QSAR Modeling: Where Have You Been? Where Are You

Journal of Medicinal Chemistry
57, 4977-5010
DOI: 10.1021/jm4004285

Citation Report

#	Article	IF	Citations
2	Defining Molecular Initiating Events in the Adverse Outcome Pathway Framework for Risk Assessment. Chemical Research in Toxicology, 2014, 27, 2100-2112.	1.7	138
3	Drugâ€Like Proteinï£¿Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. Molecular Informatics, 2014, 33, 414-437.	1.4	93
4	Insights into the adsorption of simple benzene derivatives on carbon nanotubes. RSC Advances, 2014, 4, 58036-58046.	1.7	19
5	Chemometrics approach for the prediction of structureâ€“activity relationship for membrane transporter bilitranslocase. SAR and QSAR in Environmental Research, 2014, 25, 853-872.	1.0	3
6	Prediction of Compound Potency Changes in Matched Molecular Pairs Using Support Vector Regression. Journal of Chemical Information and Modeling, 2014, 54, 2654-2663.	2.5	18
7	Translation of off-target effects: prediction of ADRs by integrated experimental and computational approach. Toxicology Research, 2014, 3, 433-444.	0.9	11
8	Multiscale quantum chemical approaches to QSAR modeling and drug design. Drug Discovery Today, 2014, 19, 1921-1927.	3.2	21
9	QSAR design of triazolopyridine mGlu2 receptor positive allosteric modulators. Journal of Molecular Graphics and Modelling, 2014, 53, 82-91.	1.3	20
10	Endocrine Disruptomeâ€”An Open Source Prediction Tool for Assessing Endocrine Disruption Potential through Nuclear Receptor Binding. Journal of Chemical Information and Modeling, 2014, 54, 1254-1267.	2.5	113
11	Industrial applications of in silico ADMET. Journal of Molecular Modeling, 2014, 20, 2322.	0.8	10
12	Towards predictive resistance models for agrochemicals by combining chemical and protein similarity via proteochemometric modelling. Journal of Chemical Biology, 2014, 7, 119-123.	2.2	2
13	OOMMPPAA: A Tool To Aid Directed Synthesis by the Combined Analysis of Activity and Structural Data. Journal of Chemical Information and Modeling, 2014, 54, 2636-2646.	2.5	9
14	Is regression through origin useful in external validation of QSAR models?. European Journal of Pharmaceutical Sciences, 2014, 59, 31-35.	1.9	46
17	Natural Products as Leads in Schistosome Drug Discovery. Molecules, 2015, 20, 1872-1903.	1.7	70
18	Improved Chemical Structureâ€“Activity Modeling Through Data Augmentation. Journal of Chemical Information and Modeling, 2015, 55, 2682-2692.	2.5	37
19	RRegrs: an R package for computer-aided model selection with multiple regression models. Journal of Cheminformatics, 2015, 7, 46.	2.8	43
20	Smiles2Monomers: a link between chemical and biological structures for polymers. Journal of Cheminformatics, 2015, 7, 62.	2.8	10
21	In silico Prediction of Aqueous Solubility: a Comparative Study of Local and Global Predictive Models. Molecular Informatics, 2015, 34, 417-430.	1.4	27

#	Article	IF	Citations
22	Quantitative Structure-Antioxidant Activity Models of Isoflavonoids: A Theoretical Study. International Journal of Molecular Sciences, 2015, 16, 12891-12906.	1.8	22
23	Structure-Thermodynamics-Antioxidant Activity Relationships of Selected Natural Phenolic Acids and Derivatives: An Experimental and Theoretical Evaluation. PLoS ONE, 2015, 10, e0121276.	1.1	117
25	Computer-aided drug discovery. F1000Research, 2015, 4, 630.	0.8	49
26	Relating Caco-2 permeability to molecular properties using block relevance analysis. MedChemComm, 2015, 6, 626-629.	3.5	12
27	Newer Directions in QSAR/QSPR. Springer Briefs in Molecular Science, 2015, , 105-121.	0.1	2
28	A Primer on QSAR/QSPR Modeling. Springer Briefs in Molecular Science, 2015, , .	0.1	197
29	Biomolecular recognition of antagonists by Î±7 nicotinic acetylcholine receptor: Antagonistic mechanism and structureâ€“activity relationships studies. European Journal of Pharmaceutical Sciences, 2015, 76, 119-132.	1.9	5
30	Alternative Toxicity Testing: Analyses on Skin Sensitization, ToxCast Phases I and II, and Carcinogenicity Provide Indications on How to Model Mechanisms Linked to Adverse Outcome Pathways. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2015, 33, 422-443.	2.9	7
31	Ligand-based 3D QSAR analysis of reactivation potency of mono- and bis-pyridinium aldoximes toward VX-inhibited rat acetylcholinesterase. Journal of Molecular Graphics and Modelling, 2015, 56, 113-129.	1.3	17
32	Rcpi: R/Bioconductor package to generate various descriptors of proteins, compounds and their interactions. Bioinformatics, 2015, 31, 279-281.	1.8	110
33	Prediction and interpretation of the lipophilicity of small peptides. Journal of Computer-Aided Molecular Design, 2015, 29, 361-370.	1.3	5
34	In silico design of low molecular weight proteinâ€“protein interaction inhibitors: Overall concept and recent advances. Progress in Biophysics and Molecular Biology, 2015, 119, 20-32.	1.4	56
35	Predicting Hepatotoxicity Using ToxCast in Vitro Bioactivity and Chemical Structure. Chemical Research in Toxicology, 2015, 28, 738-751.	1.7	124
37	Role of computer-aided drug design in modern drug discovery. Archives of Pharmacal Research, 2015, 38, 1686-1701.	2.7	477
38	Monte Carlo method based QSAR modeling of maleimide derivatives as glycogen synthase kinase-3Î² inhibitors. Computers in Biology and Medicine, 2015, 64, 276-282.	3.9	22
39	4-Fluoro-3â€²,4â€²,5â€²-trimethoxychalcone as a new anti-invasive agent. From discovery to initial validation in an inÂvivo metastasis model. European Journal of Medicinal Chemistry, 2015, 101, 627-639.	2.6	13
40	Development of quantitative structure activity relationship (QSAR) model for disinfection byproduct (DBP) research: A review of methods and resources. Journal of Hazardous Materials, 2015, 299, 260-279.	6.5	88
41	On a simple approach for determining applicability domain of QSAR models. Chemometrics and Intelligent Laboratory Systems, 2015, 145, 22-29.	1.8	534

#	Article	IF	Citations
42	Cytotoxicity of cardiotonic steroids in sensitive and multidrug-resistant leukemia cells and the link with Na+/K+-ATPase. Journal of Steroid Biochemistry and Molecular Biology, 2015, 150, 97-111.	1.2	40
43	Rational drug design applied to myeloperoxidase inhibition. Free Radical Research, 2015, 49, 711-720.	1.5	9
44	In silicotools used for compound selection during target-based drug discovery and development. Expert Opinion on Drug Discovery, 2015, 10, 901-923.	2.5	16
45	kâ€Nearest neighbors optimizationâ€based outlier removal. Journal of Computational Chemistry, 2015, 36, 493-506.	1.5	20
46	Refining the chemical toolbox to be fit for educational and practical purpose for drug discovery in the 21st Century. Drug Discovery Today, 2015, 20, 1018-1026.	3.2	23
47	Prediction of cytochrome P450 mediated metabolism. Advanced Drug Delivery Reviews, 2015, 86, 61-71.	6.6	78
48	Future Avenues. , 2015, , 455-462.		3
49	Discovery and Development of Lead Compounds from Natural Sources Using Computational Approaches. , 2015, , 455-475.		10
50	Greedy and Linear Ensembles of Machine Learning Methods Outperform Single Approaches for QSPR Regression Problems. Molecular Informatics, 2015, 34, 634-647.	1.4	10
51	Activity and property landscape modeling is at the interface of chemoinformatics and medicinal chemistry. Future Medicinal Chemistry, 2015, 7, 1197-1211.	1.1	26
52	Analysis of B-Raf $$^{mathrm{V600E}}$$ V 600 E inhibitors using 2D and 3D-QSAR, molecular docking and pharmacophore studies. Molecular Diversity, 2015, 19, 915-930.	2.1	8
53	Hologram quantitative structureâ€“activity relationship and comparative molecular interaction field analysis of aminothiazole and thiazolesulfonamide as reversible LSD1 inhibitors. Future Medicinal Chemistry, 2015, 7, 1381-1394.	1.1	12
54	Predicting the Minimal Inhibitory Concentration for Antimicrobial Peptides with Rana-Box Domain. Journal of Chemical Information and Modeling, 2015, 55, 2275-2287.	2.5	17
55	Data Mining and Regression Algorithms for the Development of a QSPR Model Relating Solvent Structure and Ibuprofen Crystal Morphology. Computer Aided Chemical Engineering, 2015, , 1439-1444.	0.3	7
56	A Multi-Objective Genetic Algorithm for Outlier Removal. Journal of Chemical Information and Modeling, 2015, 55, 2507-2518.	2.5	7
57	Target-Specific Native/Decoy Pose Classifier Improves the Accuracy of Ligand Ranking in the CSAR 2013 Benchmark. Journal of Chemical Information and Modeling, 2015, 55, 63-71.	2.5	14
58	Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. Chemistry of Materials, 2015, 27, 735-743.	3.2	209
59	The utilisation of structural descriptors to predict metabolic constants of xenobiotics in mammals. Environmental Toxicology and Pharmacology, 2015, 39, 247-258.	2.0	18

#	Article	IF	Citations
60	Benefits of statistical molecular design, covariance analysis, and reference models in QSAR: a case study on acetylcholinesterase. Journal of Computer-Aided Molecular Design, 2015, 29, 199-215.	1.3	16
61	Methods for generating and applying pharmacophore models as virtual screening filters and for bioactivity profiling. Methods, 2015, 71, 113-134.	1.9	76
62	Computational design and chemometric QSAR modeling of Plasmodium falciparum carbonic anhydrase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 133-141.	1.0	12
63	Small molecule compounds targeting miRNAs for cancer therapy. Advanced Drug Delivery Reviews, 2015, 81, 104-116.	6.6	142
64	Prediction of perception using structureâ€“activity models. , 2016, , 181-200.		1
65	Is conformation a fundamental descriptor in QSAR? A case for halogenated anesthetics. Beilstein Journal of Organic Chemistry, 2016, 12, 760-768.	1.3	12
66	The History and Development of Quantitative Structure-Activity Relationships (QSARs). International Journal of Quantitative Structure-Property Relationships, 2016, 1, 1-44.	1.1	99
67	Chemoinformatics: Achievements and Challenges, a Personal View. Molecules, 2016, 21, 151.	1.7	63
68	Drug Design for CNS Diseases: Polypharmacological Profiling of Compounds Using Cheminformatic, 3D-QSAR and Virtual Screening Methodologies. Frontiers in Neuroscience, 2016, 10, 265.	1.4	62
69	MetMaxStruct: A Tversky-Similarity-Based Strategy for Analysing the (Sub)Structural Similarities of Drugs and Endogenous Metabolites. Frontiers in Pharmacology, 2016, 7, 266.	1.6	26
70	Combining QSAR Modeling and Text-Mining Techniques to Link Chemical Structures and Carcinogenic Modes of Action. Frontiers in Pharmacology, 2016, 07, 284.	1.6	11
71	Innovative Strategies to Develop Chemical Categories Using a Combination of Structural and Toxicological Properties. Frontiers in Pharmacology, 2016, 7, 321.	1.6	5
72	Optimization Algorithms for Chemoinformatics and Material-informatics. , 0, , .		1
73	Discovery of New Anti-Schistosomal Hits by Integration of QSAR-Based Virtual Screening and High Content Screening. Journal of Medicinal Chemistry, 2016, 59, 7075-7088.	2.9	67
74	Filtered circular fingerprints improve either prediction or runtime performance while retaining interpretability. Journal of Cheminformatics, 2016, 8, 60.	2.8	20
75	Prediction of CO 2 loading of amines in carbon capture process using membrane contactors: A molecular modeling. Journal of Natural Gas Science and Engineering, 2016, 33, 388-396.	2.1	17
76	Aminopyrimidine derivatives as protein kinases inhibitors. Molecular design, synthesis, and biologic activity. Russian Journal of Organic Chemistry, 2016, 52, 139-177.	0.3	26
77	Modern approaches to accelerate discovery of new antischistosomal drugs. Expert Opinion on Drug Discovery, 2016, 11, 557-567.	2.5	19

#	Article	IF	Citations
78	A comprehensive company database analysis of biological assay variability. Drug Discovery Today, 2016, 21, 1213-1221.	3.2	20
79	Hybrid Docking-Nano-QSPR: An Alternative Approach for Prediction of Chemicals Adsorption on Nanoparticles. Nano, 2016, 11, 1650078.	0.5	10
80	Secondary pharmacology: screening and interpretation of off-target activities â€“ focus on translation. Drug Discovery Today, 2016, 21, 1232-1242.	3.2	52
81	Experimental Binding Energies in Supramolecular Complexes. Chemical Reviews, 2016, 116, 5216-5300.	23.0	395
82	QSAR modeling for predicting reproductive toxicity of chemicals in rats for regulatory purposes. Toxicology Research, 2016, 5, 1029-1038.	0.9	21
83	Computational Structureâ€“Activity Relationship Studies of Epigenetic Target Inhibitors. , 2016, , 359-384.		1
84	A D3R prospective evaluation of machine learning for protein-ligand scoring. Journal of Computer-Aided Molecular Design, 2016, 30, 761-771.	1.3	15
85	Using Molecular Initiating Events To Generate 2D Structureâ€“Activity Relationships for Toxicity Screening. Chemical Research in Toxicology, 2016, 29, 1611-1627.	1.7	15
86	Automatically updating predictive modeling workflows support decision-making in drug design. Future Medicinal Chemistry, 2016, 8, 1779-1796.	1.1	13
87	Computational Modeling of Î²-Secretase 1 (BACE-1) Inhibitors Using Ligand Based Approaches. Journal of Chemical Information and Modeling, 2016, 56, 1936-1949.	2.5	166
88	QSAR models of human data can enrich or replace LLNA testing for human skin sensitization. Green Chemistry, 2016, 18, 6501-6515.	4.6	42
89	Learnings from quantitative structureâ€“activity relationship (QSAR) studies with respect to food protein-derived bioactive peptides: a review. RSC Advances, 2016, 6, 75400-75413.	1.7	73
90	Computational Method for the Systematic Identification of Analog Series and Key Compounds Representing Series and Their Biological Activity Profiles. Journal of Medicinal Chemistry, 2016, 59, 7667-7676.	2.9	50
91	Preselection of A- and B- modified d-homo lactone and d-seco androstane derivatives as potent compounds with antiproliferative activity against breast and prostate cancer cells â€“ QSAR approach and molecular docking analysis. European Journal of Pharmaceutical Sciences, 2016, 93, 107-113.	1.9	11
92	Parametrization of nanoparticles: development of full-particle nanodescriptors. Nanoscale, 2016, 8, 16243-16250.	2.8	30
93	Materials Informatics: Statistical Modeling in Material Science. Molecular Informatics, 2016, 35, 568-579.	1.4	13
94	Partition coefficients for the SAMPL5 challenge using transfer free energies. Journal of Computer-Aided Molecular Design, 2016, 30, 1129-1138.	1.3	19
95	AutoQSAR: an automated machine learning tool for best-practice quantitative structureâ€“activity relationship modeling. Future Medicinal Chemistry, 2016, 8, 1825-1839.	1.1	102

#	Article	IF	Citations
96	Comprehensive QSRR modeling as a starting point in characterization and further development of anticancer drugs based on 17Î±-picolyl and 17(E)-picolinylidene androstane structures. European Journal of Pharmaceutical Sciences, 2016, 93, 1-10.	1.9	15
97	Electron affinity of tricyclic, bicyclic, and monocyclic compounds containing cyanoenones correlates with their potency as inducers of a cytoprotective enzyme. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 4345-4349.	1.0	2
99	Structural and Physico-Chemical Interpretation (SPCI) of QSAR Models and Its Comparison with Matched Molecular Pair Analysis. Journal of Chemical Information and Modeling, 2016, 56, 1455-1469.	2.5	35
100	Ligand Affinity Prediction with Multi-pattern Kernels. Lecture Notes in Computer Science, 2016, , 474-489.	1.0	4
101	QSAR modeling of bis-quinolinium and bis-isoquinolinium compounds as acetylcholine esterase inhibitors based on the Monte Carlo methodâ€"the implication for Myasthenia gravis treatment. Medicinal Chemistry Research, 2016, 25, 2989-2998.	1.1	9
102	Predictive toxicology today: the transition from biological knowledge to practicable models. Expert Opinion on Drug Metabolism and Toxicology, 2016, 12, 989-992.	1.5	16
103	Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. Briefings in Bioinformatics, 2018, 19, bbw105.	3.2	17
104	Support vector regression-guided unravelling: antioxidant capacity and quantitative structure-activity relationship predict reduction and promotion effects of flavonoids on acrylamide formation. Scientific Reports, 2016, 6, 32368.	1.6	4
105	Improving confidence in (Q)SAR predictions under Canadaâ€™s Chemicals Management Plan â€“ a chemical space approach. SAR and QSAR in Environmental Research, 2016, 27, 851-863.	1.0	6
106	Cheminformatics Modeling of Adverse Drug Responses by Clinically Relevant Mutants of Human Androgen Receptor. Journal of Chemical Information and Modeling, 2016, 56, 2507-2516.	2.5	16
107	The â€œdouble cross-validationâ€•software tool for MLR QSAR model development. Chemometrics and Intelligent Laboratory Systems, 2016, 159, 108-126.	1.8	72
108	Electrochemical interpretation of parabolic relation between the hydrophobicity and the permeability of tetraalkylammonium chlorides. Journal of Electroanalytical Chemistry, 2016, 782, 161-167.	1.9	2
109	Current Status and Future Challenges in Molecular Design for Reduced Hazard. ACS Sustainable Chemistry and Engineering, 2016, 4, 5900-5906.	3.2	35
110	Mixtures, metabolites, ionic liquids: a new measure to evaluate similarity between complex chemical systems. Journal of Cheminformatics, 2016, 8, 49.	2.8	10
111	Trust, but Verify II: A Practical Guide to Chemogenomics Data Curation. Journal of Chemical Information and Modeling, 2016, 56, 1243-1252.	2.5	228
112	The Consultancy Activity on In Silico Models for Genotoxic Prediction of Pharmaceutical Impurities. Methods in Molecular Biology, 2016, 1425, 511-529.	0.4	6
113	In Silico Study of In Vitro GPCR Assays by QSAR Modeling. Methods in Molecular Biology, 2016, 1425, 361-381.	0.4	14
114	Descriptors and their selection methods in QSAR analysis: paradigm for drug design. Drug Discovery Today, 2016, 21, 1291-1302.	3.2	235

#	Article	IF	Citations
115	QSAR-Driven Discovery of Novel Chemical Scaffolds Active against Schistosoma mansoni. Journal of Chemical Information and Modeling, 2016, 56, 1357-1372.	2.5	47
116	A data-based exploration of the adverse outcome pathway for skin sensitization points to the necessary requirements for its prediction with alternative methods. Regulatory Toxicology and Pharmacology, 2016, 78, 45-52.	1.3	9
117	Monte Carlo-based QSAR modeling of dimeric pyridinium compounds and drug design of new potent acetylcholine esterase inhibitors for potential therapy of myasthenia gravis. Structural Chemistry, 2016, 27, 1511-1519.	1.0	26
118	A renaissance of neural networks in drug discovery. Expert Opinion on Drug Discovery, 2016, 11, 785-795.	2.5	182
119	The Use of In Silico Models Within a Large Pharmaceutical Company. Methods in Molecular Biology, 2016, 1425, 475-510.	0.4	3
120	Alarms about structural alerts. Green Chemistry, 2016, 18, 4348-4360.	4.6	103
121	Imageâ€Based Analysis to Predict the Activity of Tariquidar Analogs as Pâ€Glycoprotein Inhibitors: The Importance of External Validation. Archiv Der Pharmazie, 2016, 349, 124-131.	2.1	4
122	Solution-Binding and Molecular Docking Approaches Combine to Provide an Expanded View of Multidrug Recognition in the MDR Gene Regulator BmrR. Journal of Chemical Information and Modeling, 2016, 56, 377-389.	2.5	4
123	How to rank and discriminate artificial neural networks? Case study: prediction of anticancer activity of 17-picolyl and 17-picolinylidene androstane derivatives. Journal of the Iranian Chemical Society, 2016, 13, 499-507.	1.2	9
124	Computer-Aided Drug Discovery Approaches against the Tropical Infectious Diseases Malaria, Tuberculosis, Trypanosomiasis, and Leishmaniasis. ACS Infectious Diseases, 2016, 2, 8-31.	1.8	48
125	QSAR studies in the discovery of novel type-II diabetic therapies. Expert Opinion on Drug Discovery, 2016, 11, 197-214.	2.5	25
126	Toward a unifying strategy for the structure-based prediction of toxicological endpoints. Archives of Toxicology, 2016, 90, 2445-2460.	1.9	9
127	Improving quantitative structureâ€“activity relationship models using Artificial Neural Networks trained with dropout. Journal of Computer-Aided Molecular Design, 2016, 30, 177-189.	1.3	42
128	Structure-guided unravelling: Phenolic hydroxyls contribute to reduction of acrylamide using multiplex quantitative structureâ€“activity relationship modelling. Food Chemistry, 2016, 199, 492-501.	4.2	24
129	Structureâ€“response relationship in electrospray ionization-mass spectrometry of sartans by artificial neural networks. Journal of Chromatography A, 2016, 1438, 123-132.	1.8	26
130	PQSAR: The membrane quantitative structure-activity relationships in cheminformatics. Expert Systems With Applications, 2016, 54, 219-227.	4.4	5
131	High-throughput imaging-based nephrotoxicity prediction for xenobiotics with diverse chemical structures. Archives of Toxicology, 2016, 90, 2793-2808.	1.9	51
132	QSAR analysis of substituent effects on tambjamine anion transporters. Chemical Science, 2016, 7, 1600-1608.	3.7	47

