 1.4 | 45 |
| 46 | 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 |
| 47 | 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 |
| 48 | Photoinduced Charge Transfer versus Fragmentation Pathways in Lanthanum Cyclopentadienyl Complexes. Journal of Chemical Theory and Computation, 2017, 13, 4281-4296. | 2.3 | 26 |
| 49 | Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale, 2017, 9, 10263-10276. | 2.8 | 29 |
| 50 | 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 |
| 51 | 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 |
| 52 | QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955. | | 0 |
| 53 | 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 |
| 54 | Classification nano-SAR modeling of metal oxides nanoparticles genotoxicity based on comet assay data. Toxicology Letters, 2016, 258, S271. | 0.4 | 3 |

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| 55 | 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 |
| 56 | Estimation of melting points of large set of persistent organic pollutants utilizing QSPR approach. Journal of Molecular Modeling, 2016, 22, 55. | 0.8 | 14 |
| 57 | 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 |
| 58 | Recent Developments in 3D QSAR and Molecular Docking Studies of Organic and Nanostructures. , 2016, , 1-29. | | 1 |
| 59 | Photofragmentation of the Gas-Phase Lanthanum Isopropylcyclopentadienyl Complex: Computational Modeling vs Experiment. Journal of Physical Chemistry A, 2015, 119, 10838-10848. | 1.1 | 26 |
| 60 | 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 |
| 61 | 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 |
| 62 | 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 |
| 63 | 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 |
| 64 | Extraordinarily Adaptive Properties of the Genetically Encoded Amino Acids. Scientific Reports, 2015, 5, 9414. | 1.6 | 54 |
| 65 | 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 |
| 66 | Causal inference methods to assist in mechanistic interpretation of classification nano-SAR models. RSC Advances, 2015, 5, 77739-77745. | 1.7 | 16 |
| 67 | Genotoxicity of metal oxide nanomaterials: review of recent data and discussion of possible mechanisms. Nanoscale, 2015, 7, 2154-2198. | 2.8 | 163 |
| 68 | Towards understanding mechanisms governing cytotoxicity of metal oxides nanoparticles: Hints from nano-QSAR studies. Nanotoxicology, 2015, 9, 313-325. | 1.6 | 147 |
| 69 | QSPR/QSAR Analyses by Means of the CORAL Software. Advances in Chemical and Materials Engineering Book Series, 2015, , 560-585. | 0.2 | 10 |
| 70 | 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 |
| 71 | Advances in In Silico Research on Nerve Agents. , 2014, , 283-322. | | 2 |
| 72 | Immunotoxicity of nanoparticles: a computational study suggests that CNTs and C<sub>60</sub> fullerenes might be recognized as pathogens by Toll-like receptors. Nanoscale, 2014, 6, 3488-3495. | 2.8 | 97 |

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| 73 | 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 |
| 74 | 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 |
| 75 | 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 |
| 76 | 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 |
| 77 | CORAL: Binary Classifications (Active/Inactive) for Liver-Related Adverse Effects of Drugs. Current Drug Safety, 2012, 7, 257-261. | 0.3 | 14 |
| 78 | Chapter 10. Nano-QSAR: Advances and Challenges. RSC Nanoscience and Nanotechnology, 2012, , 220-256. | 0.2 | 11 |
| 79 | 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 |
| 80 | Advancing risk assessment of engineered nanomaterials: Application of computational approaches. Advanced Drug Delivery Reviews, 2012, 64, 1663-1693. | 6.6 | 186 |
| 81 | Metal Oxide Nanoparticles: Size-Dependence of Quantum-Mechanical Properties. Nanoscience and Nanotechnology - Asia, 2012, 1, 53-58. | 0.3 | 12 |
| 82 | 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 |
| 83 | Room temperature synthesis of PbSe quantum dots in aqueous solution: stabilization by interactions with ligands. Nanoscale, 2012, 4, 1312. | 2.8 | 39 |
| 84 | 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 |
| 85 | 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 |
| 86 | Metal Oxide Nanoparticles: Size-Dependence of Quantum-Mechanical Properties. Nanoscience and Nanotechnology - Asia, 2012, 1, 53-58. | 0.3 | 15 |
| 87 | 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 |
| 88 | Structureâ€“Activity Relationship Investigations Of Leishmanicidal Nâ€Benzylcytisine Derivatives. Chemical Biology and Drug Design, 2011, 78, 183-189. | 1.5 | 6 |
| 89 | Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. Nature Nanotechnology, 2011, 6, 175-178. | 15.6 | 654 |
| 90 | 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 |

