Jerzy Leszczynski

List of Publications by Year
in descending order

559 papers	19,147 citations	13332 70 h-index	31191 106 g-index
579 all docs	579 docs citations	579 times ranked	15436 citing authors

#	Article	IF	Citations
1	NTO degradation by direct photolysis: DFT study. Structural Chemistry, 2023, 34, 23-31.	1.0	5
2	SARS-CoV M^{pro} inhibitory activity of aromatic disulfide compounds: QSAR model. Journal of Biomolecular Structure and Dynamics, 2022, 40, 780-786.	2.0	23
3	First-Principles Modeling of Non-covalent Interactions in Molecular Systems and Extended Materials. , 2022, , 71-124.		0
4	Application of Computational Approaches to Analysis of Multistep Chemical Reactions of Energetic Materials: Hydrolysis of Hexahydro-1,3,5-Trinitro-1,3,5-Triazine (RDX) and Octahydro-1,3,5,7-Tetranitro-1,3,5,7-Tetrazocine(HMX). , 2022, , 215-232.		0
5	Metal halide perovskites for photocatalysis applications. Journal of Materials Chemistry A, 2022, 10, 407-429.	5.2	61
6	Enhanced Perovskite Solar Cell Performance via 2-Amino-5-iodobenzoic Acid Passivation. ACS Applied Materials & Interfaces, 2022, 14, 5414-5424.	4.0	17
7	Computational approaches in assessments of mixture toxicity. Current Opinion in Toxicology, 2022, 29, 31-35.	2.6	5
8	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	23.0	155
9	In Silico Tools and Software to Predict ADMET of New Drug Candidates. Methods in Molecular Biology, 2022, 2425, 85-115.	0.4	15
10	Identification of potential antivirals against 3CLpro enzyme for the treatment of SARS-CoV-2: A multi-step virtual screening study. SAR and QSAR in Environmental Research, 2022, 33, 357-386.	1.0	9
11	Decomposition of 2,4,6-trinitrotoluene (TNT) and 5-nitro-2,4-dihydro-3H-1,2,4-triazol-3-one (NTO) by Fe13O13 nanoparticle: density functional theory study. Environmental Science and Pollution Research, 2022, 29, 68522-68531.	2.7	2
12	An effect of nitrogen incorporation on the structure and properties of amorphous SiC: First-principles molecular dynamics simulations. Thin Solid Films, 2022, 756, 139349.	0.8	1
13	Repurposing FDA approved drugs as possible anti-SARS-CoV-2 medications using ligand-based computational approaches: sum of ranking difference-based model selection. Structural Chemistry, 2022, 33, 1741-1753.	1.0	9
14	Photophysical Properties of Donorâ€“Acceptorâ^'Ï€ Bridgeâ€“Acceptor Sensitizers with a Naphthobisthiadiazole Auxiliary Acceptor: Toward Longer-Wavelength Access in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2022, 126, 11875-11888.	1.5	8
15	Protein reliability analysis and virtual screening of natural inhibitors for SARS-CoV-2 main protease (M^{pro}) through docking, molecular mechanic & dynamic, and ADMET profiling. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6810-6827.	2.0	21
16	N-arylnaphthylamines as inhibitors of human immunodeficiency virus integrase - lens epithelium-derived growth factor interactions: theoretical studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 867-880.	2.0	0
17	Efficient approach for exploring the multiple-channel bimolecular interactions of conformationally flexible reagents. Epoxide ring opening reaction. Structural Chemistry, 2021, 32, 581-589.	1.0	1
18	Evaluating the cytotoxicity of a large pool of metal oxide nanoparticles to Escherichia coli: Mechanistic understanding through InÂVitro and In Silico studies. Chemosphere, 2021, 264, 128428.	4.2	19

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19	Therapeutics for COVID-19: from computation to practicesâ€"where we are, where we are heading to. Molecular Diversity, 2021, 25, 625-659.	2.1	53
20	Catalytic role of solvated electron in the spontaneous degradation of insensitive munition compounds: computational chemistry investigation. Structural Chemistry, 2021, 32, 521-527.	1.0	4
21	Drug Databases for Development of Therapeutics Against Coronaviruses. Methods in Pharmacology and Toxicology, 2021, , 761.	0.1	1