#	Article	IF	Citations
133	Recent advances, and unresolved issues, in the application of computational modelling to the prediction of the biological effects of nanomaterials. Toxicology and Applied Pharmacology, 2016, 299, 96-100.	1.3	67
134	Novel triazolothiadiazines act as potent anticancer agents in liver cancer cells through Akt and ASK-1 proteins. Bioorganic and Medicinal Chemistry, 2016, 24, 858-872.	1.4	31
135	Systematic assessment of analog relationships between bioactive compounds and promiscuity of analog sets. MedChemComm, 2016, 7, 230-236.	3.5	4
136	In silico assessment of adverse drug reactions and associated mechanisms. Drug Discovery Today, 2016, 21, 58-71.	3.2	51
137	Cheminformatics-aided pharmacovigilance: application to Stevens-Johnson Syndrome. Journal of the American Medical Informatics Association: JAMIA, 2016, 23, 968-978.	2.2	13
138	Convergent QSAR studies on a series of NK₃ receptor antagonists for schizophrenia treatment. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 283-294.	2.5	10
139	Multitarget compounds bearing tacrine- and donepezil-like structural and functional motifs for the potential treatment of Alzheimer's disease. Progress in Neurobiology, 2017, 151, 4-34.	2.8	128
140	Computational study involving identification of endocrine disrupting potential of herbicides: Its implication in TDS and cancer progression in CRPC patients. Chemosphere, 2017, 173, 395-403.	4.2	22
141	Chembench: A Publicly Accessible, Integrated Cheminformatics Portal. Journal of Chemical Information and Modeling, 2017, 57, 105-108.	2.5	47
142	Development and evaluation of predictive model for bovine serum albumin-water partition coefficients of neutral organic chemicals. Ecotoxicology and Environmental Safety, 2017, 138, 92-97.	2.9	6
143	CADD medicine: design is the potion that can cure my disease. Journal of Computer-Aided Molecular Design, 2017, 31, 249-253.	1.3	9
144	Molecular Descriptors. , 2017, , 2065-2093.		30
145	How important is to detect systematic error in predictions and understand statistical applicability domain of QSAR models?. Chemometrics and Intelligent Laboratory Systems, 2017, 162, 44-54.	1.8	120
146	QSAR study of dipeptidyl peptidase-4 inhibitors based on the Monte Carlo method. Medicinal Chemistry Research, 2017, 26, 796-804.	1.1	24
147	QSAR analysis for 6-arylpyrazine-2-carboxamides as Trypanosoma brucei inhibitors. SAR and QSAR in Environmental Research, 2017, 28, 165-177.	1.0	16
148	The importance of the glycosylation of antimicrobial peptides: natural and synthetic approaches. Drug Discovery Today, 2017, 22, 919-926.	3.2	73
149	Prediction of acute toxicity of emerging contaminants on the water flea Daphnia magna by Ant Colony Optimizationâ€“Support Vector Machine QSTR models. Environmental Sciences: Processes and Impacts, 2017, 19, 438-448.	1.7	62
150	History of EPI Suiteâ„¢ and future perspectives on chemical property estimation in US Toxic Substances Control Act new chemical risk assessments. Environmental Sciences: Processes and Impacts, 2017, 19, 203-212.	1.7	73

#	Article	IF	Citations
151	Quantitative structureâ€“activity relationship analysis and virtual screening studies for identifying HDAC2 inhibitors from known HDAC bioactive chemical libraries. SAR and QSAR in Environmental Research, 2017, 28, 199-220.	1.0	22
152	Design, Synthesis, Structureâ€“Activity Relationship Studies, and Three-Dimensional Quantitative Structureâ€“Activity Relationship (3D-QSAR) Modeling of a Series of O-Biphenyl Carbamates as Dual Modulators of Dopamine D3 Receptor and Fatty Acid Amide Hydrolase. Journal of Medicinal Chemistry, 2017, 60, 2287-2304.	2.9	28
153	Prediction of N-Methyl-D-Aspartate Receptor GluN1-Ligand Binding Affinity by a Novel SVM-Pose/SVM-Score Combinatorial Ensemble Docking Scheme. Scientific Reports, 2017, 7, 40053.	1.6	19
154	Cheminformatics Modeling of Amine Solutions for Assessing their CO₂Absorption Properties. Molecular Informatics, 2017, 36, 1600143.	1.4	12
155	Virulence factor activity relationships (VFARs): a bioinformatics perspective. Environmental Sciences: Processes and Impacts, 2017, 19, 247-260.	1.7	16
156	Using Delaunay triangulation and Voronoi tessellation to predict the toxicities of binary mixtures containing hormetic compound. Scientific Reports, 2017, 7, 43473.	1.6	16
157	Exploring beneficial structural features of ionic surfactants for wettability alteration of carbonate rocks using QSPR modeling technique. Journal of Molecular Liquids, 2017, 240, 196-208.	2.3	4
158	QSAR-driven design, synthesis and discovery of potent chalcone derivatives with antitubercular activity. European Journal of Medicinal Chemistry, 2017, 137, 126-138.	2.6	96
159	Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 1013-1017.	2.5	79
160	QSAR studies of the bioactivity of hepatitis C virus (HCV) NS3/4A protease inhibitors by multiple linear regression (MLR) and support vector machine (SVM). Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2931-2938.	1.0	20
161	Modulating and evaluating receptor promiscuity through directed evolution and modeling. Protein Engineering, Design and Selection, 2017, 30, 455-465.	1.0	6
162	Best Practices of Computer-Aided Drug Discovery: Lessons Learned from the Development of a Preclinical Candidate for Prostate Cancer with a New Mechanism of Action. Journal of Chemical Information and Modeling, 2017, 57, 1018-1028.	2.5	92
163	In Silico ADME Techniques Used in Early-Phase Drug Discovery. AAPS Advances in the Pharmaceutical Sciences Series, 2017, , 81-117.	0.2	15
164	Quantitative structureâ€“activity relationships study of potent pyridinone scaffold derivatives as HIV-1 integrase inhibitors with therapeutic applications. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750038.	1.8	12
165	Novel 4-acetamide-2-alkylthio-N-acetanilides resembling nimesulide: Synthesis, cell viability evaluation and in silico studies. Bioorganic and Medicinal Chemistry, 2017, 25, 4304-4313.	1.4	10
166	Documenting and harnessing the biological potential of molecules in Distributed Drug Discovery (D3) virtual catalogs. Chemical Biology and Drug Design, 2017, 90, 909-918.	1.5	6
167	Predicting the Enzymatic Hydrolysis Halfâ€lives of New Chemicals Using Support Vector Regression Models Based on Stepwise Feature Elimination. Molecular Informatics, 2017, 36, 1600153.	1.4	3
168	Towards the Revival of Interpretable QSAR Models. Challenges and Advances in Computational Chemistry and Physics, 2017, , 3-55.	0.6	17

#	Article	IF	Citations
169	Exploring the QSARâ€™s predictive truthfulness of the novel N-tuple discrete derivative indices on benchmark datasets. SAR and QSAR in Environmental Research, 2017, 28, 367-389.	1.0	6
170	The advancement of multidimensional QSAR for novel drug discovery - where are we headed?. Expert Opinion on Drug Discovery, 2017, 12, 1-16.	2.5	32
171	Kinetic study of Friedel-Crafts acylation reactions over hierarchical MCM-22 zeolites. Molecular Catalysis, 2017, 434, 175-183.	1.0	19
172	An integrated approach with new strategies for QSAR models and lead optimization. BMC Genomics, 2017, 18, 104.	1.2	5
173	Molecular Modelling Approaches for the Analysis of Histamine Receptors and Their Interaction with Ligands. Handbook of Experimental Pharmacology, 2017, 241, 31-61.	0.9	3
174	Sustainable Practices in Medicinal Chemistry Part 2: Green by Design. Journal of Medicinal Chemistry, 2017, 60, 5955-5968.	2.9	17
175	Insight into the structural requirements of pyrimidine-based phosphodiesterase 10A (PDE10A) inhibitors by multiple validated 3D QSAR approaches. SAR and QSAR in Environmental Research, 2017, 28, 253-273.	1.0	22
176	A QSAR study of integrase strand transfer inhibitors based on a large set of pyrimidine, pyrimidone, and pyridopyrazine carboxamide derivatives. Journal of Molecular Structure, 2017, 1141, 252-260.	1.8	9
177	Monte Carlo method based QSAR modelling of natural lipase inhibitors using hybrid optimal descriptors. SAR and QSAR in Environmental Research, 2017, 28, 179-197.	1.0	32
178	A review of quantitative structureâ€“property relationships for the fate of ionizable organic chemicals in water matrices and identification of knowledge gaps. Environmental Sciences: Processes and Impacts, 2017, 19, 221-246.	1.7	34
179	Comprehensive comparison of twenty structural characterization scales applied as QSAM of antimicrobial dodecapeptides derived from Bac2A against P. aeruginosa. Journal of Molecular Graphics and Modelling, 2017, 71, 88-95.	1.3	4
180	In silico prediction of the mutagenicity of nitroaromatic compounds using a novel two-QSAR approach. Toxicology in Vitro, 2017, 40, 102-114.	1.1	24
181	Fragment Prioritization on a Large Mutagenicity Dataset. Molecular Informatics, 2017, 36, 1600133.	1.4	10
182	Azolium analogues as CDK4 inhibitors: Pharmacophore modeling, 3D QSAR study and new lead drug discovery. Journal of Molecular Structure, 2017, 1134, 482-491.	1.8	13
183	Distinguishing between expert and statistical systems for application under ICH M7. Regulatory Toxicology and Pharmacology, 2017, 84, 124-130.	1.3	25
184	Advantages of Relative versus Absolute Data for the Development of Quantitative Structureâ€“Activity Relationship Classification Models. Journal of Chemical Information and Modeling, 2017, 57, 2776-2788.	2.5	12
185	Assessment of predictivity of volatile organic compounds carcinogenicity and mutagenicity by freeware in silico models. Regulatory Toxicology and Pharmacology, 2017, 91, 1-8.	1.3	16
186	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. Journal of Physical Chemistry A, 2017, 121, 8086-8096.	1.1	15

#	Article	IF	Citations
187	Support Vector Machine Classification and Regression Prioritize Different Structural Features for Binary Compound Activity and Potency Value Prediction. ACS Omega, 2017, 2, 6371-6379.	1.6	75
188	Interpretation of Quantitative Structureâ€“Activity Relationship Models: Past, Present, and Future. Journal of Chemical Information and Modeling, 2017, 57, 2618-2639.	2.5	168
189	Integrating computational methods to predict mutagenicity of aromatic azo compounds. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2017, 35, 239-257.	2.9	7
190	Quantitative Nanostructureâ€“Activity Relationships: Methods, Case Studies, and Perspectives. Nanomedicine and Nanotoxicology, 2017, , 361-376.	0.1	2
191	Building Predictive Adverse Outcome Pathway Models: Role of Molecular Initiating Events and Structureâ€“Activity Relationships. Applied in Vitro Toxicology, 2017, 3, 265-270.	0.6	2
192	Reaction: Molecular Modeling for Novel Antibacterials. CheM, 2017, 3, 13-14.	5.8	3
193	Comparison of the Predictive Performance and Interpretability of Random Forest and Linear Models on Benchmark Data Sets. Journal of Chemical Information and Modeling, 2017, 57, 1773-1792.	2.5	88
194	Convolutional Embedding of Attributed Molecular Graphs for Physical Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 1757-1772.	2.5	317
195	In silico identification of milk antihypertensive di- and tripeptides involved in angiotensin Iâ€“converting enzyme inhibitory activity. Nutrition Research, 2017, 46, 22-30.	1.3	26
196	3D-QSAR studies on Maslinic acid analogs for Anticancer activity against Breast Cancer cell line MCF-7. Scientific Reports, 2017, 7, 6019.	1.6	68
197	QSPR studies on the photoinduced-fluorescence behaviour of pharmaceuticals and pesticides. SAR and QSAR in Environmental Research, 2017, 28, 609-620.	1.0	6
198	Rapid Life-Cycle Impact Screening Using Artificial Neural Networks. Environmental Science & Technology, 2017, 51, 10777-10785.	4.6	67
199	Molecular Structure-Based Large-Scale Prediction of Chemical-Induced Gene Expression Changes. Journal of Chemical Information and Modeling, 2017, 57, 2194-2202.	2.5	5
200	Development of a pharmacophore for cruzain using oxadiazoles as virtual molecular probes: quantitative structureâ€“activity relationship studies. Journal of Computer-Aided Molecular Design, 2017, 31, 801-816.	1.3	9
201	Shallow Representation Learning via Kernel PCA Improves QSAR Modelability. Journal of Chemical Information and Modeling, 2017, 57, 1859-1867.	2.5	13
203	The Future of Animal Research: Guesstimates on Technical and Ethical Developments. , 0, , 163-174.		0
204	Predicting Nanoâ€“Bio Interactions by Integrating Nanoparticle Libraries and Quantitative Nanostructure Activity Relationship Modeling. ACS Nano, 2017, 11, 12641-12649.	7.3	80
205	Synthesis meets theory: Past, present and future of rational chemistry. Physical Sciences Reviews, 2017, 2, .	0.8	3

#	Article	IF	Citations
206	Topological pattern for the search of new active drugs against methicillin resistant Staphylococcus aureus. European Journal of Medicinal Chemistry, 2017, 138, 807-815.	2.6	16
207	Towards molecular design using 2D-molecular contour maps obtained from PLS regression coefficients. Molecular Physics, 2017, 115, 3044-3050.	0.8	4
208	Review of (Q)SAR models for regulatory assessment of nanomaterials risks. NanoImpact, 2017, 8, 48-58.	2.4	45
209	Impact of geometry optimization methods on QSAR modelling: A case study for predicting human serum albumin binding affinity. SAR and QSAR in Environmental Research, 2017, 28, 491-509.	1.0	10
210	Predictive cartography of metal binders using generative topographic mapping. Journal of Computer-Aided Molecular Design, 2017, 31, 701-714.	1.3	6
211	A Mechanistic Model for Predicting Lung Inflammogenicity of Oxide Nanoparticles. Toxicological Sciences, 2017, 159, 339-353.	1.4	7
212	Helping to improve the practice of cheminformatics. Journal of Cheminformatics, 2017, 9, 40.	2.8	3
213	RANdom SAmple Consensus (RANSAC) algorithm for material-informatics: application to photovoltaic solar cells. Journal of Cheminformatics, 2017, 9, 34.	2.8	18
214	Comprehensive Network Map of ADMEâ€Tox Databases. Molecular Informatics, 2017, 36, 1700029.	1.4	5
215	Sweetness prediction of natural compounds. Food Chemistry, 2017, 221, 1421-1425.	4.2	47
216	QSAR modeling for anti-human African trypanosomiasis activity of substituted 2-Phenylimidazopyridines. Journal of Molecular Structure, 2017, 1130, 711-718.	1.8	26
217	Public (Q)SAR Services, Integrated Modeling Environments, and Model Repositories on the Web: State of the Art and Perspectives for Future Development. Molecular Informatics, 2017, 36, 1600082.	1.4	32
218	Computational platform Way2Drug: from the prediction of biological activity to drug repurposing. Russian Chemical Bulletin, 2017, 66, 1832-1841.	0.4	60
219	Computer-Assisted Decision Support for Student Admissions Based on Their Predicted Academic Performance. American Journal of Pharmaceutical Education, 2017, 81, 46.	0.7	16
220	vNN Web Server for ADMET Predictions. Frontiers in Pharmacology, 2017, 8, 889.	1.6	148
221	A Systematic Review of Computational Drug Discovery, Development, and Repurposing for Ebola Virus Disease Treatment. Molecules, 2017, 22, 1777.	1.7	28
222	Modernization of Enoxaparin Molecular Weight Determination Using Homogeneous Standards. Pharmaceuticals, 2017, 10, 66.	1.7	5
223	Chalcone Derivatives: Promising Starting Points for Drug Design. Molecules, 2017, 22, 1210.	1.7	261

#	Article	IF	Citations
224	Drug discovery. , 2017, , 281-420.		1
225	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. , 2017, , 329-378.		27
226	2D-QSAR and 3D-QSAR Analyses for EGFR Inhibitors. BioMed Research International, 2017, 2017, 1-11.	0.9	26
227	Computational Models to Predict Toxicological Endpoints in Drug Discovery and Strategies for Data Integration. , 2017, , 233-258.		2
228	The use of QSAR methods for determination of n-octanol/water partition coefficient using the example of hydroxyester HE-1. E3S Web of Conferences, 2017, 19, 02034.	0.2	1
229	Knowledge graph prediction of unknown adverse drug reactions and validation in electronic health records. Scientific Reports, 2017, 7, 16416.	1.6	69
230	Structural Chemogenomics Databases to Navigate Proteinâ€“Ligand Interaction Space. , 2017, , 444-471.		1
231	EXPERIMENTAL STUDY AND HIGH DIMENSIONAL QSAR MODELLING OF PHENYLPROPANOIDS OF ALPINIA GALANGA AS CORROSION INHIBITORS ON MILD STEEL. Jurnal Teknologi (Sciences and Engineering), 2017, 79, .	0.3	1
232	Precision and recall oncology: combining multiple gene mutations for improved identification of drug-sensitive tumours. Oncotarget, 2017, 8, 97025-97040.	0.8	31
233	Exploiting mAb structure characteristics for a directed QbD implementation in early process development. Critical Reviews in Biotechnology, 2018, 38, 957-970.	5.1	8
234	QSAR classification and regression models for Î²-secretase inhibitors using relative distance matrices. SAR and QSAR in Environmental Research, 2018, 29, 355-383.	1.0	5
235	An automated framework for QSAR model building. Journal of Cheminformatics, 2018, 10, 1.	2.8	114
236	QSAR models for describing the toxicological eï¬€ects of ILs against Candida albicans based on norm indexes. Chemosphere, 2018, 201, 417-424.	4.2	21
241	Classical and 3D QSAR studies of larvicidal monoterpenes against Aedes aegypti: new molecular insights for the rational design of more active compounds. Structural Chemistry, 2018, 29, 1287-1297.	1.0	13
242	Progress with modeling activity landscapes in drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 605-615.	2.5	21
243	In silico toxicology protocols. Regulatory Toxicology and Pharmacology, 2018, 96, 1-17.	1.3	159
244	Representing molecular and materials data for unsupervised machine learning. Molecular Simulation, 2018, 44, 905-920.	0.9	18
245	QSPR modeling of optical rotation of amino acids using specific quantum chemical descriptors. Journal of Molecular Modeling, 2018, 24, 59.	0.8	8

#	Article	IF	Citations
246	Computer-aided Discovery of Peptides that Specifically Attack Bacterial Biofilms. Scientific Reports, 2018, 8, 1871.	1.6	92
247	In-silico prediction of sweetness using structure-activity relationship models. Food Chemistry, 2018, 253, 127-131.	4.2	24
248	Consensus QSAR modelling of SIRT1 activators using simplex representation of molecular structure. SAR and QSAR in Environmental Research, 2018, 29, 277-294.	1.0	7
249	Meta-QSAR: a large-scale application of meta-learning to drug design and discovery. Machine Learning, 2018, 107, 285-311.	3.4	55
250	A Perspective and a New Integrated Computational Strategy for Skin Sensitization Assessment. ACS Sustainable Chemistry and Engineering, 2018, 6, 2845-2859.	3.2	35
251	Computational method for estimating progression saturation of analog series. RSC Advances, 2018, 8, 5484-5492.	1.7	12
252	Is it possible to improve the quality of predictions from an â€œintelligentâ€•use of multiple QSAR/QSPR/QSTR models?. Journal of Chemometrics, 2018, 32, e2992.	0.7	90
253	Application of SAR methods toward inhibition of bacterial peptidoglycan metabolizing enzymes. Journal of Chemometrics, 2018, 32, e3007.	0.7	1
254	Molecular simulations in drug delivery: Opportunities and challenges. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1358.	6.2	54
255	Ligand-based computer aided drug design reveals new tropomycin receptor kinase a (TrkA) inhibitors. Journal of Molecular Graphics and Modelling, 2018, 80, 327-352.	1.3	9
256	Assessment and Reproducibility of Quantitative Structureâ€“Activity Relationship Models by the Nonexpert. Journal of Chemical Information and Modeling, 2018, 58, 673-682.	2.5	29
257	Recent trends and analytical challenges in plant bioactive peptide separation, identification and validation. Analytical and Bioanalytical Chemistry, 2018, 410, 3425-3444.	1.9	110
258	Predictive and mechanistic multivariate linear regression models for reaction development. Chemical Science, 2018, 9, 2398-2412.	3.7	248
261	The use of a quantitative structure-activity relationship (QSAR) model to predict GABA-A receptor binding of newly emerging benzodiazepines. Science and Justice - Journal of the Forensic Science Society, 2018, 58, 219-225.	1.3	30
262	Toward the Rational Design of Sustainable Hair Dyes Using Cheminformatics Approaches: Step 1. Database Development and Analysis. ACS Sustainable Chemistry and Engineering, 2018, 6, 2344-2352.	3.2	15
263	In Silico Approaches for Predictive Toxicology. , 2018, , 91-109.		19
264	Scoping the polymer genome: A roadmap for rational polymer dielectrics design and beyond. Materials Today, 2018, 21, 785-796.	8.3	143
265	Atom Pair Contribution Method: Fast and General Procedure To Predict Molecular Formation Enthalpies. Journal of Chemical Information and Modeling, 2018, 58, 12-26.	2.5	21

#	Article	IF	Citations
266	Statistical models are able to predict ionic liquid viscosity across a wide range of chemical functionalities and experimental conditions. Molecular Systems Design and Engineering, 2018, 3, 253-263.	1.7	28
267	Combining machine learning models of in vitro and in vivo bioassays improves rat carcinogenicity prediction. Regulatory Toxicology and Pharmacology, 2018, 94, 8-15.	1.3	17
268	In Silico Studies Designed to Select Sesquiterpene Lactones with Potential Antichagasic Activity from an Inâ€House Asteraceae Database. ChemMedChem, 2018, 13, 634-645.	1.6	34
269	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. Medicinal Research Reviews, 2018, 38, 914-950.	5.0	38
270	Discrete Fourier Transform-Based Multivariate Image Analysis: Application to Modeling of Aromatase Inhibitory Activity. ACS Combinatorial Science, 2018, 20, 75-81.	3.8	14
271	In Silico Pharmacoepidemiologic Evaluation of Drug-Induced Cardiovascular Complications Using Combined Classifiers. Journal of Chemical Information and Modeling, 2018, 58, 943-956.	2.5	37
272	Computer-Aided Drug Discovery. , 2018, , 7-24.		11
273	Machine Learning in Computer-Aided Synthesis Planning. Accounts of Chemical Research, 2018, 51, 1281-1289.	7.6	430
275	Conformal Regression for Quantitative Structureâ€“Activity Relationship Modelingâ€”Quantifying Prediction Uncertainty. Journal of Chemical Information and Modeling, 2018, 58, 1132-1140.	2.5	35
276	A new data representation based on relative measurements and fingerprint patterns for the development of QSAR regression models. Chemometrics and Intelligent Laboratory Systems, 2018, 176, 53-65.	1.8	4
277	Prediction of ionic liquids viscosity at variable temperatures and pressures. Chemical Engineering Science, 2018, 184, 134-140.	1.9	46
278	Dempster-Shafer theory for combining in silico evidence and estimating uncertainty in chemical risk assessment. Computational Toxicology, 2018, 6, 16-31.	1.8	23
279	Performance of In Silico Models for Mutagenicity Prediction of Food Contact Materials. Toxicological Sciences, 2018, 163, 632-638.	1.4	14
280	Computational modeling approaches to quantitative structureâ€“binding kinetics relationships in drug discovery. Drug Discovery Today, 2018, 23, 1396-1406.	3.2	20
281	Can we accelerate medicinal chemistry by augmenting the chemist with Big Data and artificial intelligence?. Drug Discovery Today, 2018, 23, 1373-1384.	3.2	32
282	On the virtues of automated quantitative structureâ€“activity relationship: the new kid on the block. Future Medicinal Chemistry, 2018, 10, 335-342.	1.1	12
283	Discovery of an Orally Bioavailable Inhibitor of Defective in Cullin Neddylation 1 (DCN1)-Mediated Cullin Neddylation. Journal of Medicinal Chemistry, 2018, 61, 2694-2706.	2.9	41
284	Performance of machine learning algorithms for qualitative and quantitative prediction drug blockade of hERG1 channel. Computational Toxicology, 2018, 6, 55-63.	1.8	38