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| 91 | 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 |
| 92 | 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 |
| 93 | 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 |
| 94 | Structureâ€hepatoprotective activity relationship study of sesquiterpene lactones: A QSAR analysis. International Journal of Quantum Chemistry, 2009, 109, 17-27. | 1.0 | 13 |
| 95 | Prediction of rate constants for radical degradation of aromatic pollutants in water matrix: A QSAR study. Chemosphere, 2009, 75, 1128-1134. | 4.2 | 122 |
| 96 | Antiparasitic activity of certain isoquinoline alkaloids and their hypothetical complexes with oligonucleotides. Chemistry of Natural Compounds, 2008, 44, 341-345. | 0.2 | 3 |
| 97 | Estrogen activity of terpenoids from plants of the genus Ferula. Chemistry of Natural Compounds, 2008, 44, 572-577. | 0.2 | 12 |
| 98 | 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 |
| 99 | Aconitum and Delphinium sp. alkaloids as antagonist modulators of voltage-gated Na+ channels. Computational Biology and Chemistry, 2008, 32, 88-101. | 1.1 | 29 |
| 100 | Multiplicative SMILES-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2008, 457, 332-336. | 1.2 | 43 |
| 101 | QSAR modeling of acute toxicity by balance of correlations. Bioorganic and Medicinal Chemistry, 2008, 16, 5999-6008. | 1.4 | 53 |
| 102 | Aconitum and Delphinium alkaloids. Environmental Toxicology and Pharmacology, 2008, 25, 310-320. | 2.0 | 23 |
| 103 | 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 |
| 104 | Additive SMILES based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. Chemical Physics Letters, 2007, 444, 209-214. | 1.2 | 37 |
| 105 | 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 |
| 106 | Structure-toxicity relationships of nitroaromatic compounds. Molecular Diversity, 2006, 10, 233-245. | 2.1 | 79 |
| 107 | QSAR Analysis of the Structureâ€"Toxicity Relationship of Aconitum and Delphinium Diterpene Alkaloids. Chemistry of Natural Compounds, 2005, 41, 213-219. | 0.2 | 13 |
| 108 | A Quantitative Structure-Activity Relationship (QSAR) Study of the Antioxidant Activity of Flavonoids. QSAR and Combinatorial Science, 2005, 24, 1056-1065. | 1.5 | 88 |

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| 109 | 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 |
| 110 | A QSAR Toxicity Study of a Series of Alkaloids with the Lycoctonine Skeleton. Molecules, 2004, 9, 1194-1207. | 1.7 | 31 |
| 111 | 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 |
| 112 | Protein-ligand docking as a tool to predict properties and performance of plant-protein based bioplastics films. , 0, , . | | 0 |
| 113 | USEDAT: USA-Europe Data Analysis Training Worldwide Program, 2019 ed.. , 0, , . | | 1 |
| 114 | Nanoparticles mutagenicity: search for matches and potential limitations of Comet assay and Ames test. , 0, , . | | 0 |
| 115 | MOL2NET: FROM MOLECULES TO NETWORKS (PROCEEDINGS BOOK), 2016, 2nd edition.. , 0, , . | | 0 |
| 116 | Chemometric modeling of refractive index of polymers using 2D descriptors: A QSPR approach. , 0, , . | | 1 |
| 117 | Nanoparticles. , 0, , 1071-1089. | | 0 |
| 118 | Nanoparticles. , 0, , 92-110. | | 1 |