22	Application of QSPR Modeling in Designing and Prediction of Power Conversion-Efficient Solar Cell. Challenges and Advances in Computational Chemistry and Physics, 2021, , 167-186.	0.6	0
23	Combining Features of Metal Oxide Nanoparticles. , 2021, , 317-329.		1
24	Computational Screening of Organic Dye-Sensitizers for Dye-Sensitized Solar Cells: DFT/TDDFT Approach. Challenges and Advances in Computational Chemistry and Physics, 2021, , 187-205.	0.6	0
25	Another look at the structure of the (H2O)nâ€¢Ö¾ system: water anion vs. hydrated electron. Structural Chemistry, 2021, 32, 655-665.	1.0	2
26	The kernel-weighted local polynomial regression (KwLPR) approach: an efficient, novel tool for development of QSAR/QSAAR toxicity extrapolation models. Journal of Cheminformatics, 2021, 13, 9.	2.8	9
27	Z,E-Isomerism in a Series of Substituted Iminophosphonates: Quantum Chemical Research. Organics, 2021, 2, 84-97.	0.6	2
28	Zeta potentials (Î¶) of metal oxide nanoparticles: A meta-analysis of experimental data and a predictive neural networks modeling. NanoImpact, 2021, 22, 100317.	2.4	28
29	COMBINED EXPERIMENTAL AND COMPUTATIONAL APPROACH TO THE STRUCTURE OF A NEW NICKEL(II) COMPLEX WITH TRIDENTATE SCHIFF BASE LIGAND. Journal of Structural Chemistry, 2021, 62, 938-946.	0.3	1
30	Preliminary Screening of COVID-19 Infection Employing Machine Learning Techniques From Simple Blood Profile. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 35-47.	1.1	6
31	Interaction of epoxy-based hydrogels and water: A molecular dynamics simulation study. Journal of Molecular Graphics and Modelling, 2021, 106, 107915.	1.3	9
32	Using quasi-SMILES for the predictive modeling of the safety of 574 metal oxide nanoparticles measured in different experimental conditions. Environmental Toxicology and Pharmacology, 2021, 86, 103665.	2.0	19
33	Theoretical DFT Study on the Mechanisms of CO/CO2 Conversion in Chemical Looping Catalyzed by Calcium Ferrite. Journal of Physical Chemistry A, 2021, 125, 8159-8167.	1.1	2
34	Application of quasi-SMILES to the model of gold-nanoparticles uptake in A549Âcells. Computers in Biology and Medicine, 2021, 136, 104720.	3.9	8
35	QSAR and machine learning modeling of toxicity of nanomaterials: a risk assessment approach. , 2021, , 417-441.		2
36	Single site Fe on the (110) surface of Î³-Al₂O₃: insights from a DFT study including the periodic boundary approach. Physical Chemistry Chemical Physics, 2021, 23, 7164-7177.	1.3	9

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37	Jahn-Teller and Pseudo Jahn-Teller Effects: Influences on the Electronic Structures of Small Transition, Main Group and Mixed Metal Clusters. Structural Chemistry, 2020, 31, 7-23.	1.0	2
38	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	4.6	86
39	How the CORAL software can be used to select compounds for efficient treatment of neurodegenerative diseases?. Toxicology and Applied Pharmacology, 2020, 408, 115276.	1.3	6
40	From Animal to Human: Interspecies Analysis Provides a Novel Way of Ascertaining and Fighting COVID-19. Innovation(China), 2020, 1, 100021.	5.2	11
41	Effect of Microenvironment on the Geometrical Structure of d(A)₅ d(T)₅ and d(G)₅ d(C)₅ DNA Mini-Helixes and the Dickerson Dodecamer: A Density Functional Theory Study. Journal of Physical Chemistry B, 2020, 124, 9343-9353.	1.2	5
42	Revealing the Photophysical Mechanism of N,Nâ€²-Diphenyl-aniline Based Sensitizers with the Dâ€“Dâ^'Iâ€“A Framework: Theoretical Insights. ACS Sustainable Chemistry and Engineering, 2020, 8, 13328-13341.	3.2	36
43	Advancement of predictive modeling of zeta potentials (Î¶) in metal oxide nanoparticles with correlation intensity index (CII). Journal of Molecular Liquids, 2020, 317, 113929.	2.3	15
44	Open access in silico tools to predict the ADMET profiling of drug candidates. Expert Opinion on Drug Discovery, 2020, 15, 1473-1487.	2.5	99