#	Article	IF	Citations
285	The Application of Modeling and Prediction to the Formation and Stability of Amorphous Solid Dispersions. Journal of Pharmaceutical Sciences, 2018, 107, 57-74.	1.6	62
286	The application of molecular topology for ulcerative colitis drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 89-101.	2.5	2
287	From Classical Toxicology to Tox21: Some Critical Conceptual and Technological Advances in the Molecular Understanding of the Toxic Response Beginning From the Last Quarter of the 20th Century. Toxicological Sciences, 2018, 161, 5-22.	1.4	29
288	Perspectives from the NanoSafety Modelling Cluster on the validation criteria for (Q)SAR models used in nanotechnology. Food and Chemical Toxicology, 2018, 112, 478-494.	1.8	27
289	QSAR study of 2,4-dihydro-3H-1,2,4-triazol-3-ones derivatives as angiotensin II AT1 receptor antagonists based on the Monte Carlo method. Structural Chemistry, 2018, 29, 441-449.	1.0	40
290	Binding affinity toward human prion protein of some anti-prion compounds â€" Assessment based on QSAR modeling, molecular docking and non-parametric ranking. European Journal of Pharmaceutical Sciences, 2018, 111, 215-225.	1.9	9
291	Multiâ€objective Optimization of Benzamide Derivatives as Rho Kinase Inhibitors. Molecular Informatics, 2018, 37, 1700080.	1.4	6
292	Integrative approaches in HIV â€1 nonâ€nucleoside reverse transcriptase inhibitor design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1328.	6.2	10
293	Interaction prediction in structure-based virtual screening using deep learning. Computers in Biology and Medicine, 2018, 100, 253-258.	3.9	76
294	Chemical reaction vector embeddings: towards predicting drug metabolism in the human gut microbiome. , 2018, , .		12
295	QSAR modeling of dihydrofolate reductase inhibitors as a therapeutic target for multiresistant bacteria. Structural Chemistry, 2018, 29, 541-551.	1.0	25
296	Identification of Novel Aurora Kinase A (AURKA) Inhibitors via Hierarchical Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2018, 58, 36-47.	2.5	24
297	Allosteric mechanism of quinoline inhibitors for <scp>HIV RT</scp>â€associated <scp>RN</scp>ase with <scp>MD</scp> simulation and dynamics fluctuation network. Chemical Biology and Drug Design, 2018, 91, 805-816.	1.5	6
298	Lessons learned in induced fit docking and metadynamics in the Drug Design Data Resource Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 45-58.	1.3	18
299	Quantitative structureâ€"activity relationship (QSAR) directed the discovery of 3â€(pyridinâ€2â€yl)benzenesulfonamide derivatives as novel herbicidal agents. Pest Management Science, 2018, 74, 189-199.	1.7	19
300	Strategies of Virtual Screening in Medicinal Chemistry. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 134-160.	1.1	12
301	IL-Net: Using Expert Knowledge to Guide the Design of Furcated Neural Networks. , 2018, , .		3
302	chemmodlab: a cheminformatics modeling laboratoryÂR package for fitting and assessing machine learning models. Journal of Cheminformatics, 2018, 10, 57.	2.8	3

#	Article	IF	Citations
303	Antimicrobial peptide similarity and classification through rough set theory using physicochemical boundaries. BMC Bioinformatics, 2018, 19, 469.	1.2	25
304	Deep learning for predicting toxicity of chemicals: a mini review. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 252-271.	2.9	61
305	Anti-flavi: A Web Platform to Predict Inhibitors of Flaviviruses Using QSAR and Peptidomimetic Approaches. Frontiers in Microbiology, 2018, 9, 3121.	1.5	19
306	Applications of Chemoinformatics in Predictive Toxicology for Regulatory Purposes, Especially in the Context of the EU REACH Legislation. International Journal of Quantitative Structure-Property Relationships, 2018, 3, 1-24.	1.1	12
307	Graph Memory Networks for Molecular Activity Prediction. , 2018, , .		10
308	Classification of HIV-1 Protease Inhibitors by Machine Learning Methods. ACS Omega, 2018, 3, 15837-15849.	1.6	10
309	Computational drug discovery for the Zika virus. Brazilian Journal of Pharmaceutical Sciences, 2018, 54, .	1.2	6
310	A review on machine learning methods forin silicotoxicity prediction. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 169-191.	2.9	91
311	Best Practices for QSAR Model Reporting: Physical and Chemical Properties, Ecotoxicity, Environmental Fate, Human Health, and Toxicokinetics Endpoints. Environmental Health Perspectives, 2018, 126, 126001.	2.8	51
312	Predicting Strategies for Lead Optimization via Learning to Rank. IPSJ Transactions on Bioinformatics, 2018, 11, 41-47.	0.2	5
313	A new semi-automated workflow for chemical data retrieval and quality checking for modeling applications. Journal of Cheminformatics, 2018, 10, 60.	2.8	56
314	Computational approaches for skin sensitization prediction. Critical Reviews in Toxicology, 2018, 48, 738-760.	1.9	38
315	Computational Method to Evaluate Progress in Lead Optimization. Journal of Medicinal Chemistry, 2018, 61, 10895-10900.	2.9	18
316	The convergence of artificial intelligence and chemistry for improved drug discovery. Future Medicinal Chemistry, 2018, 10, 2573-2576.	1.1	23
317	Using 3D-QSAR to predict the separation efficiencies of flotation collectors: Implications for rational design of non-polar side chains. Minerals Engineering, 2018, 129, 112-119.	1.8	10
318	Renewable Hydride Donors for the Catalytic Reduction of CO₂: A Thermodynamic and Kinetic Study. Journal of Physical Chemistry B, 2018, 122, 10179-10189.	1.2	13
319	Implementation of a dynamic intestinal gut-on-a-chip barrier model for transport studies of lipophilic dioxin congeners. RSC Advances, 2018, 8, 32440-32453.	1.7	36
320	Quantitative structureâ€“activity relationship of the thymidylate synthase inhibitors of Mus musculus in the series of quinazolin-4-one and quinazolin-4-imine derivatives. Journal of Molecular Graphics and Modelling, 2018, 85, 198-211.	1.3	4

#	Article	IF	Citations
321	MIA-QSAR based model for bioactivity prediction of flavonoid derivatives as acetylcholinesterase inhibitors. Journal of Theoretical Biology, 2018, 459, 103-110.	0.8	7
322	QSAR-Based Virtual Screening: Advances and Applications in Drug Discovery. Frontiers in Pharmacology, 2018, 9, 1275.	1.6	291
323	Theoretical Prediction of the Complex P-Glycoprotein Substrate Efflux Based on the Novel Hierarchical Support Vector Regression Scheme. Molecules, 2018, 23, 1820.	1.7	22
325	Chemistry-Wide Association Studies (CWAS): A Novel Framework for Identifying and Interpreting Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2018, 58, 2203-2213.	2.5	7
326	Finding the structural requirements of diverse HIV-1 protease inhibitors using multiple QSAR modelling for lead identification. SAR and QSAR in Environmental Research, 2018, 29, 911-933.	1.0	24
327	Prediction of Effective Drug Combinations by an Improved NaÃ¯ve Bayesian Algorithm. International Journal of Molecular Sciences, 2018, 19, 467.	1.8	30
328	Computer-aided drug discovery of Myc-Max inhibitors as potential therapeutics for prostate cancer. European Journal of Medicinal Chemistry, 2018, 160, 108-119.	2.6	38
329	Diagnostics of Data-Driven Models: Uncertainty Quantification of PM7 Semi-Empirical Quantum Chemical Method. Scientific Reports, 2018, 8, 13248.	1.6	8
330	How Precise Are Our Quantitative Structureâ€“Activity Relationship Derived Predictions for New Query Chemicals?. ACS Omega, 2018, 3, 11392-11406.	1.6	88
331	Regression Modelability Index: A New Index for Prediction of the Modelability of Data Sets in the Development of QSAR Regression Models. Journal of Chemical Information and Modeling, 2018, 58, 2069-2084.	2.5	7
332	Development of an allosteric inhibitor class blocking RNA elongation by the respiratory syncytial virus polymerase complex. Journal of Biological Chemistry, 2018, 293, 16761-16777.	1.6	23
333	Future of Regulatory Safety Assessments. , 2018, , 1-24.		0
334	Nanobiotechnology: 1D nanomaterial building blocks for cellular interfaces and hybrid tissues. Nano Research, 2018, 11, 5372-5399.	5.8	14
335	Novel 1,4-dihydropyridine induces apoptosis in human cancer cells through overexpression of Sirtuin1. Apoptosis: an International Journal on Programmed Cell Death, 2018, 23, 532-553.	2.2	14
336	Computational Multi-Target Drug Design. Methods in Pharmacology and Toxicology, 2018, , 51-90.	0.1	1
337	Study of Data Set Modelability: Modelability, Rivality, and Weighted Modelability Indexes. Journal of Chemical Information and Modeling, 2018, 58, 1798-1814.	2.5	17
338	Modelling methods and cross-validation variants in QSAR: a multi-level analysis[$]. SAR and QSAR in Environmental Research, 2018, 29, 661-674.	1.0	32
339	Multi-Descriptor Read Across (MuDRA): A Simple and Transparent Approach for Developing Accurate Quantitative Structureâ€“Activity Relationship Models. Journal of Chemical Information and Modeling, 2018, 58, 1214-1223.	2.5	43

#	Article	IF	Citations
340	Diverse classes of HDAC8 inhibitors: in search of molecular fingerprints that regulate activity. Future Medicinal Chemistry, 2018, 10, 1589-1602.	1.1	30
341	QSAR: What Else?. Methods in Molecular Biology, 2018, 1800, 79-105.	0.4	15
342	(Q)SAR Methods for Predicting Genotoxicity and Carcinogenicity: Scientific Rationale and Regulatory Frameworks. Methods in Molecular Biology, 2018, 1800, 447-473.	0.4	18
343	Machine Learning Methods in Computational Toxicology. Methods in Molecular Biology, 2018, 1800, 119-139.	0.4	41
344	Computational Toxicology. Methods in Molecular Biology, 2018, , .	0.4	7
345	Assessment of river sediment toxicity: Combining empirical zebrafish embryotoxicity testing with in silico toxicity characterization. Science of the Total Environment, 2018, 643, 435-450.	3.9	29
346	In Silico and in Vitro Assessment of OATP1B1 Inhibition in Drug Discovery. Molecular Pharmaceutics, 2018, 15, 3060-3068.	2.3	12
347	Quantitative-Structure-Activity-Relationship (QSAR) models for the reaction rate and temperature of nitrogenous organic compounds in supercritical water oxidation (SCWO). Chemical Engineering Journal, 2018, 354, 12-20.	6.6	25
348	Transfer and Multi-task Learning in QSAR Modeling: Advances and Challenges. Frontiers in Pharmacology, 2018, 9, 74.	1.6	87
349	QSAR-Driven Design and Discovery of Novel Compounds With Antiplasmodial and Transmission Blocking Activities. Frontiers in Pharmacology, 2018, 9, 146.	1.6	22
350	Use of Simplified Molecular Input Line Entry System and molecular graph based descriptors in prediction and design of pancreatic lipase inhibitors. Future Medicinal Chemistry, 2018, 10, 1603-1622.	1.1	25
351	Emerging Computational Methods for Predicting Chemically Induced Mutagenicity. , 2018, , 161-176.		1
352	Using Rule-Based Labels for Weak Supervised Learning. , 2018, , .		52
353	Quantitative Nano-Structureâ€“Property Relationships for the Nanoporous Carbon: Predicting the Performance of Energy Storage Materials. ACS Applied Energy Materials, 2018, 1, 4016-4024.	2.5	14
354	Deep reinforcement learning for de novo drug design. Science Advances, 2018, 4, eaap7885.	4.7	740
355	Natural Products for Drug Discovery in the 21st Century: Innovations for Novel Drug Discovery. International Journal of Molecular Sciences, 2018, 19, 1578.	1.8	703
356	Combining traditional 2D and modern physical organic-derived descriptors to predict enhanced enantioselectivity for the key aza-Michael conjugate addition in the synthesis of Prevymisâ„¢ (letermovir). Chemical Science, 2018, 9, 6922-6927.	3.7	22
357	Challenges with multi-objective QSAR in drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 851-859.	2.5	26

#	Article	IF	Citations
358	The Design, Synthesis, and Characterizations of Spore Germination Inhibitors Effective against an Epidemic Strain of Clostridium difficile. Journal of Medicinal Chemistry, 2018, 61, 6759-6778.	2.9	16
359	Discovery and design of new PI3K inhibitors through pharmacophore-based virtual screening, molecular docking, and binding free energy analysis. Structural Chemistry, 2018, 29, 1753-1766.	1.0	11
360	Toward sustainable environmental quality: Priority research questions for Europe. Environmental Toxicology and Chemistry, 2018, 37, 2281-2295.	2.2	98
361	Networking of Smart Drugs: A Chem-Bioinformatic Approach to Cancer Treatment. Methods in Pharmacology and Toxicology, 2018, , 529-555.	0.1	0
362	Insight Analysis of Promiscuous Estrogen Receptor Î±-Ligand Binding by a Novel Machine Learning Scheme. Chemical Research in Toxicology, 2018, 31, 799-813.	1.7	8
363	Outâ€compute drug side effects: Focus on cytochrome P450 2D6 modeling. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1366.	6.2	9
364	Machine learning in chemoinformatics and drug discovery. Drug Discovery Today, 2018, 23, 1538-1546.	3.2	630
365	Machine learning and molecular design of self-assembling -conjugated oligopeptides. Molecular Simulation, 2018, 44, 930-945.	0.9	26
366	QSAR study and rustic ligand-based virtual screening in a search for aminooxadiazole derivatives as PIM1 inhibitors. Chemistry Central Journal, 2018, 12, 32.	2.6	9
367	A perspective on multiâ€target drug discovery and design for complex diseases. Clinical and Translational Medicine, 2018, 7, 3.	1.7	481
368	The OECD Principles for (Q)SAR Models in the Context of Knowledge Discovery in Databases (KDD). Advances in Protein Chemistry and Structural Biology, 2018, 113, 85-117.	1.0	17
369	QSAR modelling: a therapeutic patent review 2010-present. Expert Opinion on Therapeutic Patents, 2018, 28, 467-476.	2.4	29
370	Synthesis of 2-alkylthio-N-(quinazolin-2-yl)benzenesulfonamide derivatives: anticancer activity, QSAR studies, and metabolic stability. Monatshefte FÃ¼r Chemie, 2018, 149, 1885-1898.	0.9	5
371	Machine Learning Based Toxicity Prediction: From Chemical Structural Description to Transcriptome Analysis. International Journal of Molecular Sciences, 2018, 19, 2358.	1.8	122
372	Classifying antimicrobial and multifunctional peptides with Bayesian network models. Peptide Science, 2018, 110, e24079.	1.0	15
373	Predictive classification models and targets identification for betulin derivatives as Leishmania donovani inhibitors. Journal of Cheminformatics, 2018, 10, 40.	2.8	2
374	Natural products as inhibitors of Leishmania major dihydroorotate dehydrogenase. European Journal of Medicinal Chemistry, 2018, 157, 852-866.	2.6	20
375	Computational Predictions for Multi-Target Drug Design. Methods in Pharmacology and Toxicology, 2018, , 27-50.	0.1	6

#	Article	IF	Citations
376	Discovering Highly Potent Molecules from an Initial Set of Inactives Using Iterative Screening. Journal of Chemical Information and Modeling, 2018, 58, 2000-2014.	2.5	28
377	Cheminformatics Approaches to Study Drug Polypharmacology. Methods in Pharmacology and Toxicology, 2018, , 3-25.	0.1	2
378	Advanced Chemometric Modeling Approaches for the Design of Multitarget Drugs Against Neurodegenerative Diseases. Methods in Pharmacology and Toxicology, 2018, , 155-186.	0.1	3
379	Synthesis, bioactivity and mode of action of 5_A5_B6_C tricyclic spirolactones as novel antiviral lead compounds. Pest Management Science, 2019, 75, 292-301.	1.7	23
380	In silico approaches to genetic toxicology: progress and future. Mutagenesis, 2019, 34, 1-2.	1.0	2
381	Multiple quantitative structure-activity relationships (QSARs) analysis for orally active trypanocidal N-myristoyltransferase inhibitors. Journal of Molecular Structure, 2019, 1175, 481-487.	1.8	25
382	Chemoinformatics: From Chemical Art to Chemistry in Silico. , 2019, , 601-618.		5
383	On the Misleading Use of for QSAR Model Comparison. Molecular Informatics, 2019, 38, e1800029.	1.4	31
384	Delfos: deep learning model for prediction of solvation free energies in generic organic solvents. Chemical Science, 2019, 10, 8306-8315.	3.7	49
385	Predicting Synergism of Cancer Drug Combinations Using NCI-ALMANAC Data. Frontiers in Chemistry, 2019, 7, 509.	1.8	101
386	QSAR studies of the antioxidant activity of anthocyanins. Journal of Food Science and Technology, 2019, 56, 5518-5530.	1.4	17
387	Investigation of Factors Affecting the Performance of in silico Volume Distribution QSAR Models for Human, Rat, Mouse, Dog & Monkey. Molecular Informatics, 2019, 38, 1900059.	1.4	9
388	Using Physicochemical Measurements to Influence Better Compound Design. SLAS Discovery, 2019, 24, 791-801.	1.4	24
389	Celebrating 40 Years of Career. Molecular Informatics, 2019, 38, e1980831.	1.4	0
390	From Target to Drug: Generative Modeling for the Multimodal Structure-Based Ligand Design. Molecular Pharmaceutics, 2019, 16, 4282-4291.	2.3	81
391	Precise modelling and interpretation of bioactivities of ligands targeting G protein-coupled receptors. Bioinformatics, 2019, 35, i324-i332.	1.8	12
392	Metoprolol and metoprolol acid degradation in UV/H2O2 treated wastewaters: An integrated screening approach for the identification of hazardous transformation products. Journal of Hazardous Materials, 2019, 380, 120851.	6.5	32
393	In Silico Prediction of PAMPA Effective Permeability Using a Two-QSAR Approach. International Journal of Molecular Sciences, 2019, 20, 3170.	1.8	34

#	Article	IF	Citations
394	Bayesian semi-supervised learning for uncertainty-calibrated prediction of molecular properties and active learning. Chemical Science, 2019, 10, 8154-8163.	3.7	85
395	Towards quantitative read across: Prediction of Ames mutagenicity in a large database. Regulatory Toxicology and Pharmacology, 2019, 108, 104434.	1.3	8
396	Cheminformatics approach to exploring and modeling trait-associated metabolite profiles. Journal of Cheminformatics, 2019, 11, 43.	2.8	10
397	Physics-Based Method for Modeling Passive Membrane Permeability and Translocation Pathways of Bioactive Molecules. Journal of Chemical Information and Modeling, 2019, 59, 3198-3213.	2.5	41
398	Continuous molecular fields and the concept of molecular co-fields in structureâ€“activity studies. Future Medicinal Chemistry, 2019, 11, 2701-2713.	1.1	2
399	www.3d-qsar.com: a web portal that brings 3-D QSAR to all electronic devicesâ€”the Py-CoMFA web application as tool to build models from pre-aligned datasets. Journal of Computer-Aided Molecular Design, 2019, 33, 855-864.	1.3	37
400	Improved 3D-QSAR prediction by multiple-conformational alignment: A case study on PTP1B inhibitors. Computational Biology and Chemistry, 2019, 83, 107134.	1.1	7
401	Shortcuts to schistosomiasis drug discovery: The state-of-the-art. Annual Reports in Medicinal Chemistry, 2019, , 139-180.	0.5	3
402	In silico model for mutagenicity (Ames test), taking into account metabolism. Mutagenesis, 2019, 34, 41-48.	1.0	10
403	Computational modelling of mechanical properties for new polymeric materials with high molecular weight. Chemometrics and Intelligent Laboratory Systems, 2019, 193, 103851.	1.8	8
404	SAR-mediated Similarity Assessment of the Property Profile for New, Silicon-Based AChE/BChE Inhibitors. International Journal of Molecular Sciences, 2019, 20, 5385.	1.8	10
405	Using Machine Learning to Classify Bioactivity for 3486 Per- and Polyfluoroalkyl Substances (PFASs) from the OECD List. Environmental Science & Technology, 2019, 53, 13970-13980.	4.6	68
406	Alignment-Free Method to Predict Enzyme Classes and Subclasses. International Journal of Molecular Sciences, 2019, 20, 5389.	1.8	19
407	Current computational methods for predicting protein interactions of natural products. Computational and Structural Biotechnology Journal, 2019, 17, 1367-1376.	1.9	36
408	Identification of prodigious and under-privileged structural features for RG7834 analogs as Hepatitis B virus expression inhibitor. Medicinal Chemistry Research, 2019, 28, 2270-2278.	1.1	3
409	Molecule Property Prediction Based on Spatial Graph Embedding. Journal of Chemical Information and Modeling, 2019, 59, 3817-3828.	2.5	76
410	Descriptor Free QSAR Modeling Using Deep Learning With Long Short-Term Memory Neural Networks. Frontiers in Artificial Intelligence, 2019, 2, 17.	2.0	64
411	Rivality index neighbourhood algorithm with density and distances weighted schemes for the building of robust QSAR classification models with high reliable applicability domain. SAR and QSAR in Environmental Research, 2019, 30, 587-615.	1.0	3