45	Negative thermal quenching of photoluminescence in a copperâ€“organic framework emitter. Chemical Communications, 2020, 56, 12057-12060.	2.2	22
46	Single Fe Site on the Surface of Î³-Al₂O₃: Insights from Density Functional Theory Periodic Boundary Approach. Journal of Physical Chemistry C, 2020, 124, 20931-20941.	1.5	7
47	Evaluating Donor Effects in Isoindigo-Based Small Molecular Fluorophores. Journal of Physical Chemistry A, 2020, 124, 10777-10786.	1.1	9
48	Chemometric Modeling of the Ecotoxicity of Industrial Chemicals to an Avian Species Anas Platyrhynchos. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 1-16.	1.1	3
49	Is intraspecies QSTR model answer to toxicity data gap filling: Ecotoxicity modeling of chemicals to avian species. Science of the Total Environment, 2020, 738, 139858.	3.9	9
50	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for in silico nanosafety assessment. Computational and Structural Biotechnology Journal, 2020, 18, 583-602.	1.9	74
51	A density functional theory study of simplest nanocomposites formed by graphene oxide and polyvinyl alcohol: geometry, interaction energy and vibrational spectrum. Journal of Molecular Modeling, 2020, 26, 183.	0.8	2
52	The index of ideality of correlation: models of the flash points of ternary mixtures. New Journal of Chemistry, 2020, 44, 4858-4868.	1.4	12
53	First-Principles Approach for Assessing Cold Electron Injection Efficiency of Dye-Sensitized Solar Cell: Elucidation of Mechanism of Charge Injection and Recombination. Journal of Physical Chemistry C, 2020, 124, 2817-2836.	1.5	25
54	Cleftâ€Induced Ditopic Binding of Spherical Halides with a Hexaurea Receptor. ChemistrySelect, 2020, 5, 1401-1409.	0.7	4

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55	Chemometric modeling of power conversion efficiency of organic dyes in dye sensitized solar cells for the future renewable energy. Nano Energy, 2020, 70, 104537.	8.2	35
56	Ecotoxicity Databases for QSAR Modeling. Methods in Pharmacology and Toxicology, 2020, , 709-758.	0.1	6
57	First-principles investigations of the pressure-induced phase transformations and properties of crystalline and amorphous AlN. Physical Review Materials, 2020, 4, .	0.9	7
58	Semi-correlations combined with the index of ideality of correlation: a tool to build up model of mutagenic potential. Molecular and Cellular Biochemistry, 2019, 452, 133-140.	1.4	13
59	Accurate and transferable multitask prediction of chemical properties with an atoms-in-molecules neural network. Science Advances, 2019, 5, eaav6490.	4.7	148
60	Role of Singlet Oxygen in the Degradation of Selected Insensitive Munitions Compounds: A Comprehensive, Quantum Chemical Investigation. Journal of Physical Chemistry A, 2019, 123, 7597-7608.	1.1	5
61	Computational and experimental approach to understanding the structural interplay of self-assembled end-terminated alkanethiolates on gold surfaces. Physical Chemistry Chemical Physics, 2019, 21, 23320-23328.	1.3	6
62	Optoelectronic Properties of C60 and C70 Fullerene Derivatives: Designing and Evaluating Novel Candidates for Efficient P3HT Polymer Solar Cells. Materials, 2019, 12, 2282.	1.3	15
63	Characterization and Simulation of Natural Pyrite Surfaces: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 26397-26405.	1.5	13
64	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
65	A first-principles study of the stability and mechanical properties of ternary transition metal carbide alloys. Journal of Applied Physics, 2019, 125, .	1.1	16
66	Combining Features of Metal Oxide Nanoparticles. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 28-40.	1.1	5
67	InÂvitro and in silico modeling of perfluoroalkyl substances mixture toxicity in an amphibian fibroblast cell line. Chemosphere, 2019, 233, 25-33.	4.2	44