#	Article	IF	Citations
412	Data-Driven Construction of Antitumor Agents with Controlled Polypharmacology. Journal of the American Chemical Society, 2019, 141, 15700-15709.	6.6	12
413	4D- quantitative structureâ€“activity relationship modeling: making a comeback. Expert Opinion on Drug Discovery, 2019, 14, 1227-1235.	2.5	23
414	Exploring structural features of EGFRâ€“HER2 dual inhibitors as anti-cancer agents using G-QSAR approach. Journal of Receptor and Signal Transduction Research, 2019, 39, 243-252.	1.3	1
415	Molecular Field Analysis Using Intermediates in Enantio-Determining Steps Can Extract Information for Data-Driven Molecular Design in Asymmetric Catalysis. Bulletin of the Chemical Society of Japan, 2019, 92, 1701-1706.	2.0	13
416	Computer-Aided Discovery of Small Molecule Inhibitors of Thymocyte Selection-Associated High Mobility Group Box Protein (TOX) as Potential Therapeutics for Cutaneous T-Cell Lymphomas. Molecules, 2019, 24, 3459.	1.7	6
417	Linking synthesis and structure descriptors from a large collection of synthetic records of zeolite materials. Nature Communications, 2019, 10, 4459.	5.8	74
418	In silico toxicity evaluation of dioxins using structureâ€“activity relationship (SAR) and two-dimensional quantitative structureâ€“activity relationship (2D-QSAR). Archives of Toxicology, 2019, 93, 3207-3218.	1.9	14
419	Modeling MEK4 Kinase Inhibitors through Perturbed Electrostatic Potential Charges. Journal of Chemical Information and Modeling, 2019, 59, 4460-4466.	2.5	4
420	Food ingredient safety evaluation: Utility and relevance of toxicokinetic methods. Toxicology and Applied Pharmacology, 2019, 382, 114759.	1.3	9
421	Making use of available and emerging data to predict the hazards of engineered nanomaterials by means of in silico tools: A critical review. NanoImpact, 2019, 13, 76-99.	2.4	47
422	Conformational Effects on Physical-Organic Descriptors: The Case of Sterimol Steric Parameters. ACS Catalysis, 2019, 9, 2313-2323.	5.5	96
423	In silico prediction of chemical reproductive toxicity using machine learning. Journal of Applied Toxicology, 2019, 39, 844-854.	1.4	34
424	Rational Use of Heterogeneous Data in Quantitative Structureâ€“Activity Relationship (QSAR) Modeling of Cyclooxygenase/Lipoxygenase Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 713-730.	2.5	17
425	Cyclin dependent kinase 4 inhibitory activity of Thieno[2,3-d] pyrimidin-4-ylhydrazones â€“ Multiple QSAR and docking studies. Journal of Molecular Structure, 2019, 1183, 263-273.	1.8	8
426	Redesigning hazardous chemicals by learning from structure-based drug discovery. Green Chemistry, 2019, 21, 1935-1946.	4.6	11
427	Identifying Structureâ€“Property Relationships through SMILES Syntax Analysis with Self-Attention Mechanism. Journal of Chemical Information and Modeling, 2019, 59, 914-923.	2.5	78
428	Predicting the Electrochemical Properties of Lithium-Ion Battery Electrode Materials with the Quantum Neural Network Algorithm. Journal of Physical Chemistry C, 2019, 123, 4682-4690.	1.5	8
429	Predicting Skin Permeability by Means of Computational Approaches: Reliability and Caveats in Pharmaceutical Studies. Journal of Chemical Information and Modeling, 2019, 59, 1759-1771.	2.5	35

#	Article	IF	Citations
430	Background, Tasks, Modeling Methods, and Challenges for Computational Toxicology. Challenges and Advances in Computational Chemistry and Physics, 2019, , 15-36.	0.6	2
431	Exploring the Potential of Spherical Harmonics and PCVM for Compounds Activity Prediction. International Journal of Molecular Sciences, 2019, 20, 2175.	1.8	2
432	Analysis and Comparison of Vector Space and Metric Space Representations in QSAR Modeling. Molecules, 2019, 24, 1698.	1.7	17
433	KekuleScope: prediction of cancer cell line sensitivity and compound potency using convolutional neural networks trained on compound images. Journal of Cheminformatics, 2019, 11, 41.	2.8	57
434	Cheminformatics-driven discovery of polymeric micelle formulations for poorly soluble drugs. Science Advances, 2019, 5, eaav9784.	4.7	34
435	Molecular Modelling of Potential Candidates for the Treatment of Depression. Molecular Informatics, 2019, 38, 1900024.	1.4	1
436	Application of Computational Methods for the Safety Assessment of Food Ingredients. Challenges and Advances in Computational Chemistry and Physics, 2019, , 233-257.	0.6	2
437	Mode-of-Action-Guided, Molecular Modeling-Based Toxicity Prediction: A Novel Approach for In Silico Predictive Toxicology. Challenges and Advances in Computational Chemistry and Physics, 2019, , 99-118.	0.6	2
438	The effect of the structure of derivatives of nitrogen-containing heterocycles on their anti-influenza activity. Chemistry of Heterocyclic Compounds, 2019, 55, 455-462.	0.6	4
439	Exploring the chemical space for freeze-drying excipients. International Journal of Pharmaceutics, 2019, 566, 254-263.	2.6	11
440	An exploration strategy improves the diversity of de novo ligands using deep reinforcement learning: a case for the adenosine A2A receptor. Journal of Cheminformatics, 2019, 11, 35.	2.8	58
441	Quinoxalinones Based Aldose Reductase Inhibitors: 2D and 3Dâ€QSAR Analysis. Molecular Informatics, 2019, 38, e1800149.	1.4	9
442	Novel criteria for elimination of the outliers in QSPR studies, when the â€˜forward stepwiseâ€™ procedure is used. Journal of Mathematical Chemistry, 2019, 57, 1770-1796.	0.7	0
443	Binding affinity in drug design: experimental and computational techniques. Expert Opinion on Drug Discovery, 2019, 14, 755-768.	2.5	75
444	An integrated quantitative structure and mechanism of action-activity relationship model of human serum albumin binding. Journal of Cheminformatics, 2019, 11, 38.	2.8	17
445	A Brief Review of Random Forests for Water Scientists and Practitioners and Their Recent History in Water Resources. Water (Switzerland), 2019, 11, 910.	1.2	336
446	Combining Features of Metal Oxide Nanoparticles. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 28-40.	1.1	5
447	Design and Optimization of Catalysts Based on Mechanistic Insights Derived from Quantum Chemical Reaction Modeling. Chemical Reviews, 2019, 119, 6509-6560.	23.0	130

#	Article	IF	Citations
448	Design and development of novel therapeutics for brucellosis treatment based on carbonic anhydrase inhibition. Journal of Biomolecular Structure and Dynamics, 2019, 38, 1-10.	2.0	7
449	Structure-Based Approach for the Prediction of Mu-opioid Binding Affinity of Unclassified Designer Fentanyl-Like Molecules. International Journal of Molecular Sciences, 2019, 20, 2311.	1.8	16
450	QSAR-Co: An Open Source Software for Developing Robust Multitasking or Multitarget Classification-Based QSAR Models. Journal of Chemical Information and Modeling, 2019, 59, 2538-2544.	2.5	73
451	Predicting skin permeability using the 3D-RISM-KH theory based solvation energy descriptors for a diverse class of compounds. Journal of Computer-Aided Molecular Design, 2019, 33, 605-611.	1.3	4
452	Evaluation of the applicability of existing (Q)SAR models for predicting the genotoxicity of pesticides and similarity analysis related with genotoxicity of pesticides for facilitating of grouping and read across. EFSA Supporting Publications, 2019, 16, 1598E.	0.3	20
453	Searching for the Optimized Luminescent Lanthanide Phosphor Using Heuristic Algorithms. Inorganic Chemistry, 2019, 58, 6458-6466.	1.9	12
454	Integrating the Structureâ€“Activity Relationship Matrix Method with Molecular Grid Maps and Activity Landscape Models for Medicinal Chemistry Applications. ACS Omega, 2019, 4, 7061-7069.	1.6	19
455	Search for Catalysts by Inverse Design: Artificial Intelligence, Mountain Climbers, and Alchemists. Chemical Reviews, 2019, 119, 6595-6612.	23.0	142
456	Improved Chemical Prediction from Scarce Data Sets via Latent Space Enrichment. Journal of Physical Chemistry A, 2019, 123, 4295-4302.	1.1	27
457	In Silico Drug Design Methods for Drug Repurposing. , 2019, , 47-84.		10
458	Encodings and models for antimicrobial peptide classification for multi-resistant pathogens. BioData Mining, 2019, 12, 7.	2.2	68
459	Proteochemometric Modeling for Drug Repositioning. , 2019, , 281-302.		7
460	Aug-MIA-QSAR based strategy in bioactivity prediction of a series of flavonoid derivatives as HIV-1 inhibitors. Journal of Theoretical Biology, 2019, 469, 18-24.	0.8	5
461	Regulatory acceptance of in silico approaches for the safety assessment of cosmetic-related substances. Computational Toxicology, 2019, 11, 82-89.	1.8	28
462	One Drug Multiple Targets: An Approach To Predict Drug Efficacies on Bacterial Strains Differing in Membrane Composition. ACS Omega, 2019, 4, 4977-4983.	1.6	6
463	Optimal Piecewise Linear Regression Algorithm for QSAR Modelling. Molecular Informatics, 2019, 38, e1800028.	1.4	19
465	A new tool to rationally design highly efficient organic sensitizers for dye-sensitized solar cells: A three-dimensional quantitative structure-activity relationship (3D-QSAR) perspective. Solar Energy, 2019, 184, 187-194.	2.9	10
466	Methodology of aiQSAR: a group-specific approach to QSAR modelling. Journal of Cheminformatics, 2019, 11, 27.	2.8	16

#	Article	IF	Citations
467	Informatics and Computational Methods in Natural Product Drug Discovery: A Review and Perspectives. Frontiers in Genetics, 2019, 10, 368.	1.1	95
468	Integration of target discovery, drug discovery and drug delivery: A review on computational strategies. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2019, 11, e1554.	3.3	27
469	BCL::Mol2Dâ€"a robust atom environment descriptor for QSAR modeling and lead optimization. Journal of Computer-Aided Molecular Design, 2019, 33, 477-486.	1.3	7
470	Intercorrelation Limits in Molecular Descriptor Preselection for QSAR/QSPR. Molecular Informatics, 2019, 38, e1800154.	1.4	34
471	A quantitative structure-biodegradation relationship (QSBR) approach to predict biodegradation rates of aromatic chemicals. Water Research, 2019, 157, 181-190.	5.3	34
472	A Safeâ€byâ€Design Strategy towards Safer Nanomaterials in Nanomedicines. Advanced Materials, 2019, 31, e1805391.	11.1	109
473	Development and application of a comprehensive machine learning program for predicting molecular biochemical and pharmacological properties. Physical Chemistry Chemical Physics, 2019, 21, 5189-5199.	1.3	10
474	Predictive Computational Tools for Assessment of Ecotoxicological Activity of Organic Micropollutants in Various Water Sources in Brazil. Molecular Informatics, 2019, 38, e1800156.	1.4	6
475	Universal transformation and non-linear connection between experimental and calculated property vectors in QSPR. Journal of Mathematical Chemistry, 2019, 57, 1075-1087.	0.7	5
476	Estudio in Silico de la reactividad y propiedades fisicoquÃmicas de aductos de EpÃ³xido de Eugenol y 2-Metoxi-4-alilideno-2,5-ciclohexadieno-1-ona con glutation en Candida albicans. Revista De La Facultad De Ciencias, 2019, 8, 124-137.	0.0	0
477	Identification of potential CRAC channel inhibitors: Pharmacophore mapping, 3D-QSAR modelling, and molecular docking approach. SAR and QSAR in Environmental Research, 2019, 30, 81-108.	1.0	9
478	Construction of a Quantitative Structure Activity Relationship (QSAR) Model to Predict the Absorption of Cephalosporins in Zebrafish for Toxicity Study. Frontiers in Pharmacology, 2019, 10, 31.	1.6	11
479	Imputation of Assay Bioactivity Data Using Deep Learning. Journal of Chemical Information and Modeling, 2019, 59, 1197-1204.	2.5	48
480	Development of Predictive Linear and Non-linear QSTR Models for Aliivibrio Fischeri Toxicity of Deep Eutectic Solvents. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 50-69.	1.1	4
481	Benchmarking multi-task learning in predictive models for drug discovery. , 2019, , .		2
482	Machine learning algorithms used in Quantitative structure-activity relationships studies as new approaches in drug discovery. , 2019, , .		2
483	Integrated Safety and Risk Assessment for Medical Devices and Combination Products. , 2019, , .		1
484	Toward Interpretable Machine Learning Models for Materials Discovery. Advanced Intelligent Systems, 2019, 1, 1900045.	3.3	25

#	Article	IF	Citations
485	Reliable and explainable machine-learning methods for accelerated material discovery. Npj Computational Materials, 2019, 5, .	3.5	111
486	Development of novel therapeutics for glaucoma filtration surgery based on transforming growth factor-Î² receptor 1 inhibition. New Journal of Chemistry, 2019, 43, 19265-19273.	1.4	0
487	Using Machine Learning To Inform Decisions in Drug Discovery: An Industry Perspective. ACS Symposium Series, 2019, , 81-101.	0.5	1
488	Bioinformatics Approaches for Anti-cancer Drug Discovery. Current Drug Targets, 2019, 21, 3-17.	1.0	73
489	Towards a reliable prediction of the aquatic toxicity of dyes. Environmental Sciences Europe, 2019, 31, .	2.6	12
490	Integrative Multi-Kinase Approach for the Identification of Potent Antiplasmodial Hits. Frontiers in Chemistry, 2019, 7, 773.	1.8	19
491	Multi-task learning with a natural metric for quantitative structure activity relationship learning. Journal of Cheminformatics, 2019, 11, 68.	2.8	14
492	Computational estimation of the acidities of purines and indoles. Journal of Molecular Modeling, 2019, 25, 12.	0.8	9
493	The integration of pharmacophore-based 3D QSAR modeling and virtual screening in safety profiling: A case study to identify antagonistic activities against adenosine receptor, A2A, using 1,897 known drugs. PLoS ONE, 2019, 14, e0204378.	1.1	25
494	A Distance-Based Boolean Applicability Domain for Classification of High Throughput Screening Data. Journal of Chemical Information and Modeling, 2019, 59, 463-476.	2.5	13
495	Discovery of new potent hits against intracellular Trypanosoma cruzi by QSAR-based virtual screening. European Journal of Medicinal Chemistry, 2019, 163, 649-659.	2.6	25
496	Important considerations for the validation of QSAR models for in vitro mutagenicity. Mutagenesis, 2019, 34, 25-32.	1.0	2
497	3D perspective into <scp>MIA</scp>â€<scp>QSAR</scp>: A case for antiâ€<scp>HCV</scp> agents. Chemical Biology and Drug Design, 2019, 93, 1096-1104.	1.5	6
498	Prediction of the datasets modelability for the building of QSAR classification models by means of the centroid based rivality index. Journal of Mathematical Chemistry, 2019, 57, 1374-1393.	0.7	2
499	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
500	In silico evaluation of 5-hydroxypyrazoles as LSD1 inhibitors based on molecular docking derived descriptors. Journal of Molecular Structure, 2019, 1179, 514-524.	1.8	6
501	A Systems Toxicology Approach for the Prediction of Kidney Toxicity and Its Mechanisms In Vitro. Toxicological Sciences, 2019, 169, 54-69.	1.4	16
502	Future of Regulatory Safety Assessments. , 2019, , 1-24.		0

#	Article	IF	Citations
503	Large scale comparison of QSAR and conformal prediction methods and their applications in drug discovery. Journal of Cheminformatics, 2019, 11, 4.	2.8	93
504	Deep Confidence: A Computationally Efficient Framework for Calculating Reliable Prediction Errors for Deep Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 1269-1281.	2.5	66
505	Three-Dimensional Activity Landscape Models of Different Design and Their Application to Compound Mapping and Potency Prediction. Journal of Chemical Information and Modeling, 2019, 59, 993-1004.	2.5	9
506	Closed-loop discovery platform integration is needed for artificial intelligence to make an impact in drug discovery. Expert Opinion on Drug Discovery, 2019, 14, 1-4.	2.5	37
507	Comprehensive 3D-QSAR Model Predicts Binding Affinity of Structurally Diverse Sigma 1 Receptor Ligands. Journal of Chemical Information and Modeling, 2019, 59, 486-497.	2.5	12
508	Synthesis, in vitro evaluation and QSAR modelling of potential antitumoral 3,4-dihydropyrimidin-2-(1H)-thiones. Arabian Journal of Chemistry, 2019, 12, 5086-5102.	2.3	12
509	Chemoinformatics. , 2020, , 635-676.		2
510	MaNGA: a novel multi-niche multi-objective genetic algorithm for QSAR modelling. Bioinformatics, 2020, 36, 145-153.	1.8	15
511	Design and development of novel therapeutics for coronary heart disease treatment based on cholesteryl ester transfer protein inhibition â€“ in silico approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2304-2313.	2.0	2
512	Deep learning on chaos game representation for proteins. Bioinformatics, 2020, 36, 272-279.	1.8	37
513	Big Data and Artificial Intelligence Modeling for Drug Discovery. Annual Review of Pharmacology and Toxicology, 2020, 60, 573-589.	4.2	209
514	An Overview of Machine Learning and Big Data for Drug Toxicity Evaluation. Chemical Research in Toxicology, 2020, 33, 20-37.	1.7	108
515	Autonomous Discovery in the Chemical Sciences Partâ€…I: Progress. Angewandte Chemie - International Edition, 2020, 59, 22858-22893.	7.2	180
516	Graph Classification of Molecules Using Force Field Atom and Bond Types. Molecular Informatics, 2020, 39, e1800155.	1.4	18
517	Autonome Entdeckung in den chemischen Wissenschaften, Teilâ€…I: Fortschritt. Angewandte Chemie, 2020, 132, 23054-23091.	1.6	11
518	Nonanimal toxicology testing approaches for traditional and deemed tobacco products in a complex regulatory environment: Limitations, possibilities, and future directions. Toxicology in Vitro, 2020, 62, 104684.	1.1	7
519	Computational basis for the design of PLK-2 inhibitors. Structural Chemistry, 2020, 31, 275-292.	1.0	1
520	Interpretation of Compound Activity Predictions from Complex Machine Learning Models Using Local Approximations and Shapley Values. Journal of Medicinal Chemistry, 2020, 63, 8761-8777.	2.9	178

#	Article	IF	Citations
521	Effect of hydrophobic and hydrogen bonding interactions on the potency of ÃŸâ€•alanine analogs of Gâ€protein coupled glucagon receptor inhibitors. Proteins: Structure, Function and Bioinformatics, 2020, 88, 327-344.	1.5	14
522	Application of in silico approaches for the generation of milk protein-derived bioactive peptides. Journal of Functional Foods, 2020, 64, 103636.	1.6	91
523	Why hasnâ€™t there been more progress in new Chagas disease drug discovery?. Expert Opinion on Drug Discovery, 2020, 15, 145-158.	2.5	44
524	Elucidating the aryl hydrocarbon receptor antagonism from a chemical-structural perspective. SAR and QSAR in Environmental Research, 2020, 31, 209-226.	1.0	11
525	Toward Rigorous Materials Production: New Approach Methodologies Have Extensive Potential to Improve Current Safety Assessment Practices. Small, 2020, 16, e1904749.	5.2	43
526	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	4.6	86
527	Influence of feature rankers in the construction of molecular activity prediction models. Journal of Computer-Aided Molecular Design, 2020, 34, 305-325.	1.3	1
528	Efficient identification of novel anti-glioma lead compounds by machine learning models. European Journal of Medicinal Chemistry, 2020, 189, 111981.	2.6	5
529	Structural Alerts and Random Forest Models in a Consensus Approach for Receptor Binding Molecular Initiating Events. Chemical Research in Toxicology, 2020, 33, 388-401.	1.7	12
530	Organic structure and solid characteristics determine reactivity of phenolic compounds with synthetic and reclaimed manganese oxides. Environmental Science: Water Research and Technology, 2020, 6, 540-553.	1.2	14
531	Machine Learning for Catalysis Informatics: Recent Applications and Prospects. ACS Catalysis, 2020, 10, 2260-2297.	5.5	309
532	Off-Pocket Activity Cliffs: A Puzzling Facet of Molecular Recognition. Journal of Chemical Information and Modeling, 2020, 60, 152-161.	2.5	9
533	Accelerating medical device biocompatibility evaluation: An industry perspective. , 2020, , 223-262.		1
534	A review on created QSPR models for predicting ionic liquids properties and their reliability from chemometric point of view. Journal of Molecular Liquids, 2020, 297, 112013.	2.3	39
535	Chemometrics for QSAR Modeling. , 2020, , 599-634.		6
536	Molecular Modeling of Âµ Opioid Receptor Ligands with Various Functional Properties: PZM21, SR-17018, Morphine, and Fentanylâ€"Simulated Interaction Patterns Confronted with Experimental Data. Molecules, 2020, 25, 4636.	1.7	19
537	Introduction: An Overview of AI in Oncology Drug Discovery and Development. , 0, , .		6
538	Molecular modelling guided design, synthesis and QSAR analysis of new small molecule non-lipid autotaxin inhibitors. Bioorganic Chemistry, 2020, 103, 104188.	2.0	5

#	Article	IF	Citations
539	Guiding Conventional Proteinâ€“Ligand Docking Software with Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2020, 60, 4594-4602.	2.5	15
540	Machine learning-based QSAR models to predict sodium ion channel (Nav 1.5) blockers. Future Medicinal Chemistry, 2020, 12, 1829-1843.	1.1	7
541	Structure features of peptide-type SARS-CoV main protease inhibitors: Quantitative structure activity relationship study. Chemometrics and Intelligent Laboratory Systems, 2020, 206, 104172.	1.8	10
542	Thermodynamics and Kinetics of Drug-Target Binding by Molecular Simulation. Chemical Reviews, 2020, 120, 12788-12833.	23.0	126
543	Using Topomer Comparative Molecular Field Analysis to Elucidate Activity Differences of Aminomethylenethiophene Derivatives as Lysyl Oxidase Inhibitors: Implications for Rational Design of Antimetastatic Agents for Cancer Therapy. Journal of Chemistry, 2020, 2020, 1-10.	0.9	0
544	High-Throughput Experimentation in Olefin Polymerization Catalysis: Facing the Challenges of Miniaturization. Industrial & Engineering Chemistry Research, 2020, 59, 13940-13947.	1.8	26
545	The Advent of Generative Chemistry. ACS Medicinal Chemistry Letters, 2020, 11, 1496-1505.	1.3	64
546	Artificial Intelligence-Based Drug Design and Discovery. , 2020, , .		6
547	Green Toxicology: Connecting Green Chemistry and Modern Toxicology. Chemical Research in Toxicology, 2020, 33, 2919-2931.	1.7	11
548	Adding Substituent Nonadditivity in Protein Allostery by NMR. Biophysical Journal, 2020, 119, 1043-1044.	0.2	0
549	A Review of In Silico Tools as Alternatives to Animal Testing: Principles, Resources and Applications. ATLA Alternatives To Laboratory Animals, 2020, 48, 146-172.	0.7	100
550	Overview of Antifungal Drugs against Paracoccidioidomycosis: How Do We Start, Where Are We, and Where Are We Going?. Journal of Fungi (Basel, Switzerland), 2020, 6, 300.	1.5	15
551	Chemical Diversity of Soft Coral Steroids and Their Pharmacological Activities. Marine Drugs, 2020, 18, 613.	2.2	27
552	Prediction of Proteinâ€“ligand Interaction Based on Sequence Similarity and Ligand Structural Features. International Journal of Molecular Sciences, 2020, 21, 8152.	1.8	6
553	Allosteric Mechanisms of Nonadditive Substituent Contributions to Protein-Ligand Binding. Biophysical Journal, 2020, 119, 1135-1146.	0.2	11
554	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	1.8	32
555	Synthesis of 1,2,3â€Triazoles Bearing a 4â€Hydroxyisoxazolidine Moiety from 4,5â€Unsubstituted 2,3â€Dihydroisoxazoles. European Journal of Organic Chemistry, 2020, 2020, 4775-4786.	1.2	2
556	Toward Building a Failsafe Hospital: The Impending Drug Resistant Pandemic. Insight, 2020, 23, 8-13.	0.1	0