68	Exploration of Computational Approaches to Predict the Toxicity of Chemical Mixtures. Toxics, 2019, 7, 15.	1.6	84
69	â€œIdeal correlationsâ€•for biological activity of peptides. BioSystems, 2019, 181, 51-57.	0.9	11
70	Predicting Thermal Conductivity Enhancement of Al2O3/Water and CuO/Water Nanofluids Using Quantitative Structure-Property Relationship Approach. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 18-27.	1.1	4
71	Modeling of Glass Transition Temperatures for Polymeric Coating Materials: Application of QSPR Mixtureâ€based Approach. Molecular Informatics, 2019, 38, e1800150.	1.4	3
72	Stability of SiC and SiN interfaces in titanium carbide and nitride based heterostructures. Journal of Applied Physics, 2019, 125, 075303.	1.1	3

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73	Theoretical study of formate, tartrate, tartronate, and glycolate production from 6-carbon trioxylate intermediate in the citric acid cycle. Journal of Molecular Modeling, 2019, 25, 347.	0.8	0
74	How water affects mercuryâ€“halogen interaction in the atmosphere. Journal of Molecular Modeling, 2019, 25, 357.	0.8	1
75	A density functional theory investigation of degradation of Nitroguanidine in the photoactivated triplet state. Journal of Molecular Modeling, 2019, 25, 372.	0.8	0
76	Adsorption of nitrogen-containing compounds on hydroxylated Î±-quartz surfaces. RSC Advances, 2019, 9, 36066-36074.	1.7	0
77	Ecotoxicological Modeling, Ranking and Prioritization of Pharmaceuticals Using QSTR and iâ€QSTTR Approaches: Application of 2D and Fragment Based Descriptors. Molecular Informatics, 2019, 38, e1800078.	1.4	24
78	Electronic Structure and Optical Properties of Designed Photo-Efficient Indoline-Based Dye-Sensitizers with Dâ€“Aâ^Ï€â€“A Framework. Journal of Physical Chemistry C, 2019, 123, 3309-3320.	1.5	46
79	Is clay-polycation adsorbent future of the greener society? In silico modeling approach with comprehensive virtual screening. Chemosphere, 2019, 220, 1108-1117.	4.2	6
80	Toward comprehension of multiple human cells uptake of engineered nano metal oxides: quantitative inter cell line uptake specificity (QICLUS) modeling. Nanotoxicology, 2019, 13, 14-34.	1.6	23
81	Multiple e-Pharmacophore modeling to identify a single molecule that could target both streptomycin and paromomycin binding sites for 30S ribosomal subunit inhibition. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1582-1596.	2.0	13
82	Diffusion of energetic compounds through biological membrane: Application of classical MD and COSMOmic approximations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 247-255.	2.0	6
83	Recent Advances of In-Silico Modeling of Potent Antagonists for the Adenosine Receptors. Current Pharmaceutical Design, 2019, 25, 750-773.	0.9	14
84	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 148-153.	0.9	4
85	Interactions of Substituted Nitroaromatics with Model Graphene Systems: Applicability of Hammett Substituent Constants To Predict Binding Energies. ACS Omega, 2018, 3, 2773-2785.	1.6	3
86	Structure and Energetics of (111) Surface of Î³-Al₂O₃: Insights from DFT Including Periodic Boundary Approach. ACS Omega, 2018, 3, 1881-1888.	1.6	34
87	Fullerene quinazolinone conjugates targeting Mycobacterium tuberculosis: a combined molecular docking, QSAR, and ONIOM approach. Structural Chemistry, 2018, 29, 765-775.	1.0	6
88	QSPR modeling of optical rotation of amino acids using specific quantum chemical descriptors. Journal of Molecular Modeling, 2018, 24, 59.	0.8	8
89	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
90	Second generation periodic table-based descriptors to encode toxicity of metal oxide nanoparticles to multiple species: QSTR modeling for exploration of toxicity mechanisms. Environmental Science: Nano, 2018, 5, 2742-2760.	2.2	26