#	Article	IF	Citations
557	The Use of Methods of Computer-Aided Drug Discovery in the Development of Topoisomerase II Inhibitors: Applications and Future Directions. Journal of Chemical Information and Modeling, 2020, 60, 3703-3721.	2.5	15
558	BNNmix: A new approach for predicting the mixture toxicity of multiple components based on the back-propagation neural network. Science of the Total Environment, 2020, 738, 140317.	3.9	19
559	Rapid Prediction of Chemical Ecotoxicity Through Genetic Algorithm Optimized Neural Network Models. ACS Sustainable Chemistry and Engineering, 2020, 8, 12168-12176.	3.2	18
560	Uncertainty Quantification Using Neural Networks for Molecular Property Prediction. Journal of Chemical Information and Modeling, 2020, 60, 3770-3780.	2.5	129
562	Cloud 3D-QSAR: a web tool for the development of quantitative structureâ€“activity relationship models in drug discovery. Briefings in Bioinformatics, 2021, 22, .	3.2	36
563	Site-Level Bioactivity of Small-Molecules from Deep-Learned Representations of Quantum Chemistry. Journal of Physical Chemistry A, 2020, 124, 9194-9202.	1.1	7
564	Comparative study between deep learning and QSAR classifications for TNBC inhibitors and novel GPCR agonist discovery. Scientific Reports, 2020, 10, 16771.	1.6	49
565	Theoretical investigation on QSAR of (2-Methyl-3-biphenylyl) methanol analogs as PD-L1 inhibitor. Chinese Journal of Chemical Physics, 2020, 33, 459-467.	0.6	2
566	In silico evaluation of inhibitory potential of novel triazole derivatives against therapeutic target myristoyl-CoA: protein N-myristoyltransferase (NMT) of Candida albicans. Network Modeling Analysis in Health Informatics and Bioinformatics, 2020, 9, 1.	1.2	2
567	Extending the identification of structural features responsible for anti-SARS-CoV activity of peptide-type compounds using QSAR modelling. SAR and QSAR in Environmental Research, 2020, 31, 643-654.	1.0	24
568	Solving the Nonalignment of Methods and Approaches Used in Microplastic Research to Consistently Characterize Risk. Environmental Science & Technology, 2020, 54, 12307-12315.	4.6	154
569	Theoretical Insights into the Anti-SARS-CoV-2 Activity of Chloroquine and Its Analogs and In Silico Screening of Main Protease Inhibitors. Journal of Proteome Research, 2020, 19, 4706-4717.	1.8	20
570	QSAR modelling and structural aspects concerning synthetic heterocycles with larvicidal activity against Aedes aegypti. Structural Chemistry, 2020, 31, 2501-2512.	1.0	1
571	Emulating Docking Results Using a Deep Neural Network: A New Perspective for Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4246-4262.	2.5	22
572	Molecular modelling study on pyrrolo[2,3-b]pyridine derivatives as c-Met kinase inhibitors: a combined approach using molecular docking, 3D-QSAR modelling and molecular dynamics simulation. Molecular Simulation, 2020, 46, 1265-1280.	0.9	6
573	Neuraldecipher â€“ reverse-engineering extended-connectivity fingerprints (ECFPs) to their molecular structures. Chemical Science, 2020, 11, 10378-10389.	3.7	28
574	Selection of antileishmanial sesquiterpene lactones from SistematX database using a combined ligand-/structure-based virtual screening approach. Molecular Diversity, 2021, 25, 2411-2427.	2.1	15
575	On the intrinsic reactivity of highly potent trypanocidal cruzain inhibitors. RSC Medicinal Chemistry, 2020, 11, 1275-1284.	1.7	7

#	Article	IF	Citations
576	Predicting The Molecular Structure Relationship and The Biological Activity of DPP-4 Inhibitor Using Deep Neural Network with CatBoost Method as Feature Selection. , 2020, , .		5
577	Predicting molecular activity on nuclear receptors by multitask neural networks. Journal of Chemometrics, 2022, 36, e3325.	0.7	13
578	Prediction of Compound Bioactivities Using Heat-Diffusion Equation. Patterns, 2020, 1, 100140.	3.1	3
579	Confidence in Inactive and Active Predictions from Structural Alerts. Chemical Research in Toxicology, 2020, 33, 3010-3022.	1.7	3
580	Do we need different machine learning algorithms for QSAR modeling? A comprehensive assessment of 16 machine learning algorithms on 14 QSAR data sets. Briefings in Bioinformatics, 2021, 22, .	3.2	70
581	Comprehensive Study on Molecular Supervised Learning with Graph Neural Networks. Journal of Chemical Information and Modeling, 2020, 60, 5936-5945.	2.5	18
582	QSAR Implementation for HIC Retention Time Prediction of mAbs Using Fab Structure: A Comparison between Structural Representations. International Journal of Molecular Sciences, 2020, 21, 8037.	1.8	6
583	Interpretation of machine learning models using shapley values: application to compound potency and multi-target activity predictions. Journal of Computer-Aided Molecular Design, 2020, 34, 1013-1026.	1.3	248
584	QSPR Models for Predicting of the Melting Points and Refractive Indices for Inorganic Substances. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 1-21.	1.1	3
585	InterPred: a webtool to predict chemical autofluorescence and luminescence interference. Nucleic Acids Research, 2020, 48, W586-W590.	6.5	11
586	Construction of a web-based nanomaterial database by big data curation and modeling friendly nanostructure annotations. Nature Communications, 2020, 11, 2519.	5.8	77
587	In Silico Prediction of Critical Micelle Concentration (CMC) of Classic and Extended Anionic Surfactants from Their Molecular Structural Descriptors. Arabian Journal for Science and Engineering, 2020, 45, 7445-7454.	1.7	8
588	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. Scientific Data, 2020, 7, 137.	2.4	71
589	A machine learning workflow for molecular analysis: application to melting points. Machine Learning: Science and Technology, 2020, 1, 025015.	2.4	23
590	Microgeometry-independent equation for measuring infinite dilution activity coefficients using gas-liquid chromatography with static-wall-coated open-tubular columns. Journal of Chromatography A, 2020, 1624, 461264.	1.8	3
591	QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping. Journal of Cheminformatics, 2020, 12, 39.	2.8	26
592	An Integrated High Throughput Experimentation/Predictive QSAR Modeling Approach to ansa-Zirconocene Catalysts for Isotactic Polypropylene. Polymers, 2020, 12, 1005.	2.0	29
593	Quantitative structure-activity relationship study for prediction of antifungal properties of phenolic compounds. Structural Chemistry, 2020, 31, 1621-1630.	1.0	5

#	Article	IF	Citations
594	QSAR modeling, docking, ADME and reactivity of indazole derivatives as antagonizes of estrogen receptor alpha (ER-Î±) positive in breast cancer. Journal of Molecular Structure, 2020, 1217, 128442.	1.8	14
595	Chemists: AI Is Here; Unite To Get the Benefits. Journal of Medicinal Chemistry, 2020, 63, 8695-8704.	2.9	28
596	Inductive transfer learning for molecular activity prediction: Next-Gen QSAR Models with MolPMoFiT. Journal of Cheminformatics, 2020, 12, 27.	2.8	74
597	New pharmacological findings linked to biphenyl DHPMs, kinesin Eg5 ligands: anticancer and antioxidant effects. Future Medicinal Chemistry, 2020, 12, 1137-1154.	1.1	6
598	A QSAR modeling approach for predicting myeloid antimicrobial peptides with high sequence similarity. Chemical Biology and Drug Design, 2020, 96, 1408-1417.	1.5	2
599	Predicting Binding from Screening Assays with Transformer Network Embeddings. Journal of Chemical Information and Modeling, 2020, 60, 4191-4199.	2.5	20
600	In silico models for genotoxicity and drug regulation. Expert Opinion on Drug Metabolism and Toxicology, 2020, 16, 651-662.	1.5	23
601	Computer-Aided Ligand Discovery for Estrogen Receptor Alpha. International Journal of Molecular Sciences, 2020, 21, 4193.	1.8	33
602	What place does molecular topology have in todayâ€™s drug discovery?. Expert Opinion on Drug Discovery, 2020, 15, 1133-1144.	2.5	18
603	Towards a Digital Bioprocess Replica: Computational Approaches in Biopharmaceutical Development and Manufacturing. Trends in Biotechnology, 2020, 38, 1141-1153.	4.9	64
604	Software tools for toxicology and risk assessment. , 2020, , 791-812.		1
605	Computational methods and tools for sustainable and green approaches in drug discovery. , 2020, , 965-988.		3
606	Artificial Intelligence: Emerging Applications in Biotechnology and Pharma. , 2020, , 399-417.		1
607	Machine learning models for drugâ€“target interactions: current knowledge and future directions. Drug Discovery Today, 2020, 25, 748-756.	3.2	105
608	A self-attention based message passing neural network for predicting molecular lipophilicity and aqueous solubility. Journal of Cheminformatics, 2020, 12, 15.	2.8	73
609	Integrating computational lead optimization diagnostics with analog design and candidate selection. Future Science OA, 2020, 6, FSO451.	0.9	6
610	Modeling pesticides toxicity to Sheepshead minnow using QSAR. Ecotoxicology and Environmental Safety, 2020, 193, 110352.	2.9	24
611	QSAR studies on hepatitis C virus NS5A protein tetracyclic inhibitors in wild type and mutants by CoMFA and CoMSIA. SAR and QSAR in Environmental Research, 2020, 31, 281-311.	1.0	7

#	Article	IF	Citations
612	Going All In: A Strategic Investment in In Silico Toxicology. Chemical Research in Toxicology, 2020, 33, 880-888.	1.7	21
613	VISAR: an interactive tool for dissecting chemical features learned by deep neural network QSAR models. Bioinformatics, 2020, 36, 3610-3612.	1.8	9
614	Perspectives, Tendencies, and Guidelines in Affinity-Based Strategies for the Recovery and Purification of PEGylated Proteins. Advances in Polymer Technology, 2020, 2020, 1-12.	0.8	2
615	Predicting the safety of medicines in pregnancy: A workshop report. Reproductive Toxicology, 2020, 93, 199-210.	1.3	7
616	High-Throughput Screening to Predict Chemical-Assay Interference. Scientific Reports, 2020, 10, 3986.	1.6	28
617	An Analysis of Proteochemometric and Conformal Prediction Machine Learning Protein-Ligand Binding Affinity Models. Frontiers in Molecular Biosciences, 2020, 7, 93.	1.6	10
618	The TTC Data Mart: An interactive browser for threshold of toxicological concern calculations. Computational Toxicology, 2020, 15, 100128.	1.8	3
620	Computer-Aided Discovery of New Solubility-Enhancing Drug Delivery System. Biomolecules, 2020, 10, 913.	1.8	10
621	Construction of pioneering quantitative structure activity relationship screening models for abuse potential of designer drugs using index of ideality of correlation in monte carlo optimization. Archives of Toxicology, 2020, 94, 3069-3086.	1.9	22
622	3Î²-Acetoxy cholest-5-ene crystals: Catalytic synthesis, structural elucidation, contribution of intermolecular interactions and density functional theory calculations. Journal of Molecular Structure, 2020, 1221, 128833.	1.8	0
623	QSAR-derived affinity fingerprints (part 2): modeling performance for potency prediction. Journal of Cheminformatics, 2020, 12, 41.	2.8	14
624	Benchmarking 2D/3D/MD-QSAR Models for Imatinib Derivatives: How Far Can We Predict?. Journal of Chemical Information and Modeling, 2020, 60, 3342-3360.	2.5	12
625	In silico development of anesthetics based on barbiturate and thiobarbiturate inhibition of GABAA. Computational Biology and Chemistry, 2020, 88, 107318.	1.1	2
626	Developing novel computational prediction models for assessing chemical-induced neurotoxicity using naÃ¯ve Bayes classifier technique. Food and Chemical Toxicology, 2020, 143, 111513.	1.8	10
627	Neural network activation similarity: a new measure to assist decision making in chemical toxicology. Chemical Science, 2020, 11, 7335-7348.	3.7	14
628	Selecting Adsorbents to Separate Diverse Near-Azeotropic Chemicals. Journal of Physical Chemistry C, 2020, 124, 3664-3670.	1.5	29
629	Application of chemometric methods and QSAR models to support pesticide risk assessment starting from ecotoxicological datasets. Water Research, 2020, 174, 115583.	5.3	26
630	Applicability Domains Enhance Application of PPARÎ³ Agonist Classifiers Trained by Drug-like Compounds to Environmental Chemicals. Chemical Research in Toxicology, 2020, 33, 1382-1388.	1.7	20

#	Article	IF	Citations
631	Novel Directions in Free Energy Methods and Applications. Journal of Chemical Information and Modeling, 2020, 60, 1-5.	2.5	36
632	In Silico Strategies in Tuberculosis Drug Discovery. Molecules, 2020, 25, 665.	1.7	50
633	Computational Approaches to Identify Structural Alerts and Their Applications in Environmental Toxicology and Drug Discovery. Chemical Research in Toxicology, 2020, 33, 1312-1322.	1.7	46
634	Entering the era of computationally driven drug development. Drug Metabolism Reviews, 2020, 52, 283-298.	1.5	25
635	QSAR studies on benzothiophene derivatives as Plasmodium falciparum Nâ€myristoyltransferase inhibitors: Molecular insights into affinity and selectivity. Drug Development Research, 2020, , .	1.4	6
636	Computational Estimation of the Gas-Phase and Aqueous Acidities of Carbon Acids. Journal of Physical Chemistry A, 2020, 124, 2152-2159.	1.1	9
637	In silico Strategies to Support Fragment-to-Lead Optimization in Drug Discovery. Frontiers in Chemistry, 2020, 8, 93.	1.8	122
638	Deep Learning-driven research for drug discovery: Tackling Malaria. PLoS Computational Biology, 2020, 16, e1007025.	1.5	34
639	Targeting Tumors Using Peptides. Molecules, 2020, 25, 808.	1.7	42
640	Development of Prediction Models for Drug-Induced Cholestasis, Cirrhosis, Hepatitis, and Steatosis Based on Drug and Drug Metabolite Structures. Frontiers in Pharmacology, 2020, 11, 67.	1.6	22
641	Combinatorial Effect of Ligand and Ligand-Binding Site Hydrophobicities on Binding Affinity. Journal of Chemical Information and Modeling, 2020, 60, 1678-1684.	2.5	4
642	Homologous G Protein-Coupled Receptors Boost the Modeling and Interpretation of Bioactivities of Ligand Molecules. Journal of Chemical Information and Modeling, 2020, 60, 1865-1875.	2.5	8
643	Building Highly Reliable Quantitative Structureâ€“Activity Relationship Classification Models Using the Rivality Index Neighborhood Algorithm with Feature Selection. Journal of Chemical Information and Modeling, 2020, 60, 133-151.	2.5	7
644	In silico Methods for Design of Kinase Inhibitors as Anticancer Drugs. Frontiers in Chemistry, 2019, 7, 873.	1.8	71
645	Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. Polymers, 2020, 12, 163.	2.0	95
646	Hierarchical Quantitative Structureâ€“Activity Relationship Modeling Approach for Integrating Binary, Multiclass, and Regression Models of Acute Oral Systemic Toxicity. Chemical Research in Toxicology, 2020, 33, 353-366.	1.7	20
647	A comparison of molecular representations for lipophilicity quantitative structureâ€“property relationships with results from the SAMPL6 logP Prediction Challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 523-534.	1.3	13
648	Cinnamic Derivatives as Antitubercular Agents: Characterization by Quantitative Structureâ€“Activity Relationship Studies. Molecules, 2020, 25, 456.	1.7	9

#	Article	IF	Citations
649	Mixtures of QSAR models: Learning application domains of p K predicto rs. Journal of Chemometrics, 2020, 34, e3223.	0.7	2
650	Principles of QSAR Modeling. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 61-97.	1.1	115
651	Prototype Selection Method Based on the Rivality and Reliability Indexes for the Improvement of the Classification Models and External Predictions. Journal of Chemical Information and Modeling, 2020, 60, 3009-3021.	2.5	3
652	Exploring the Use of Compound-Induced Transcriptomic Data Generated From Cell Lines to Predict Compound Activity Toward Molecular Targets. Frontiers in Chemistry, 2020, 8, 296.	1.8	12
653	Quantitative structureâ€“toxicity relationships in translational toxicology. Current Opinion in Toxicology, 2020, 23-24, 46-49.	2.6	4
654	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
655	Computational strategies towards developing novel antimelanogenic agents. Life Sciences, 2020, 250, 117602.	2.0	1
656	Quantitative Structureâ€“Activity Relationship Modeling and Docking of Monoterpenes with Insecticidal Activity Against Reticulitermes chinensis Snyder and Drosophila melanogaster. Journal of Agricultural and Food Chemistry, 2020, 68, 4687-4698.	2.4	14
657	Development of novel therapeutics for the treatment of glaucoma based on actin-binding kinase inhibition â€“ in silico approach. New Journal of Chemistry, 2020, 44, 6923-6931.	1.4	4
658	Computer-Driven Development of an in Silico Tool for Finding Selective Histone Deacetylase 1 Inhibitors. Molecules, 2020, 25, 1952.	1.7	15
659	Molecular Design of Environment-Friendly PAE Derivatives Based on 3D-QSAR Assisted with a Comprehensive Evaluation Method Combining Toxicity and Estrogen Activities. Water, Air, and Soil Pollution, 2020, 231, 1.	1.1	8
660	Evaluation of the applicability of existing (Q)SAR models for predicting the genotoxicity of pesticides and similarity analysis related with genotoxicity of pesticides for facilitating of grouping and read across: An EFSA funded project. Regulatory Toxicology and Pharmacology, 2020, 114, 104658.	1.3	21
661	Discriminant models on mitochondrial toxicity improved by consensus modeling and resolving imbalance in training. Chemosphere, 2020, 253, 126768.	4.2	19
662	Synthesis, Characterization, and Antifungal Evaluation of Thiolactomycin Derivatives. Engineering, 2020, 6, 560-568.	3.2	5
663	Thyroid-Disrupting Effects of 6:2 and 8:2 Polyfluoroalkyl Phosphate Diester (diPAPs) at Environmentally Relevant Concentrations from Integrated In Silico and In Vivo Studies. Environmental Science and Technology Letters, 2020, 7, 330-336.	3.9	13
664	Cheminformatics Analysis and Modeling with MacrolactoneDB. Scientific Reports, 2020, 10, 6284.	1.6	15
665	Ranking Molecules with Vanishing Kernels and a Single Parameter: Active Applicability DomainIncluded. Journal of Chemical Information and Modeling, 2020, 60, 4376-4387.	2.5	2
666	Virtual screening web servers: designing chemical probes and drug candidates in the cyberspace. Briefings in Bioinformatics, 2021, 22, 1790-1818.	3.2	81

#	Article	IF	Citations
667	Improvement the performance of the classification models of Cyclooxygenase-2 inhibitors using undersampling methods based on the rivality and reliability indexes. Journal of Mathematical Chemistry, 2021, 59, 131-160.	0.7	0
668	Quantitative structure-toxicity relationship model for acute toxicity of organophosphates via multiple administration routes in rats and mice. Journal of Hazardous Materials, 2021, 401, 123724.	6.5	17
669	COMPARE Analysis, a Bioinformatic Approach to Accelerate Drug Repurposing against Covid-19 and Other Emerging Epidemics. SLAS Discovery, 2021, 26, 345-351.	1.4	14
670	Development of classification models for predicting inhibition of mitochondrial fusion and fission using machine learning methods. Chemosphere, 2021, 273, 128567.	4.2	12
671	Cheminformatics Analysis of Fluoroquinolones and their Inhibition Potency Against Four Pathogens. Molecular Informatics, 2021, 40, 2000215.	1.4	0
672	Computer-assisted discovery of compounds with insecticidal activity against Musca domestica and Mythimna separata. Food and Chemical Toxicology, 2021, 147, 111899.	1.8	7
673	Systematic Activity Maturation of a Single-Domain Antibody with Non-canonical Amino Acids through Chemical Mutagenesis. Cell Chemical Biology, 2021, 28, 70-77.e5.	2.5	15
674	Balanced QSAR analysis to identify the structural requirements of ABBV-075 (Mivebresib) analogues as bromodomain and extraterminal domain (BET) family bromodomain inhibitor. Journal of Molecular Structure, 2021, 1229, 129597.	1.8	5
675	Artificial Intelligence Applied to the Rapid Identification of New Antimalarial Candidates with Dualâ€Stage Activity. ChemMedChem, 2021, 16, 1093-1103.	1.6	5
676	Cross-species extrapolation of chemical sensitivity. Science of the Total Environment, 2021, 753, 141800.	3.9	24
677	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. Molecular Therapy, 2021, 29, 873-885.	3.7	78
678	Laboratory bioassay, greenhouse experiment and <scp>3Dâ€QSAR</scp> studies on berberine analogues: a search for new herbicides based on natural products. Pest Management Science, 2021, 77, 2054-2067.	1.7	7
679	Prediction of the Partition Coefficient between Adipose Tissue and Blood for Environmental Chemicals: From Single QSAR Models to an Integrated Approach. Molecular Informatics, 2021, 40, e2000072.	1.4	3
680	A semi-supervised learning framework for quantitative structureâ€“activity regression modelling. Bioinformatics, 2021, 37, 342-350.	1.8	5
681	Machine learning approaches for elucidating the biological effects of natural products. Natural Product Reports, 2021, 38, 346-361.	5.2	56
682	Developing the QSPR model for predicting the storage lipid/water distribution coefficient of organic compounds. Frontiers of Environmental Science and Engineering, 2021, 15, 1.	3.3	3
683	DeepDSC: A Deep Learning Method to Predict Drug Sensitivity of Cancer Cell Lines. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 575-582.	1.9	67
684	Molecular modeling of a series of dehydroquinate dehydratase type II inhibitors of Mycobacterium tuberculosis and design of new binders. Molecular Diversity, 2021, 25, 1-12.	2.1	3