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91	Reply to the comment on â€œCausation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR modelsâ€•by D. A. Tasi, J. Csontos, B. Nagy, Z. KÃ³nya and G. Tasi, Nanoscale, 2018, 10, C8NR02377H. Nanoscale, 2018, 10, 20867-20868.	2.8	2
92	Light-dependent isomeric effects of polycyclic aromatic hydrocarbons on the predication of DNA cleavage factor efficiency. Structural Chemistry, 2018, 29, 1697-1707.	1.0	1
93	The index of ideality of correlation: hierarchy of Monte Carlo models for glass transition temperatures of polymers. Journal of Polymer Research, 2018, 25, 1.	1.2	12
94	QSAR modeling of adipose/blood partition coefficients of Alcohols, PCBs, PBDEs, PCDDs and PAHs: A data gap filling approach. Environment International, 2018, 121, 1193-1203.	4.8	17
95	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. BioSystems, 2018, 169-170, 5-12.	0.9	13
96	Impact of Pharmaceuticals on the Environment: Risk Assessment Using QSAR Modeling Approach. Methods in Molecular Biology, 2018, 1800, 395-443.	0.4	32
97	Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling. Methods in Molecular Biology, 2018, 1800, 141-169.	0.4	61
98	Insight into mechanism of iron-oxides reduction in atmospheres of CH4 and CO. Chemical Physics Letters, 2018, 706, 708-714.	1.2	8
99	Single or mixture halogenated chemicals? Risk assessment and developmental toxicity prediction on zebrafish embryos based on weighted descriptors approach. Chemosphere, 2018, 210, 588-596.	4.2	23
100	Insight into the optoelectronic properties of designed solar cells efficient tetrahydroquinoline dye-sensitizers on TiO2(101) surface: first principles approach. Scientific Reports, 2018, 8, 10997.	1.6	44
101	High-temperature thermoelectric transport behavior of the Al/Î³-Al‹sub›2‹/sub›O‹sub›3‹/sub›interface: impact of electron and phonon scattering at nanoscale metalâ€“ceramic contacts. Physical Chemistry Chemical Physics, 2018, 20, 14513-14524.	1.3	4
102	Catalytic abiotic synthesis of uracil from cysteine and urea: Theoretical studies. Chemical Physics Letters, 2018, 710, 16-25.	1.2	0
103	Towards the Development of Global Nano-Quantitative Structureâ€“Property Relationship Models: Zeta Potentials of Metal Oxide Nanoparticles. Nanomaterials, 2018, 8, 243.	1.9	31
104	Recent Advances of Computational Modeling for Predicting Drug Metabolism: A Perspective. Current Drug Metabolism, 2018, 18, 1106-1122.	0.7	19
105	Novel Imprinted Polymer for the Preconcentration of Cadmium with Determination by Inductively Coupled Plasma Mass Spectrometry. Analytical Letters, 2017, 50, 482-499.	1.0	14
106	Geometry optimization of steroid sulfatase inhibitors - the influence on the free binding energy with STS. Structural Chemistry, 2017, 28, 1017-1032.	1.0	10
107	Computational Modeling of DNA and RNA Fragments. , 2017, , 1803-1826.		1
108	Application of Quantum Mechanics and Molecular Mechanics in Chemoinformatics. , 2017, , 2041-2063.		0

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109	Chlorophenol sorption on multi-walled carbon nanotubes: DFT modeling and structureâ€“property relationship analysis. Journal of Molecular Modeling, 2017, 23, 39.	0.8	4
110	CORAL and Nano-QFAR: Quantitative feature â€“ Activity relationships (QFAR) for bioavailability of nanoparticles (ZnO, CuO, Co 3 O 4 , and TiO 2). Ecotoxicology and Environmental Safety, 2017, 139, 404-407.	2.9	29
111	A quantum chemical based toxicity study of estimated reduction potential and hydrophobicity in series of nitroaromatic compounds. SAR and QSAR in Environmental Research, 2017, 28, 133-150.	1.0	12
112	In silico modeling of functionalized graphene oxide-metal cluster conjugates as Raman probe: Raman activity of pyridine. Structural Chemistry, 2017, 28, 379-389.	1.0	2
113	In vivo toxicity of nitroaromatics: A comprehensive quantitative structureâ€“activity relationship study. Environmental Toxicology and Chemistry, 2017, 36, 2227-2233.	2.2	26