#	Article	IF	Citations
685	Computational Approaches for Drug-Induced Liver Injury (DILI) Prediction: State of the Art and Challenges. , 2021, , 308-329.		4
686	A comparative analysis of the ensemble methods for drug design. AIP Conference Proceedings, 2021, , .	0.3	3
688	Towards Rational Biosurfactant Designâ€"Predicting Solubilization in Rhamnolipid Solutions. Molecules, 2021, 26, 534.	1.7	4
689	Parsing Sage and Rosemary in Time: The Machine Learning Race to Crack Olfactory Perception. Chemical Senses, 2021, 46, .	1.1	11
690	Accuracy or novelty: what can we gain from target-specific machine-learning-based scoring functions in virtual screening?. Briefings in Bioinformatics, 2021, 22, .	3.2	26
691	Evaluation of the performance of various machine learning methods on the discrimination of the active compounds. Chemical Biology and Drug Design, 2021, 97, 930-943.	1.5	4
692	Current computer-aided drug design methodologies in discovery of novel drug candidates for neuropsychiatric and inflammatory diseases. Arhiv Za Farmaciju, 2021, 71, 225-256.	0.2	0
693	Nature Identification of Chinese Herbal Medicine Compounds Based on Molecular Descriptors. Journal of AOAC INTERNATIONAL, 2021, 104, 1754-1759.	0.7	4
694	â€œPredictive in silico toxicology.â€•An update on modern approaches and a critical analysis of its strong and weak points. , 2021, , 75-83.		0
695	Combining machine learning and high-throughput experimentation to discover photocatalytically active organic molecules. Chemical Science, 2021, 12, 10742-10754.	3.7	52
696	Chemoinformatics and QSAR. , 2021, , 183-212.		1
697	Accelerating Big Data Analysis through LASSO-Random Forest Algorithm in QSAR Studies. Bioinformatics, 2022, 38, 469-475.	1.8	17
698	Application of Quantitative Structureâ€"Property Relationship Predictive Models to Water Treatment: A Critical Review. ACS ES&T Water, 2021, 1, 498-517.	2.3	21
699	Simulating drug concentrations in PDMS microfluidic organ chips. Lab on A Chip, 2021, 21, 3509-3519.	3.1	50
700	Automated and enabling technologies for medicinal chemistry. Progress in Medicinal Chemistry, 2021, 60, 191-272.	4.1	4
701	Predicting Chemical Properties using Self-Attention Multi-task Learning based on SMILES Representation. , 2021, , .		9
702	Structureâ€"property models of organic compounds based on molecular graphs with elements of the spatial structures of the molecules. Fine Chemical Technologies, 2021, 15, 84-103.	0.1	1
703	Development of a Hierarchical Support Vector Regression-Based In Silico Model for Caco-2 Permeability. Pharmaceutics, 2021, 13, 174.	2.0	11

#	Article	IF	Citations
704	Impact of chemoinformatics approaches and tools on current chemical research. , 2021, , 1-26.		1
705	Computational methods (in silico) and stem cells as alternatives to animals in research. , 2021, , 389-421.		0
706	Commentary toward the 20th Anniversary of the Society ofComputer Chemistry, Japan. Journal of Computer Chemistry Japan, 2021, 20, A26-A40.	0.0	0
707	Combining Features of Metal Oxide Nanoparticles. , 2021, , 317-329.		1
708	A review on machine learning algorithms for the ionic liquid chemical space. Chemical Science, 2021, 12, 6820-6843.	3.7	80
709	Molecular modelling of compounds used for corrosion inhibition studies: a review. Physical Chemistry Chemical Physics, 2021, 23, 19987-20027.	1.3	78
710	Regio-selectivity prediction with a machine-learned reaction representation and on-the-fly quantum mechanical descriptors. Chemical Science, 2021, 12, 2198-2208.	3.7	75
711	Computer-Aided Drug Designing. , 2021, , 151-182.		10
712	Biological activity-based modeling identifies antiviral leads against SARS-CoV-2. Nature Biotechnology, 2021, 39, 747-753.	9.4	38
713	Permutationally Invariant Deep Learning Approach to Molecular Fingerprinting with Application to Compound Mixtures. Journal of Chemical Information and Modeling, 2021, 61, 631-640.	2.5	1
714	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
715	In-silico driven design and development of spirobenzimidazo-quinazolines as potential DNA gyrase inhibitors. Biomedicine and Pharmacotherapy, 2021, 134, 111132.	2.5	9
716	Integrated approaches to testing and assessment as a tool for the hazard assessment and risk characterization of cosmetic preservatives. Journal of Applied Toxicology, 2021, 41, 1687-1699.	1.4	11
717	Antiplasmodial activity of sulfonylhydrazones: in vitro and in silico approaches. Future Medicinal Chemistry, 2021, 13, 233-250.	1.1	2
718	MAIP: a web service for predicting bloodâ€stage malaria inhibitors. Journal of Cheminformatics, 2021, 13, 13.	2.8	20
719	Novel Development of Predictive Feature Fingerprints to Identify Chemistry-Based Features for the Effective Drug Design of SARS-CoV-2 Target Antagonists and Inhibitors Using Machine Learning. ACS Omega, 2021, 6, 4857-4877.	1.6	8
720	Advances in De Novo Drug Design: From Conventional to Machine Learning Methods. International Journal of Molecular Sciences, 2021, 22, 1676.	1.8	131
721	Trends in application of advancing computational approaches in GPCR ligand discovery. Experimental Biology and Medicine, 2021, 246, 1011-1024.	1.1	5

#	Article	IF	Citations
722	Evaluation of multi-target deep neural network models for compound potency prediction under increasingly challenging test conditions. Journal of Computer-Aided Molecular Design, 2021, 35, 285-295.	1.3	10
723	100th Anniversary of Macromolecular Science Viewpoint: Data-Driven Protein Design. ACS Macro Letters, 2021, 10, 327-340.	2.3	30
724	Gains from no real PAINS: Where â€˜Fair Trial Strategyâ€™ stands in the development of multi-target ligands. Acta Pharmaceutica Sinica B, 2021, 11, 3417-3432.	5.7	10
725	Synthesis and Hybrid SAR Property Modeling of Novel Cholinesterase Inhibitors. International Journal of Molecular Sciences, 2021, 22, 3444.	1.8	18
726	An Inverse QSAR Method Based on a Two-Layered Model and Integer Programming. International Journal of Molecular Sciences, 2021, 22, 2847.	1.8	5
727	The challenges of generalizability in artificial intelligence for ADME/Tox endpoint and activity prediction. Expert Opinion on Drug Discovery, 2021, 16, 1045-1056.	2.5	13
728	Predicting Reaction Yields via Supervised Learning. Accounts of Chemical Research, 2021, 54, 1856-1865.	7.6	72
729	Linear Regression Model Development for Analysis of Asymmetric Copper-Bisoxazoline Catalysis. ACS Catalysis, 2021, 11, 3916-3922.	5.5	28
731	Outliers in SAR and QSAR: 3. Importance of considering the role of water molecules in proteinâ€“ligand interactions and quantitative structureâ€“activity relationship studies. Journal of Computer-Aided Molecular Design, 2021, 35, 371-396.	1.3	4
732	A Novel Graph Neural Network Methodology to Investigate Dihydroorotate Dehydrogenase Inhibitors in Small Cell Lung Cancer. Biomolecules, 2021, 11, 477.	1.8	7
733	Developing a variation of 3Dâ€QSAR / MD method in drug design. Journal of Computational Chemistry, 2021, 42, 917-929.	1.5	6
734	QSAR-Based Virtual Screening of Natural Products Database for Identification of Potent Antimalarial Hits. Biomolecules, 2021, 11, 459.	1.8	13
735	Automation and computer-assisted planning for chemical synthesis. Nature Reviews Methods Primers, 2021, 1, .	11.8	83
736	QSAR and Pharmacophore Modeling of Nitrogen Heterocycles as Potent Human N-Myristoyltransferase (Hs-NMT) Inhibitors. Molecules, 2021, 26, 1834.	1.7	11
737	PySmash: Python package and individual executable program for representative substructure generation and application. Briefings in Bioinformatics, 2021, 22, .	3.2	6
738	Classification and QSAR models of leukotriene A4 hydrolase (LTA4H) inhibitors by machine learning methods. SAR and QSAR in Environmental Research, 2021, 32, 411-431.	1.0	6
739	Inhibitory mechanism of an antifungal drug, caspofungin against amyloid Î² peptide aggregation: Repurposing via neuroinformatics and an experimental approach. Molecular and Cellular Neurosciences, 2021, 112, 103612.	1.0	3
741	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

#	Article	IF	Citations
742	Molecular-Based Guide to Predict the pH of Eutectic Solvents: Promoting an Efficient Design Approach for New Green Solvents. ACS Sustainable Chemistry and Engineering, 2021, 9, 5783-5808.	3.2	44
743	Hyperbolic relational graph convolution networks plus: a simple but highly efficient QSAR-modeling method. Briefings in Bioinformatics, 2021, 22, .	3.2	22
744	QSAR modeling for predicting the antifungal activities of gemini imidazolium surfactants against Candida albicans using GA-MLR methods. Journal of Applied Pharmaceutical Science, 0, , .	0.7	0
746	Exploring in vitro to in vivo extrapolation for exposure and health impacts of e-cigarette flavor mixtures. Toxicology in Vitro, 2021, 72, 105090.	1.1	7
747	An Overview of Biological and Computational Methods for Designing Mechanism-Informed Anti-biofilm Agents. Frontiers in Microbiology, 2021, 12, 640787.	1.5	25
748	Predicting the reproductive toxicity of chemicals using ensemble learning methods and molecular fingerprints. Toxicology Letters, 2021, 340, 4-14.	0.4	27
749	QSAR Modeling and Prediction of Triptan Binding Affinities. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 19-28.	1.1	0
750	Critical assessment of AI in drug discovery. Expert Opinion on Drug Discovery, 2021, 16, 937-947.	2.5	25
751	Application of deep learning and molecular modeling to identify small drug-like compounds as potential HIV-1 entry inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7555-7573.	2.0	15
752	Flame: an open source framework for model development, hosting, and usage in production environments. Journal of Cheminformatics, 2021, 13, 31.	2.8	9
753	Clinical pharmacokinetic study of latrepirdine via in silico sublingual administration. In Silico Pharmacology, 2021, 9, 29.	1.8	8
754	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 1: Theory and characteristicsâ€. Journal of Cheminformatics, 2021, 13, 32.	2.8	25
755	Machine Learning in Discovery of New Antivirals and Optimization of Viral Infections Therapy. Current Medicinal Chemistry, 2021, 28, .	1.2	4
756	Identification of Kaurane-Type Diterpenes as Inhibitors of Leishmania Pteridine Reductase I. Molecules, 2021, 26, 3076.	1.7	11
757	Two Decades of 4D-QSAR: A Dying Art or Staging a Comeback?. International Journal of Molecular Sciences, 2021, 22, 5212.	1.8	14
758	An effective self-supervised framework for learning expressive molecular global representations to drug discovery. Briefings in Bioinformatics, 2021, 22, .	3.2	55
759	In silico development of potential therapeutic for the pain treatment by inhibiting voltage-gated sodium channel 1.7. Computers in Biology and Medicine, 2021, 132, 104346.	3.9	5
760	Ensemble machine learning to evaluate the in vivo acute oral toxicity and in vitro human acetylcholinesterase inhibitory activity of organophosphates. Archives of Toxicology, 2021, 95, 2443-2457.	1.9	13

#	Article	IF	Citations
762	Curated Data In â€" Trustworthy In Silico Models Out: The Impact of Data Quality on the Reliability of Artificial Intelligence Models as Alternatives to Animal Testing. ATLA Alternatives To Laboratory Animals, 2021, 49, 73-82.	0.7	20
763	In silico Prediction of Skin Sensitization: Quo vadis?. Frontiers in Pharmacology, 2021, 12, 655771.	1.6	14
764	Schistosomiasis Drug Discovery in the Era of Automation and Artificial Intelligence. Frontiers in Immunology, 2021, 12, 642383.	2.2	10
765	Drug design of new 5-HT6R antagonists aided by artificial neural networks. Journal of Molecular Graphics and Modelling, 2021, 104, 107844.	1.3	3
766	Multiomic Big Data Analysis Challenges: Increasing Confidence in the Interpretation of Artificial Intelligence Assessments. Analytical Chemistry, 2021, 93, 7763-7773.	3.2	18
767	XGraphBoost: Extracting Graph Neural Network-Based Features for a Better Prediction of Molecular Properties. Journal of Chemical Information and Modeling, 2021, 61, 2697-2705.	2.5	41
768	Directionally sensitive homogeneously weighted moving average control charts. Quality and Reliability Engineering International, 0, , .	1.4	1
769	Evaluation of the OECD QSAR toolbox automatic workflow for the prediction of the acute toxicity of organic chemicals to fathead minnow. Regulatory Toxicology and Pharmacology, 2021, 122, 104893.	1.3	7
770	QSAR analysis and molecular docking study of pyrrolo- and pyridoquinolinecarboxamides with diuretic activity. ScienceRise: Pharmaceutical Science, 2021, , 19-27.	0.1	0
772	Simplex representation of molecular structure as universal QSAR/QSPR tool. Structural Chemistry, 2021, 32, 1365-1392.	1.0	17
773	PolyMaS: A new software to generate high molecular weight polymer macromolecules from repeating structural units. Polimery, 2021, 66, 293-297.	0.4	2
774	Machine learning models to select potential inhibitors of acetylcholinesterase activity from SistematX: a natural products database. Molecular Diversity, 2021, 25, 1553-1568.	2.1	10
775	An Updated Review of Computer-Aided Drug Design and Its Application to COVID-19. BioMed Research International, 2021, 2021, 1-18.	0.9	95
776	Computational Methods and Tools in Antimicrobial Peptide Research. Journal of Chemical Information and Modeling, 2021, 61, 3172-3196.	2.5	51
777	Molecular spaces and the dimension paradox. Pure and Applied Chemistry, 2021, 93, 1189-1196.	0.9	3
779	Antitumor Profile of Carbon-Bridged Steroids (CBS) and Triterpenoids. Marine Drugs, 2021, 19, 324.	2.2	6
780	Global Analysis of Models for Predicting Human Absorption: QSAR, In Vitro, and Preclinical Models. Journal of Medicinal Chemistry, 2021, 64, 9389-9403.	2.9	13
781	Data Science in Chemical Engineering: Applications to Molecular Science. Annual Review of Chemical and Biomolecular Engineering, 2021, 12, 15-37.	3.3	9

#	Article	IF	Citations
782	ERpred: a web server for the prediction of subtype-specific estrogen receptor antagonists. PeerJ, 2021, 9, e11716.	0.9	4
783	Machine learning models for predicting the activity of AChE and BACE1 dual inhibitors for the treatment of Alzheimerâ€™s disease. Molecular Diversity, 2022, 26, 1501-1517.	2.1	19
784	Identification of Novel HBV/HDV Entry Inhibitors by Pharmacophore- and QSAR-Guided Virtual Screening. Viruses, 2021, 13, 1489.	1.5	9
785	Leveraging high-throughput screening data, deep neural networks, and conditional generative adversarial networks to advance predictive toxicology. PLoS Computational Biology, 2021, 17, e1009135.	1.5	23
786	Evidential Deep Learning for Guided Molecular Property Prediction and Discovery. ACS Central Science, 2021, 7, 1356-1367.	5.3	73
787	MLSolvA: solvation free energy prediction from pairwise atomistic interactions by machine learning. Journal of Cheminformatics, 2021, 13, 56.	2.8	17
788	Recent trends in artificial intelligence-driven identification and development of anti-neurodegenerative therapeutic agents. Molecular Diversity, 2021, 25, 1517-1539.	2.1	8
789	Machine Learning in Chemical Engineering: Strengths, Weaknesses, Opportunities, and Threats. Engineering, 2021, 7, 1201-1211.	3.2	118
790	Learning protein-ligand binding affinity with atomic environment vectors. Journal of Cheminformatics, 2021, 13, 59.	2.8	29
791	Comparative analysis of molecular fingerprints in prediction of drug combination effects. Briefings in Bioinformatics, 2021, 22, .	3.2	47
792	Machine learning and big data provide crucial insight for future biomaterials discovery and research. Acta Biomaterialia, 2021, 130, 54-65.	4.1	32
793	SAG-DTA: Prediction of Drugâ€“Target Affinity Using Self-Attention Graph Network. International Journal of Molecular Sciences, 2021, 22, 8993.	1.8	26
794	Mechanistic and Predictive QSAR Analysis of Diverse Molecules to Capture Salient and Hidden Pharmacophores for Anti-Thrombotic Activity. International Journal of Molecular Sciences, 2021, 22, 8352.	1.8	4
795	Development and Application of Liquid Chromatographic Retention Time Indices in HRMS-Based Suspect and Nontarget Screening. Analytical Chemistry, 2021, 93, 11601-11611.	3.2	79
796	A Decade of Indonesian Atmosphere in Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 5276-5288.	2.5	3
797	Toward Application and Implementation of in Silico Tools and Workflows within Benign by Design Approaches. ACS Sustainable Chemistry and Engineering, 2021, 9, 12461-12475.	3.2	19
798	Insight into the structural requirement of aryl sulphonamide based gelatinases (MMP-2 and MMP-9) inhibitors â€“ Part I: 2D-QSAR, 3D-QSAR topomer CoMFA and NaÃ¯ve Bayes studies â€“ First report of 3D-QSAR Topomer CoMFA analysis for MMP-9 inhibitors and jointly inhibitors of gelatinases together. SAR and QSAR in Environmental Research, 2021, 32, 655-687.	1.0	4
800	Quantitative Structureâ€“Activity Relationship Evaluation of MDA-MB-231 Cell Anti-Proliferative Leads. Molecules, 2021, 26, 4795.	1.7	1

#	Article	IF	Citations
801	Development of blood brain barrier permeation prediction models for organic and inorganic biocidal active substances. Chemosphere, 2021, 277, 130330.	4.2	11
802	Reverse chemical ecology in a moth: machine learning on odorant receptors identifies new behaviorally active agonists. Cellular and Molecular Life Sciences, 2021, 78, 6593-6603.	2.4	11
803	Accelerating the pace of ecotoxicological assessment using artificial intelligence. Ambio, 2022, 51, 598-610.	2.8	12
804	Machine Learning Models Identify Inhibitors of SARS-CoV-2. Journal of Chemical Information and Modeling, 2021, 61, 4224-4235.	2.5	31
805	Comparisons of Molecular Structure Generation Methods Based on Fragment Assemblies and Genetic Graphs. Journal of Chemical Information and Modeling, 2021, 61, 4245-4258.	2.5	7
806	Hafnium vs. Zirconium, the Perpetual Battle for Supremacy in Catalytic Olefin Polymerization: A Simple Matter of Electrophilicity?. Polymers, 2021, 13, 2621.	2.0	9
807	Learning to SMILES: BAN-based strategies to improve latent representation learning from molecules. Briefings in Bioinformatics, 2021, 22, .	3.2	25
808	X-ray Crystallography-Guided Design, Antitumor Efficacy, and QSAR Analysis of Metabolically Stable Cyclopenta-Pyrimidinyl Dihydroquinoxalinone as a Potent Tubulin Polymerization Inhibitor. Journal of Medicinal Chemistry, 2021, 64, 13072-13095.	2.9	13
809	Preliminary modelling as the first stage of targeted organic synthesis. Russian Chemical Reviews, 2021, 90, 831-867.	2.5	3
810	Web-Based Quantitative Structureâ€“Activity Relationship Resources Facilitate Effective Drug Discovery. Topics in Current Chemistry, 2021, 379, 37.	3.0	8
811	QSAR analysis of sodium glucose coâ€“transporter 2 (SGLT2) inhibitors for anti-hyperglycaemic lead development. SAR and QSAR in Environmental Research, 2021, 32, 731-744.	1.0	1
812	Accelerating antibiotic discovery through artificial intelligence. Communications Biology, 2021, 4, 1050.	2.0	68
813	Dose-effect and structure-activity relationships of haloquinoline toxicity towards Vibrio fischeri. Environmental Science and Pollution Research, 2022, 29, 10858-10864.	2.7	2
814	ADMET Predictability at Boehringer Ingelheim: Stateâ€ofâ€theâ€Art, and Do Bigger Datasets or Algorithms Make a Difference?. Molecular Informatics, 2022, 41, e2100113.	1.4	18
815	A robust classification-dependent multi-molecular modelling study on some biphenyl sulphonamide based MMP-8 inhibitors. SAR and QSAR in Environmental Research, 2021, 32, 835-861.	1.0	5
816	Using molecular embeddings in QSAR modeling: does it make a difference?. Briefings in Bioinformatics, 2022, 23, .	3.2	14
817	Hybrid SFO and TLBO optimization for biodegradable classification. Soft Computing, 2021, 25, 15417-15443.	2.1	3
818	Machine learning analysis of microwave dielectric properties for seven structure types: The role of the processing and composition. Journal of Physics and Chemistry of Solids, 2021, 156, 110178.	1.9	6

#	Article	IF	Citations
819	Comprehensive strategies of machine-learning-based quantitative structure-activity relationship models. IScience, 2021, 24, 103052.	1.9	58
820	Quantum chemical descriptors in quantitative structureâ€“activity relationship models and their applications. Chemometrics and Intelligent Laboratory Systems, 2021, 217, 104384.	1.8	30
821	Chemical safety assessment of transformation products of landfill leachate formed during the Fenton process. Journal of Hazardous Materials, 2021, 419, 126438.	6.5	3
822	Assessing the chemical-induced estrogenicity using in silico and in vitro methods. Environmental Toxicology and Pharmacology, 2021, 87, 103688.	2.0	2
823	Theoretical modeling of structure-toxicity relationship of cyanides. Toxicology Letters, 2021, 349, 30-39.	0.4	7
824	Identification of concealed structural alerts using QSTR modeling for Pseudokirchneriella subcapitata. Aquatic Toxicology, 2021, 239, 105962.	1.9	5
825	Application of Deep Neural Network Models in Drug Discovery Programs. ChemMedChem, 2021, 16, 3772-3786.	1.6	15
826	Predicting zebrafish (Danio rerio) embryo developmental toxicity through a non-conformational QSAR approach. Science of the Total Environment, 2021, 796, 148820.	3.9	11
827	Representative feature selection of molecular descriptors in QSAR modeling. Journal of Molecular Structure, 2021, 1244, 131249.	1.8	12
828	Prenylated (iso)flavonoids as antifungal agents against the food spoiler Zygosaccharomyces parabailii. Food Control, 2022, 132, 108434.	2.8	14
829	Patent Toxicity. Research Policy, 2022, 51, 104329.	3.3	11
830	The Role of Natural Products as Sources of Therapeutic Agents for Innovative Drug Discovery. , 2022, , 408-422.		42
831	Computational identification of chemical compounds with potential anti-Chagas activity using a classification tree. SAR and QSAR in Environmental Research, 2021, 32, 71-83.	1.0	3
832	In Silico Methods to Predict Relevant Toxicological Endpoints of Bioactive Substances. Engineering Materials, 2021, , 649-676.	0.3	2
833	Deep Learning Techniques and COVID-19 Drug Discovery: Fundamentals, State-of-the-Art and Future Directions. Studies in Systems, Decision and Control, 2021, , 9-31.	0.8	24
834	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	18.7	128
835	QSAR: Descriptor calculations, model generation, validation and their application. , 2021, , 29-63.		1
836	Development of potential therapeutics for pain treatment by inducing Sigma 1 receptor antagonism â€“ in silico approach. New Journal of Chemistry, 2021, 45, 12286-12295.	1.4	4