114	Endocrine-disrupting activity of per- and polyfluoroalkyl substances: Exploring combined approaches of ligand and structure based modeling. Chemosphere, 2017, 184, 514-523.	4.2	79
115	Predicting Physical Properties of Nanofluids by Computational Modeling. Journal of Physical Chemistry C, 2017, 121, 1910-1917.	1.5	23
116	Addressing a bottle neck for regulation of nanomaterials: quantitative read-across (Nano-QRA) algorithm for cases when only limited data is available. Environmental Science: Nano, 2017, 4, 346-358.	2.2	45
117	4d and 5d bimetal doped tubular silicon clusters Si₁₂M₂ with M = Nb, Ta, Mo and W: a bimetallic configuration model. Physical Chemistry Chemical Physics, 2017, 19, 3115-3124.	1.3	36
118	In silico kinetics of alkaline hydrolysis of 1,3,5-trinitro-1,3,5-triazinane (RDX): M06-2X investigation. Environmental Sciences: Processes and Impacts, 2017, 19, 388-394.	1.7	18
119	Binding of Alkali Metal Ions with 1,3,5-Tri(phenyl)benzene and 1,3,5-Tri(naphthyl)benzene: The Effect of Phenyl and Naphthyl Ring Substitution on Cationâ^'Î€ Interactions Revealed by DFT Study. Journal of Physical Chemistry A, 2017, 121, 8927-8938.	1.1	5
120	d(A)3d(T)3 and d(G)3d(C)3 B-DNA mini-helixes: the DFT/M06-2x and DFT/B97-D3 comparison of geometrical and energetic characteristics. Journal of Molecular Modeling, 2017, 23, 289.	0.8	8
121	Exploiting a single intramolecular conformational switching Ni-TPP molecule to probe charge transfer dynamics at the nanoscale on bare Si(100)-2 Ã— 1. Physical Chemistry Chemical Physics, 2017, 19, 28982-28992.	1.3	2
122	An Ideal C₃-Symmetric Sulfate Complex: Molecular Recognition of Oxoanions by m-Nitrophenyl- and Pentafluorophenyl-Functionalized Hexaurea Receptors. ACS Omega, 2017, 2, 5840-5849.	1.6	14
123	Remarkable hexafunctional anion receptor with operational urea-based inner cleft and thiourea-based outer cleft: Novel design with high-efficiency for sulfate binding. Scientific Reports, 2017, 7, 6032.	1.6	18
124	In silico designing of power conversion efficient organic lead dyes for solar cells using todays innovative approaches to assure renewable energy for future. Npj Computational Materials, 2017, 3, .	3.5	43
125	Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale, 2017, 9, 10263-10276.	2.8	29
126	Understanding the influence of low-frequency vibrations on the hydrogen bonds of acetic acid and acetamide dimers. Physical Chemistry Chemical Physics, 2017, 19, 24866-24878.	1.3	10

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127	Drug-Nanoparticle Composites. Journal of Nanotoxicology and Nanomedicine, 2017, 2, 1-10.	0.7	4
128	Modeling of Interactions between the Zebrafish Hatching Enzyme ZHE1 and A Series of Metal Oxide Nanoparticles: Nano-QSAR and Causal Analysis of Inactivation Mechanisms. Nanomaterials, 2017, 7, 330.	1.9	17
129	Power Conversion Efficiency of Arylamine Organic Dyes for Dye-Sensitized Solar Cells (DSSCs) Explicit to Cobalt Electrolyte: Understanding the Structural Attributes Using a Direct QSPR Approach. Computation, 2017, 5, 2.	1.0	17
130	Evaluating the toxicity of TiO2-based nanoparticles to Chinese hamster ovary cells and Escherichia coli: a complementary experimental and computational approach. Beilstein Journal of Nanotechnology, 2017, 8, 2171-2180.	1.5	29
131	Review of Current and Emerging Approaches for Quantitative Nanostructure-Activity Relationship Modeling. , 2017, , 1704-1721.		1
132	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
133	QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955.		0
134	Theoretical Studies on Hydrogen Bonds in Anions Encapsulated by an Azamacrocyclic Receptor. Crystals, 2016, 6, 31.	1.0	2
135	Review of Current and Emerging Approaches for Quantitative Nanostructure-Activity Relationship Modeling. Journal of Nanotoxicology and Nanomedicine, 2016, 1, 1-16.	0.7	20