#	Article	IF	Citations
837	QSAR/QSPR Revisited. , 0, , 465-495.		6
838	<scp>HCVpred</scp>: A web server for predicting the bioactivity of hepatitis C virus <scp>NS5B</scp> inhibitors. Journal of Computational Chemistry, 2020, 41, 1820-1834.	1.5	16
839	Computational Approaches to Evaluate Ecotoxicity of Biocides: Cases from the Project COMBASE. Methods in Pharmacology and Toxicology, 2020, , 387-404.	0.1	4
840	QSAR Modeling of Dye Ecotoxicity. Methods in Pharmacology and Toxicology, 2020, , 405-436.	0.1	2
841	Ecotoxicological QSARs of Mixtures. Methods in Pharmacology and Toxicology, 2020, , 437-475.	0.1	4
842	Environmental Toxicity (Q)SARs for Polymers as an Emerging Class of Materials in Regulatory Frameworks, with a Focus on Challenges and Possibilities Regarding Cationic Polymers. Methods in Pharmacology and Toxicology, 2020, , 681-705.	0.1	8
843	Ecotoxicity Databases for QSAR Modeling. Methods in Pharmacology and Toxicology, 2020, , 709-758.	0.1	6
845	On the Relevance of Feature Selection Algorithms While Developing Non-linear QSARs. Methods in Pharmacology and Toxicology, 2020, , 177-194.	0.1	3
846	Interpretable Deep Learning in Drug Discovery. Lecture Notes in Computer Science, 2019, , 331-345.	1.0	62
847	Development of a Neural Network-Based Approach for Prediction of Potential HIV-1 Entry Inhibitors Using Deep Learning and Molecular Modeling Methods. Lecture Notes in Computer Science, 2020, , 304-311.	1.0	4
848	Structural, Physicochemical and Stereochemical Interpretation of QSAR Models Based on Simplex Representation of Molecular Structure. Challenges and Advances in Computational Chemistry and Physics, 2017, , 107-147.	0.6	3
849	Quantitative Structure-Epigenetic Activity Relationships. Challenges and Advances in Computational Chemistry and Physics, 2017, , 303-338.	0.6	4
850	QSAR/QSPR Modeling in the Design of Drug Candidates with Balanced Pharmacodynamic and Pharmacokinetic Properties. Challenges and Advances in Computational Chemistry and Physics, 2017, , 339-384.	0.6	3
851	Quantitative Structure Activity Relationship. , 2017, , 3855-3859.		1
852	Molecular Descriptors. , 2016, , 1-29.		13
853	Why are most phospholipidosis inducers also hERG blockers?. Archives of Toxicology, 2017, 91, 3885-3895.	1.9	22
855	Predictive modeling of aryl hydrocarbon receptor (AhR) agonism. Chemosphere, 2020, 256, 127068.	4.2	11
856	Semi-supervised regression trees with application to QSAR modelling. Expert Systems With Applications, 2020, 158, 113569.	4.4	13

#	Article	IF	Citations
858	Applications of Deep Learning in Molecule Generation and Molecular Property Prediction. Accounts of Chemical Research, 2021, 54, 263-270.	7.6	133
859	CHAPTER 6. Chemical Similarity, Shape Matching and QSAR. Issues in Toxicology, 2017, , 120-173.	0.2	1
860	Chapter 6. A Prediction of Future States: AI-powered Chemical Innovation for Defense Applications. RSC Theoretical and Computational Chemistry Series, 2020, , 136-168.	0.7	1
861	Chapter 15. Representation Learning in Chemistry. RSC Theoretical and Computational Chemistry Series, 2020, , 372-397.	0.7	3
862	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. Toxicology Research, 2016, 5, 883-894.	0.9	10
869	WONKAandOOMMPPAA: analysis of proteinâ€“ligand interaction data to direct structure-based drug design. Acta Crystallographica Section D: Structural Biology, 2017, 73, 279-285.	1.1	5
870	Computational-experimental approach to drug-target interaction mapping: A case study on kinase inhibitors. PLoS Computational Biology, 2017, 13, e1005678.	1.5	84
871	Systematic Artifacts in Support Vector Regression-Based Compound Potency Prediction Revealed by Statistical and Activity Landscape Analysis. PLoS ONE, 2015, 10, e0119301.	1.1	26
872	Template CoMFA Generates Single 3D-QSAR Models that, for Twelve of Twelve Biological Targets, Predict All ChEMBL-Tabulated Affinities. PLoS ONE, 2015, 10, e0129307.	1.1	13
873	Computational Approaches to Identify a Hidden Pharmacological Potential in Large Chemical Libraries. Supercomputing Frontiers and Innovations, 2020, 7, .	0.5	6
874	Toward Good Read-Across Practice (GRAP) guidance. ALTEX: Alternatives To Animal Experimentation, 2016, 33, 149-166.	0.9	134
875	Computational approaches to chemical hazard assessment. ALTEX: Alternatives To Animal Experimentation, 2017, 34, 459-478.	0.9	41
876	Whither QSAR?. Pharmaceutical Sciences, 2017, 23, 82-83.	0.1	7
877	Aromatase inhibitory activity of 1,4-naphthoquinone derivatives and QSAR study. EXCLI Journal, 2017, 16, 714-726.	0.5	16
878	Rational Drug Design of Antineoplastic Agents Using 3D-QSAR, Cheminformatic, and Virtual Screening Approaches. Current Medicinal Chemistry, 2019, 26, 3874-3889.	1.2	20
879	In Silico Chemogenomics Drug Repositioning Strategies for Neglected Tropical Diseases. Current Medicinal Chemistry, 2019, 26, 4355-4379.	1.2	24
880	An Overview of Antiretroviral Agents for Treating HIV Infection in Paediatric Population. Current Medicinal Chemistry, 2020, 27, 760-794.	1.2	5
881	Ligand-Based Virtual Screening Using Tailored Ensembles: A Prioritization Tool for Dual A_{2A} Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. Current Pharmaceutical Design, 2016, 22, 3082-3096.	0.9	13

#	Article	IF	Citations
882	Lipophilic Guanylhydrazone Analogues as Promising Trypanocidal Agents: An Extended SAR Study. Current Pharmaceutical Design, 2020, 26, 838-866.	0.9	4
883	Setting New Routes for Antifungal Drug Discovery Against Pathogenic Fungi. Current Pharmaceutical Design, 2020, 26, 1509-1520.	0.9	8
884	A Random Forest Model to Predict the Activity of a Large Set of Soluble Epoxide Hydrolase Inhibitors Solely Based on a Set of Simple Fragmental Descriptors. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 555-569.	0.6	7
885	Machine Learning in Quantitative Proteinâ€“peptide Affinity Prediction: Implications for Therapeutic Peptide Design. Current Drug Metabolism, 2019, 20, 170-176.	0.7	79
886	Aqueous Drug Solubility: What Do We Measure, Calculate and QSPR Predict?. Mini-Reviews in Medicinal Chemistry, 2019, 19, 362-372.	1.1	15
887	The Application of the Combination of Monte Carlo Optimization Method based QSAR Modeling and Molecular Docking in Drug Design and Development. Mini-Reviews in Medicinal Chemistry, 2020, 20, 1389-1402.	1.1	17
888	Applications of Quantitative Structure-Activity Relationships (QSAR) based Virtual Screening in Drug Design: A Review. Mini-Reviews in Medicinal Chemistry, 2020, 20, 1375-1388.	1.1	30
889	Tuning hERG Out: Antitarget QSAR Models for Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1399-1415.	1.0	82
890	Perspectives in Medicinal Chemistry: The Evolution of Medicinal Chemistry. Current Topics in Medicinal Chemistry, 2015, 16, 897-898.	1.0	2
891	Molecular Modeling Approaches for the Prediction of Selected Pharmacokinetic Properties. Current Topics in Medicinal Chemistry, 2019, 18, 2230-2238.	1.0	2
892	Virtual Screening Techniques in Drug Discovery: Review and Recent Applications. Current Topics in Medicinal Chemistry, 2019, 19, 1751-1767.	1.0	99
893	Current Advances and Limitations of Deep Learning in Anticancer Drug Sensitivity Prediction. Current Topics in Medicinal Chemistry, 2020, 20, 1858-1867.	1.0	8
894	QSAR Modeling of Histamine H3R Antagonists/inverse Agonists as Future Drugs for Neurodegenerative Diseases. Current Neuropharmacology, 2018, 16, 749-757.	1.4	7
895	Quantitative Structure-Activity Relationship Study for HIV-1 LEDGF/p75 Inhibitors. Current Computer-Aided Drug Design, 2020, 16, 654-666.	0.8	2
896	Dapsone is not a Pharmacodynamic Lead Compound for its Aryl Derivatives. Current Computer-Aided Drug Design, 2020, 16, 327-339.	0.8	2
897	Communicative Representation Learning on Attributed Molecular Graphs. , 2020, , .		50
898	In Silico Prediction of Intestinal Permeability by Hierarchical Support Vector Regression. International Journal of Molecular Sciences, 2020, 21, 3582.	1.8	11
899	Experimental Data Based Machine Learning Classification Models with Predictive Ability to Select in Vitro Active Antiviral and Non-Toxic Essential Oils. Molecules, 2020, 25, 2452.	1.7	19

#	Article	IF	Citations
900	Predictive Modeling of Critical Temperatures in Superconducting Materials. Molecules, 2021, 26, 8.	1.7	6
901	QSAR and Molecular Docking Studies on Non-Imidazole-Based Histamine H3 Receptor Antagonists. Pharmaceutical Sciences, 2020, 26, 165-174.	0.1	6
902	The History and Development of Quantitative Structure-Activity Relationships (QSARs). , 2017, , 67-117.		21
903	Computational Tools and Techniques to Predict Aquatic Toxicity of Some Halogenated Pollutants. Advances in Environmental Engineering and Green Technologies Book Series, 2019, , 318-337.	0.3	3
904	Computational maturation of a single-domain antibody against AÎ²42 aggregation. Chemical Science, 2021, 12, 13940-13948.	3.7	4
906	Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. Molecular Diversity, 2022, 26, 1893-1913.	2.1	35
907	Quantum Artificial Neural Network Approach to Derive a Highly Predictive 3D-QSAR Model for Bloodâ€“Brain Barrier Passage. International Journal of Molecular Sciences, 2021, 22, 10995.	1.8	8
908	Computer Aided Drug Design Methodologies with Natural Products in the Drug Research Against Alzheimerâ€™s Disease. Current Neuropharmacology, 2022, 20, 857-885.	1.4	6
909	Drug Repurposing to Identify Nilotinib as a Potential SARS-CoV-2 Main Protease Inhibitor: Insights from a Computational and In Vitro Study. Journal of Chemical Information and Modeling, 2021, 61, 5469-5483.	2.5	26
910	Using computers to ESKAPE the antibiotic resistance crisis. Drug Discovery Today, 2022, 27, 456-470.	3.2	7
911	Suggestion of active 3-chymotrypsin like protease (3CL^{Pro}) inhibitors as potential anti-SARS-CoV-2 agents using predictive QSAR model based on the combination of ALASSO with an ANN model. SAR and QSAR in Environmental Research, 2021, 32, 863-888.	1.0	2
913	The Computer â€“ Your Virgil in the World of Atoms. Visnik Nacional Noi Academii Nauk Ukrai Ni, 2014, , 22-31.	0.0	0
914	Cheminformatics and Molecular Modeling. Journal of Molecular and Genetic Medicine: an International Journal of Biomedical Research, 2015, 09, .	0.1	0
915	The review of the most used computational methods for studies of the relationships between molecular structure and biological activity. ScienceRise, 2015, 10, 9.	0.1	0
916	Virtual screening tailored ensembles of QSAR models for the discovery of dual A_{2A} Adenosine Receptor Antagonists / Monoamine Oxidase B Inhibitors. , 0, , .		0
917	Molecular Fields to Assess Recognition Forces and Property Spacesâ€†. , 2016, , .		1
918	New Microbiological and Pharmacokinetic models. , 0, , .		0
919	New Drugs - From Necessity to Delivery. Current Issues in Pharmacy and Medical Sciences, 2018, 31, 69-75.	0.1	2

#	Article	IF	Citations
922	Medical Devices Biological Safety Assessment: Towards Animal-free Testing. Derecho Animal, 2019, 10, 91.	0.1	0
923	Methods for Biodegradability and Toxicity Assessment of Ionic Liquid. , 2019, , 1-6.		0
924	Assessment of Exposures in Vulnerable Populations: Exposure and Response Modelling for Environmental Contaminants Through a Lifetime. Encyclopedia of the UN Sustainable Development Goals, 2019, , 1-13.	0.0	0
925	An Introduction to (Q)SAR with Respect to Regulatory Submissions. , 2019, , 321-337.		0
926	Predictive Power of Time-Series Based Machine Learning Models for DMPK Measurements in Drug Discovery. Lecture Notes in Computer Science, 2019, , 741-746.	1.0	1
927	Image-based QSAR Model for the Prediction of P-gp Inhibitory Activity of Epigallocatechin and Gallocatechin Derivatives. Current Computer-Aided Drug Design, 2019, 15, 212-224.	0.8	2
928	Estudio computacional de la reactividad y propiedades fisicoquÃmicas del eugenol, 2-metoxi-4-oxiranilmetilfenol y quinona metilada. Revista Colombiana De Ciencias QuÃmico FarmacÃ©uticas, 2019, 48, 245-259.	0.3	0
929	Quantitative Prediction of Toxicity of Substituted Phenols Using Deep Learning. Smart Innovation, Systems and Technologies, 2020, , 123-130.	0.5	0
931	Assessment of Exposures in Vulnerable Populations: Exposure and Response Modelling for Environmental Contaminants Through a Lifetime. Encyclopedia of the UN Sustainable Development Goals, 2020, , 38-50.	0.0	0
932	Future of Regulatory Safety Assessments. , 2020, , 1145-1168.		0
933	QSAR-ANALYSIS OF POLYSUBSTITUTED FUNCTIONALIZED AMINOTHIAZOLES WITH ANTIHYPERTENSIVE ACTIVITY. International Journal of Medicine and Medical Research, 2020, 5, 98-104.	0.0	1
936	Nonantimicrobial Actions of Macrolides: Overview and Perspectives for Future Development. Pharmacological Reviews, 2021, 73, 1404-1433.	7.1	40
937	Virtual screening of dipeptidyl peptidase-4 inhibitors using quantitative structureâ€“activity relationship-based artificial intelligence and molecular docking of hit compounds. Computational Biology and Chemistry, 2021, 95, 107597.	1.1	10
938	Unsupervised Machine Learning Neural Gas Algorithm for Accurate Evaluations of the Hessian Matrix in Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 6733-6746.	2.3	7
939	Knowledge-based approaches to drug discovery for rare diseases. Drug Discovery Today, 2022, 27, 490-502.	3.2	15
940	Evaluating High-Variance Leaves as Uncertainty Measure for Random Forest Regression. Molecules, 2021, 26, 6514.	1.7	5
941	How doppelgÃnger effects in biomedical data confound machine learning. Drug Discovery Today, 2022, 27, 678-685.	3.2	6
942	Diversity and Chemical Library Networks of Large Data Sets. Journal of Chemical Information and Modeling, 2022, 62, 2186-2201.	2.5	22

#	Article	IF	Citations
943	Multi-objective optimization methods in novel drug design. Expert Opinion on Drug Discovery, 2021, 16, 647-658.	2.5	23
944	Rational Design of Potential Bcr-Abl Tyrosine Kinase Inhibitors by the Methods of Molecular Modeling. Mathematical Biology and Bioinformatics, 2020, 15, 396-415.	0.1	1
945	Approaches using AI in medicinal chemistry. , 2022, , 111-159.		0
946	Use of Machine Learning and Classical QSAR Methods in Computational Ecotoxicology. Methods in Pharmacology and Toxicology, 2020, , 151-175.	0.1	2
947	Benchmarking Small-Dataset Structure-Activity-Relationship Models for Prediction of Wnt Signaling Inhibition. IEEE Access, 2020, 8, 228831-228840.	2.6	9
948	Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches. , 2020, , 81-108.		0
949	Machine Learning and Big Data Provide Crucial Insight for Future Biomaterials Discovery and Research. SSRN Electronic Journal, 0, , .	0.4	0
950	Computational Modeling of Nonlinear Phenomena Using Machine Learning. AAPS Introductions in the Pharmaceutical Sciences, 2020, , 53-62.	0.1	0
951	Generating Explainable and Effective Data Descriptors Using Relational Learning: Application to Cancer Biology. Lecture Notes in Computer Science, 2020, , 374-385.	1.0	2
952	Strategies of Virtual Screening in Medicinal Chemistry. , 2020, , 194-225.		1
953	QSAR model of phenols generated by deep neural network. , 2020, , .		0
954	The development of a predictive model to identify potential HIV-1 attachment inhibitors. Computers in Biology and Medicine, 2020, 120, 103743.	3.9	1
955	Deep Neural Networks for QSAR. Methods in Molecular Biology, 2022, 2390, 233-260.	0.4	13
956	Artificial Intelligence in Compound Design. Methods in Molecular Biology, 2022, 2390, 349-382.	0.4	4
957	Applications of Artificial Intelligence in Drug Design: Opportunities and Challenges. Methods in Molecular Biology, 2022, 2390, 1-59.	0.4	11
958	New insights into toxicity of microcystins produced by cyanobacteria using in silico ADMET prediction. Toxicon, 2021, 204, 64-71.	0.8	3
960	Molecular docking and QSAR theoretical model for prediction of phthalazinone derivatives as new class of potent dengue virus inhibitors. Beni-Suef University Journal of Basic and Applied Sciences, 2020, 9, .	0.8	14
961	Application of Deep Learning and Molecular Modelling Methods to Identify Potential HIV-1 Entry Inhibitors. , 0, , .		0

#	Article	IF	Citations
962	Molecular Docking of Novel 5-O-benzoylpinostrobin Derivatives as SARS-CoV-2 Main Protease Inhibitors. Pharmaceutical Sciences, 2020, 26, S63-S77.	0.1	2
963	Chemoinformatics for Data Scientists. , 2020, , .		0
965	Chemical reaction vector embeddings: towards predicting drug metabolism in the human gut microbiome. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2018, 23, 56-67.	0.7	7
966	Pharmacophore modeling and its applications. , 2022, , 269-289.		5
971	In Silico Prediction of Steroids and Triterpenoids as Potential Regulators of Lipid Metabolism. Marine Drugs, 2021, 19, 650.	2.2	18
972	Transformational machine learning: Learning how to learn from many related scientific problems. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11
973	QSAR, pharmacophore modeling and molecular docking studies to identify structural alerts for some nitrogen heterocycles as dual inhibitor of telomerase reverse transcriptase and human telomeric G-quadruplex DNA. Future Journal of Pharmaceutical Sciences, 2021, 7, .	1.1	1
974	Towards Property Profiling: SYNTHESIS and SAR Probing of New Tetracyclic Diazaphenothiazine Analogues. International Journal of Molecular Sciences, 2021, 22, 12826.	1.8	7
975	The effect of noise on the predictive limit of QSAR models. Journal of Cheminformatics, 2021, 13, 92.	2.8	15
976	TargetTox: A Feature Selection Pipeline for Identifying Predictive Targets Associated with Drug Toxicity. Journal of Chemical Information and Modeling, 2021, 61, 5386-5394.	2.5	7
977	Application of Machine Learning and Reaction Optimization for the Iterative Improvement of Enantioselectivity of Cinchona-Derived Phase Transfer Catalysts. Organic Process Research and Development, 2022, 26, 670-682.	1.3	14
978	Unsupervised Representation Learning for Proteochemometric Modeling. International Journal of Molecular Sciences, 2021, 22, 12882.	1.8	5
979	Molecular Modeling Techniques Applied to the Design of Multitarget Drugs: Methods and Applications. Current Topics in Medicinal Chemistry, 2022, 22, 333-346.	1.0	3
980	Molecular modeling in cardiovascular pharmacology: current state of the art and perspectives. Drug Discovery Today, 2021, , .	3.2	3
981	Quantitative structureâ€“activity relationship(QSAR) models for color and COD removal for some dyes subjected to electrochemical oxidation. Environmental Technology (United Kingdom), 2023, 44, 2374-2385.	1.2	7
982	Development of a QSAR model to predict comedogenic potential of some cosmetic ingredients. Computational Toxicology, 2022, 21, 100207.	1.8	3
983	Methodological aspects of assessment of the state of chemical pollution and water quality of surface waters in Ukraine. Zurnal Hromatograficnogo Tovaristva, 2020, 20, 33-61.	0.1	0
984	VIRTECS: Virtual Screening Of Therapeutic Classes Using Encodings Of Chemical Structures. , 2020, , .		0

#	Article	IF	Citations
985	Structure-Based Virtual Screening for Ligands of G Proteinâ€“Coupled Receptors: What Can Molecular Docking Do for You?. Pharmacological Reviews, 2021, 73, 1698-1736.	7.1	61
986	Hydrobiological Aspects of Saturated, Methyl-Branched, and Cyclic Fatty Acids Derived from Aquatic Ecosystems: Origin, Distribution, and Biological Activity. Hydrobiology, 2022, 1, 89-110.	0.9	1
987	Development of novel antipsychotic agents by inhibiting dopamine transporter â€“in silicoapproach. New Journal of Chemistry, 2022, 46, 2687-2696.	1.4	3
988	PlayMolecule Glimpse: Understanding Proteinâ€“Ligand Property Predictions with Interpretable Neural Networks. Journal of Chemical Information and Modeling, 2022, 62, 225-231.	2.5	11
989	QSAR studies of BBR analogues against coxsackievirus B1. Bulletin of the National Research Centre, 2022, 46, .	0.7	1
990	High-Throughput Chemical Screening and Structure-Based Models to Predict hERG Inhibition. Biology, 2022, 11, 209.	1.3	8
991	Computer-Assisted Discovery of Alkaloids with Schistosomicidal Activity. Current Issues in Molecular Biology, 2022, 44, 383-408.	1.0	7
992	Prediction of degradability of micropollutants by sonolysis in water with QSPR - a case study on phenol derivates. Ultrasonics Sonochemistry, 2022, 82, 105867.	3.8	8
993	QSAR Classification Models for Prediction of Hydroxamate Histone Deacetylase Inhibitor Activity against Malaria Parasites. ACS Infectious Diseases, 2022, 8, 106-117.	1.8	8
994	Statistical methods for in silico tools used for risk assessment and toxicology. ChemistrySelect, 2022, .	0.7	1
995	Computational Medicinal Chemistry to Target GPCRs. , 2022, , 84-114.		3
996	Skin sensitization quantitative QSAR models based on mechanistic structural alerts. Toxicology, 2022, 468, 153111.	2.0	2
997	Exploiting Endocytosis for Non-Spherical Nanoparticle Cellular Uptake. Nanomanufacturing, 2022, 2, 1-16.	1.8	16
998	The system of self-consistent models for vapour pressure. Chemical Physics Letters, 2022, 790, 139354.	1.2	9
999	Deep learning meets quantitative structureâ€“activity relationship (QSAR) for leveraging structure-based prediction of solute rejection in organic solvent nanofiltration. Journal of Membrane Science, 2022, 646, 120268.	4.1	47
1000	Benchmarking machine learning methods for modeling physical properties of ionic liquids. Journal of Molecular Liquids, 2022, 351, 118616.	2.3	24
1001	How can polydispersity information be integrated in the QSPR modeling of mechanical properties?. Science and Technology of Advanced Materials Methods, 2022, 2, 1-13.	0.4	2
1002	Sextans: A Streaming Accelerator for General-Purpose Sparse-Matrix Dense-Matrix Multiplication. , 2022, , .		24