136	Can Toxicity for Different Species be Correlated?. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 23-51.	1.1	20
137	pHâ€controlled reaction divergence of decarboxylation versus fragmentation in reactions of dihydroxyfumarate with glyoxylate and formaldehyde: parallels to biological pathways. Journal of Physical Organic Chemistry, 2016, 29, 352-360.	0.9	5
138	Efficacy of topological informational potentials for analysis of nonequivalent atoms in molecular graphs: the case of chiral fullerenes. Journal of Mathematical Chemistry, 2016, 54, 1986-1996.	0.7	1
139	Novel enhanced applications of QSPR models: Temperature dependence of aqueous solubility. Journal of Computational Chemistry, 2016, 37, 2045-2051.	1.5	15
140	Structure and electrochemical properties for complexes of nitrocompounds with inorganic ions: A theoretical approach. Journal of Computational Chemistry, 2016, 37, 1206-1213.	1.5	2
141	International conference on â€œModeling Interaction in Biomolecules VIIâ€• held in Prague, 14â€“18 September 2015. Journal of Molecular Modeling, 2016, 22, 1.	0.8	0
142	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
143	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
144	In Silico Alkaline Hydrolysis of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine: Density Functional Theory Investigation. Environmental Science & Technology, 2016, 50, 10039-10046.	4.6	14

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145	A DFT-based QSAR study on inhibition of human dihydrofolate reductase. Journal of Molecular Graphics and Modelling, 2016, 70, 23-29.	1.3	19
146	Quantitative structure-property relationship model leading to virtual screening of fullerene derivatives: Exploring structural attributes critical for photoconversion efficiency of polymer solar cell acceptors. Nano Energy, 2016, 26, 677-691.	8.2	25
147	A comprehensive computational analysis of cathinone and its metabolites using quantum mechanical approaches and docking studies. Structural Chemistry, 2016, 27, 1291-1302.	1.0	5
148	Monte Carloâ€“based quantitative structureâ€“activity relationship models for toxicity of organic chemicals to Daphnia magna. Environmental Toxicology and Chemistry, 2016, 35, 2691-2697.	2.2	24
149	Extrapolating between toxicity endpoints of metal oxide nanoparticles: Predicting toxicity to Escherichia coli and human keratinocyte cell line (HaCaT) with Nano-QTTR. Ecotoxicology and Environmental Safety, 2016, 126, 238-244.	2.9	44
150	Computational assessment of environmental hazards of nitroaromatic compounds: influence of the type and position of aromatic ring substituents on toxicity. Structural Chemistry, 2016, 27, 191-198.	1.0	11
151	Introduction of simplex-informational descriptors for QSPR analysis of fullerene derivatives. Journal of Mathematical Chemistry, 2016, 54, 698-706.	0.7	10
152	Experimental and Theoretical Aspects of Anion Complexes with a Thiophene-Based Cryptand. Comments on Inorganic Chemistry, 2016, 36, 305-326.	3.0	6
153	Estimation of melting points of large set of persistent organic pollutants utilizing QSPR approach. Journal of Molecular Modeling, 2016, 22, 55.	0.8	14
154	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. Chemosphere, 2016, 148, 294-299.	4.2	6
155	Experimental and computational study of membrane affinity for selected energetic compounds. Chemosphere, 2016, 148, 322-327.	4.2	10
156	Causation or only correlation? Application of causal inference graphs for evaluating causality in nano-QSAR models. Nanoscale, 2016, 8, 7203-7208.	2.8	23
157	Conformations, vibrational spectra and force field of 1-methyl-2-(2â€²-pyridyl)benzimidazole: experimental data and density functional theory investigation in comparison with 2-(2â€²-pyridyl)benzimidazole. Structural Chemistry, 2016, 27, 209-219.	1.0	5
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