#	Article	IF	Citations
1003	Application of artificial neural networks to the prediction of antifungal activity of imidazole derivatives against Candida albicans. Chemometrics and Intelligent Laboratory Systems, 2022, 222, 104501.	1.8	8
1004	Data-driven catalyst optimization for stereodivergent asymmetric synthesis by iridium/boron hybrid catalysis. Cell Reports Physical Science, 2021, 2, 100679.	2.8	25
1005	Improving QSAR Modeling for Predictive Toxicology using Publicly Aggregated Semantic Graph Data and Graph Neural Networks. Pacific Symposium on Biocomputing Pacific Symposium on Biocomputing, 2022, 27, 187-198.	0.7	0
1006	Increasing the Value of Data Within a Large Pharmaceutical Company Through In Silico Models. Methods in Molecular Biology, 2022, 2425, 637-674.	0.4	2
1007	Creation of Quantitative Feature Toxicity Relationship Models for Cytotoxicity of Cadmium Containing Quantum Dots towards HEK Cells using QuasiSMILES. International Journal of Quantitative Structure-Property Relationships, 2022, 7, 0-0.	1.1	0
1008	Pharmacokinetic Tools and Applications. Methods in Molecular Biology, 2022, 2425, 57-83.	0.4	3
1010	Computational Modeling of Mixture Toxicity. Methods in Molecular Biology, 2022, 2425, 561-587.	0.4	2
1012	Assisting Multitargeted Ligand Affinity Prediction of Receptor Tyrosine Kinases Associated Nonsmall Cell Lung Cancer Treatment with Multitasking Principal Neighborhood Aggregation. Molecules, 2022, 27, 1226.	1.7	3
1013	Machine Learning Analysis of Essential Oils from Cuban Plants: Potential Activity against Protozoa Parasites. Molecules, 2022, 27, 1366.	1.7	0
1014	COVIDâ€19: A systematic review and update on prevention, diagnosis, and treatment. MedComm, 2022, 3, e115.	3.1	30
1015	Computational Methods for the Interaction between Cyclodextrins and Natural Compounds: Technology, Benefits, Limitations, and Trends. Journal of Agricultural and Food Chemistry, 2022, 70, 2466-2482.	2.4	18
1016	Relationships between the Structure and Severe Drug-Induced Liver Injury for Low, Medium, and High Doses of Drugs. Chemical Research in Toxicology, 2022, 35, 402-411.	1.7	4
1017	Next-Generation Molecular Discovery: From Bottom-Up In Vivo and In Vitro Approaches to In Silico Top-Down Approaches for Therapeutics Neogenesis. Life, 2022, 12, 363.	1.1	1
1018	Extended continuous similarity indices: theory and application for QSAR descriptor selection. Journal of Computer-Aided Molecular Design, 2022, 36, 157-173.	1.3	7
1019	Working at the interfaces of data science and synthetic electrochemistry. , 2022, 1, 100012.		9
1020	Exploring the Prominent and Concealed Inhibitory Features for Cytoplasmic Isoforms of Hsp90 Using QSAR Analysis. Pharmaceuticals, 2022, 15, 303.	1.7	2
1021	AFSE: towards improving model generalization of deep graph learning of ligand bioactivities targeting GPCR proteins. Briefings in Bioinformatics, 2022, 23, .	3.2	2
1023	Limits of Prediction for Machine Learning in Drug Discovery. Frontiers in Pharmacology, 2022, 13, 832120.	1.6	4

#	Article	IF	Citations
1024	A Statistical Comparison between Zagreb indices for correlation with toxicity predictions of natural products. International Journal of Research in Pharmaceutical Sciences, 2022, 13, 121-125.	0.0	1
1025	In silico approach for the development of novel antiviral compounds based on SARS-COV-2 protease inhibition. Chemical Papers, 2022, 76, 4393-4404.	1.0	1
1026	Identification of potent aldose reductase inhibitors as antidiabetic (Anti-hyperglycemic) agents using QSAR based virtual Screening, molecular Docking, MD simulation and MMGBSA approaches. Saudi Pharmaceutical Journal, 2022, 30, 693-710.	1.2	16
1027	Multi-Strategy Assessment of Different Uses of QSAR under REACH Analysis of Alternatives to Advance Information Transparency. International Journal of Environmental Research and Public Health, 2022, 19, 4338.	1.2	4
1028	QSPR Modelling of the Solubility of Drug and Drugâ€like Compounds in Supercritical Carbon Dioxide. Molecular Informatics, 2022, 41, .	1.4	7
1029	Predicting chemical hazard across taxa through machine learning. Environment International, 2022, 163, 107184.	4.8	21
1030	Development of an in silico consensus model for the prediction of the phospholipigenic potential of small molecules. Computational Toxicology, 2022, 22, 100226.	1.8	3
1031	Predicting chemical ecotoxicity by learning latent space chemical representations. Environment International, 2022, 163, 107224.	4.8	5
1032	Nanochemistry advancing photon conversion in rare-earth nanostructures for theranostics. Coordination Chemistry Reviews, 2022, 460, 214486.	9.5	39
1033	Robust and predictive QSAR models for predicting the D2, 5-HT1A, and 5-HT2A inhibition activities of fused tricyclic heterocycle piperazine (piperidine) derivatives as atypical antipsychotic drugs. Journal of Molecular Structure, 2022, 1259, 132753.	1.8	2
1034	Hierarchical Modeling of Binding Affinity Prediction Using Machine LearningTechniques. , 2021, , .		1
1035	Leveraging nonstructural data to predict structures and affinities of proteinâ€“ligand complexes. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	17
1037	Selection of Promising Novel Fragment Sized S. aureus SrtA Noncovalent Inhibitors Based on QSAR and Docking Modeling Studies. Molecules, 2021, 26, 7677.	1.7	6
1038	Joint Decision-Making Model Based on Consensus Modeling Technology for the Prediction of Drug-Induced Liver Injury. Journal of Chemistry, 2021, 2021, 1-20.	0.9	1
1039	Disclosing incoherent sparse and low-rank patterns inside homologous GPCR tasks for better modelling of ligand bioactivities. Frontiers of Computer Science, 2022, 16, .	1.6	1
1040	Discovery of Novel Epidermal Growth Factor Receptor (EGFR) Inhibitors Using Computational Approaches. Journal of Chemical Information and Modeling, 2022, 62, 5149-5164.	2.5	6
1041	Interpreting the Physicochemical Meaning of a Molecular Descriptor Which Is Predictive of Amorphous Solid Dispersion Formation in Polyvinylpyrrolidone Vinyl Acetate. Molecular Pharmaceutics, 2022, 19, 303-317.	2.3	8
1042	Novel computational models offer alternatives to animal testing for assessing eye irritation and corrosion potential of chemicals. Artificial Intelligence in the Life Sciences, 2021, 1, 100028.	1.6	7

#	Article	IF	Citations
1043	Topological Distance-Based Electron Interaction Tensor to Apply a Convolutional Neural Network on Drug-like Compounds. ACS Omega, 2021, 6, 35757-35768.	1.6	2
1044	Dielectric Polymer Genome: Integrating Valence-Aware Polarizable Reactive Force Fields and Machine Learning. Transactions on Computational Science and Computational Intelligence, 2021, , 51-64.	0.3	2
1045	A Review on Procedure of QSAR Assessment in Organic Compounds As a Measure of Antioxidant Potentiality. , 2022, 1, 08-18.		4
1046	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	8.3	73
1047	Machine Learning in Chemoinformatics and Medicinal Chemistry. Annual Review of Biomedical Data Science, 2022, 5, 43-65.	2.8	8
1048	Investigation of potential descriptors of chemical compounds on prevention of nephrotoxicity via QSAR approach. Computational and Structural Biotechnology Journal, 2022, 20, 1876-1884.	1.9	4
1049	QSAR analysis on a large and diverse set of potent phosphoinositide 3-kinase gamma (PI3KÎ³) inhibitors using MLR and ANN methods. Scientific Reports, 2022, 12, 6090.	1.6	9
1062	Machine Learning Applications for Chemical Reactions. Chemistry - an Asian Journal, 2022, 17, .	1.7	13
1063	A novel workflow for semi-quantification of emerging contaminants in environmental samples analyzed by LC-HRMS. Analytical and Bioanalytical Chemistry, 2022, 414, 7435-7450.	1.9	25
1064	Predicting Prenatal Developmental Toxicity Based On the Combination of Chemical Structures and Biological Data. Environmental Science & Technology, 2022, 56, 5984-5998.	4.6	11
1065	Target Specific Inhibition of Protein Tyrosine Kinase in Conjunction With Cancer and SARS-COV-2 by Olive Nutraceuticals. Frontiers in Pharmacology, 2021, 12, 812565.	1.6	17
1066	The first report on predictive comparative ligand-based multi-QSAR modeling analysis of 4-pyrimidinone and 2-pyridinone based APJ inhibitors. New Journal of Chemistry, 2022, 46, 11591-11607.	1.4	9
1067	A Machine Learning Language to Build a QSAR Model of Pyrazoline Derivative Inhibitors Targeting Mycobacterium tuberculosis Strain H37Rv. Letters in Drug Design and Discovery, 2023, 20, 167-180.	0.4	0
1069	Design and Development of Novel Nutraceuticals: Current Trends and Methodologies. Nutraceuticals, 2022, 2, 71-90.	0.6	10
1070	In Silico Prediction of Skin Permeability Using a Two-QSAR Approach. Pharmaceutics, 2022, 14, 961.	2.0	3
1071	Natural Polyether Ionophores and Their Pharmacological Profile. Marine Drugs, 2022, 20, 292.	2.2	7
1072	Insight into potent TLR2 inhibitors for the treatment of disease caused by Mycoplasma pneumoniae based on machine learning approaches. Molecular Diversity, 2023, 27, 371-387.	2.1	21
1073	Application of Artificial Intelligence in Discovery and Development of Anticancer and Antidiabetic Therapeutic Agents. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-16.	0.5	5

#	Article	IF	Citations
1074	Towards quantifying the uncertainty in in silico predictions using Bayesian learning. Computational Toxicology, 2022, 23, 100228.	1.8	2
1075	In silico models to predict tubular secretion or reabsorption clearance pathway using physicochemical properties and structural characteristics. Xenobiotica, 2022, 52, 346-352.	0.5	1
1076	Machine Learning on DNA-Encoded Library Count Data Using an Uncertainty-Aware Probabilistic Loss Function. Journal of Chemical Information and Modeling, 2022, 62, 2316-2331.	2.5	20
1077	Accelerating AutoDock Vina with GPUs. Molecules, 2022, 27, 3041.	1.7	28
1078	Quantitative Structureâ€“Activity Relationship (QSAR) Study Predicts Small-Molecule Binding to RNA Structure. Journal of Medicinal Chemistry, 2022, 65, 7262-7277.	2.9	21
1079	Quantitative in vitro to in vivo extrapolation for developmental toxicity potency of valproic acid analogues. Birth Defects Research, 2022, 114, 1037-1055.	0.8	4
1080	Semi-automated harmonization and selection of chemical data for risk and impact assessment. Chemosphere, 2022, 302, 134886.	4.2	6
1081	Data considerations for predictive modeling applied to the discovery of bioactive natural products. Drug Discovery Today, 2022, 27, 2235-2243.	3.2	7
1083	Insights into the Pharmacological Effects of Flavonoids: The Systematic Review of Computer Modeling. International Journal of Molecular Sciences, 2022, 23, 6023.	1.8	16
1085	An Overview of Antiviral Peptides and Rational Biodesign Considerations. Biodesign Research, 2022, 2022, .	0.8	11
1086	Machine Learning Prediction of <scp>Structureâ€Performance</scp> Relationship in Organic Synthesis. Chinese Journal of Chemistry, 2022, 40, 2106-2117.	2.6	6
1087	Allosteric Binders of ACE2 Are Promising Anti-SARS-CoV-2 Agents. ACS Pharmacology and Translational Science, 2022, 5, 468-478.	2.5	3
1088	Analysis of the benefits of imputation models over traditional QSAR models for toxicity prediction. Journal of Cheminformatics, 2022, 14, .	2.8	7
1089	Application of Machine Learning in Developing Quantitative Structureâ€“Property Relationship for Electronic Properties of Polyaromatic Compounds. ACS Omega, 2022, 7, 22879-22888.	1.6	5
1090	Mechanistic Analysis of Chemically Diverse Bromodomain-4 Inhibitors Using Balanced QSAR Analysis and Supported by X-ray Resolved Crystal Structures. Pharmaceuticals, 2022, 15, 745.	1.7	1
1091	Quantitative structureâ€“activity relationship modeling of hydroxylated polychlorinated biphenyls as constitutive androstane receptor agonists. Structural Chemistry, 2023, 34, 477-490.	1.0	3
1092	Predicting In Vivo Compound Brain Penetration Using Multi-task Graph Neural Networks. Journal of Chemical Information and Modeling, 2022, 62, 3180-3190.	2.5	13
1093	Artificial Intelligence-Based Toxicity Prediction of Environmental Chemicals: Future Directions for Chemical Management Applications. Environmental Science & Technology, 2022, 56, 7532-7543.	4.6	34

#	Article	IF	Citations
1094	In-silico and in-vitro studies on the efficacy of mangiferin against colorectal cancer. BMC Chemistry, 2022, 16, .	1.6	2
1095	Critical features identification for chemical chronic toxicity based on mechanistic forecast models. Environmental Pollution, 2022, 307, 119584.	3.7	1
1096	QSAR modelling, molecular docking studies and ADMET predictions of polysubstituted pyridinylimidazoles as dual inhibitors of JNK3 and p38Î± MAPK. Journal of Molecular Structure, 2022, 1265, 133504.	1.8	3
1097	Machine learning hybrid approach for the prediction of surface tension profiles of hydrocarbon surfactants in aqueous solution. Journal of Colloid and Interface Science, 2022, 625, 328-339.	5.0	7
1098	Quantitative structure-activity relationships (QSARs). , 2022, , 101-123.		1
1099	Molecular field analysis for data-driven molecular design in asymmetric catalysis. Organic and Biomolecular Chemistry, 2022, 20, 6057-6071.	1.5	2
1100	Monte Carlo optimization method based QSAR modeling of postmortem redistribution of structurally diverse drugs. New Journal of Chemistry, 0, , .	1.4	0
1101	Computer-Aided Drug Design and Development: An Integrated Approach. , 0, , .		0
1102	IN SILICO ANALYSIS OF EDIBLE BIRDâ€™S NEST PROTEINS AS POTENTIAL PRECURSORS FOR BIOACTIVE PEPTIDES. , 2022, 51, 53-62.		0
1103	First report of q-RASAR modeling toward an approach of easy interpretability and efficient transferability. Molecular Diversity, 2022, 26, 2847-2862.	2.1	51
1104	Microbiological Aspects of Unique, Rare, and Unusual Fatty Acids Derived from Natural Amides and Their Pharmacological Profile. Microbiology Research, 2022, 13, 377-417.	0.8	5
1105	Computational analysis, alignmentÂand extension of analogue series from medicinal chemistry. Future Science OA, 0, , .	0.9	0
1106	First Novel Workflow for Semiquantification of Emerging Contaminants in Environmental Samples Analyzed by Gas Chromatographyâ€“Atmospheric Pressure Chemical Ionizationâ€“Quadrupole Time of Flightâ€“Mass Spectrometry. Analytical Chemistry, 2022, 94, 9766-9774.	3.2	6
1107	Computational Methods in Cooperation with Experimental Approaches to Design Protein Tyrosine Phosphatase 1B Inhibitors in Type 2 Diabetes Drug Design: A Review of the Achievements of This Century. Pharmaceuticals, 2022, 15, 866.	1.7	11
1108	Principles and procedures for assessment of acute toxicity incorporating in silico methods. Computational Toxicology, 2022, 24, 100237.	1.8	5
1109	Perceiving the Concealed and Unreported Pharmacophoric Features of the 5-Hydroxytryptamine Receptor Using Balanced QSAR Analysis. Pharmaceuticals, 2022, 15, 834.	1.7	4
1110	Natural Products from Annonaceae as Potential Antichagasic Agents. ChemMedChem, 2022, 17, .	1.6	0
1111	Chemoinformatics Analysis of the Colour Fastness Properties of Acid and Direct Dyes in Textile Coloration. Colorants, 2022, 1, 280-297.	0.9	3

#	Article	IF	Citations
1112	Quantitative predictions from chemical read-across and their confidence measures. Chemometrics and Intelligent Laboratory Systems, 2022, 227, 104613.	1.8	32
1113	Toxicity prediction of 1,2,4-triazoles compounds by QSTR and interspecies QSTTR models. Ecotoxicology and Environmental Safety, 2022, 242, 113839.	2.9	3
1114	Conformational Effects on the Passive Membrane Permeability of Synthetic Macrocycles. Journal of Medicinal Chemistry, 2022, 65, 10300-10317.	2.9	8
1115	Escaping from the Cutoff Paradox by Accumulating Long-Chain Alcohols in the Cell Membrane. Journal of Medicinal Chemistry, 2022, 65, 10471-10480.	2.9	3
1116	Unsymmetrical aromatic disulfides as SARS-CoV-2 Mpro inhibitors: Molecular docking, molecular dynamics, and ADME scoring investigations. Journal of King Saud University - Science, 2022, 34, 102226.	1.6	16
1117	QSAR Evaluations to Unravel the Structural Features in Lysine-Specific Histone Demethylase 1A Inhibitors for Novel Anticancer Lead Development Supported by Molecular Docking, MD Simulation and MMGBSA. Molecules, 2022, 27, 4758.	1.7	4
1118	Development of Novel Therapeutics for Schizophrenia Treatment Based on a Selective Positive Allosteric Modulation of Î±1-Containing GABAARsâ€"In Silico Approach. Current Issues in Molecular Biology, 2022, 44, 3398-3412.	1.0	1
1119	AI for predicting chemical-effect associations at the chemical universe levelâ€"<tt>deepFPlearn</tt>. Briefings in Bioinformatics, 2022, 23, .	3.2	2
1120	Relationships Between Aquatic Toxicity, Chemical Hydrophobicity, and Mode of Action: Log Kow Revisited. Archives of Environmental Contamination and Toxicology, 2022, 83, 326-338.	2.1	6
1121	Application of Machine Learning Technology in the Prediction of ADME- Related Pharmacokinetic Parameters. Current Medicinal Chemistry, 2023, 30, 1945-1962.	1.2	2
1122	Ligand Binding Prediction Using Protein Structure Graphs and Residual Graph Attention Networks. Molecules, 2022, 27, 5114.	1.7	5
1123	MolPredictX: Online Biological Activity Predictions by Machine Learning Models. Molecular Informatics, 2022, 41, .	1.4	5
1124	Transforming the evaluation of agrochemicals. Pest Management Science, 2022, 78, 5049-5056.	1.7	6
1125	In silico QSAR modeling to predict the safe use of antibiotics during pregnancy. Drug and Chemical Toxicology, 2023, 46, 962-971.	1.2	5
1126	Viral informatics: bioinformatics-based solution for managing viral infections. Briefings in Bioinformatics, 2022, 23, .	3.2	10
1127	Integrating concept of pharmacophore with graph neural networks for chemical property prediction and interpretation. Journal of Cheminformatics, 2022, 14, .	2.8	5
1128	Representing and describing nanomaterials in predictive nanoinformatics. Nature Nanotechnology, 2022, 17, 924-932.	15.6	23
1130	Annonaceae Terpenoids as Potential Leishmanicidal Agents. Revista Brasileira De Farmacognosia, 0, , .	0.6	0

#	Article	IF	Citations
1131	PreS/MD: Predictor of Sensitization Hazard for Chemical Substances Released From Medical Devices. Toxicological Sciences, 0, , .	1.4	2
1132	Harnessing Semi-Supervised Machine Learning to Automatically Predict Bioactivities of Per- and Polyfluoroalkyl Substances (PFASs). Environmental Science and Technology Letters, 2023, 10, 1017-1022.	3.9	10
1133	Comparison of various methods for validity evaluation of QSAR models. BMC Chemistry, 2022, 16, .	1.6	11
1134	Structural characterization of functional peptides by extending the hybrid orbital theory. EFood, 2022, 3, .	1.7	1
1135	VLA-SMILES: Variable-Length-Array SMILES Descriptors in Neural Network-Based QSAR Modeling. Machine Learning and Knowledge Extraction, 2022, 4, 715-737.	3.2	0
1136	QSAR, Molecular Docking, MD Simulation and MMGBSA Calculations Approaches to Recognize Concealed Pharmacophoric Features Requisite for the Optimization of ALK Tyrosine Kinase Inhibitors as Anticancer Leads. Molecules, 2022, 27, 4951.	1.7	9
1137	A brief guide to machine learning for antibiotic discovery. Current Opinion in Microbiology, 2022, 69, 102190.	2.3	14
1138	Concepts and applications of chemical fingerprint for hit and lead screening. Drug Discovery Today, 2022, 27, 103356.	3.2	17
1139	Virtual screening techniques in pharmaceutical research. , 2022, , 89-128.		0
1140	Anti-breast Cancer Drug Design and ADMET Prediction of ERa Antagonists Based on QSAR Study. Lecture Notes in Computer Science, 2022, , 28-40.	1.0	0
1141	Monte Carlo based QSGFEAR: prediction of Gibb's free energy of activation at different temperatures using SMILES based descriptors. New Journal of Chemistry, 2022, 46, 19062-19072.	1.4	12
1142	Cytotoxicity of Nitrogenous Disinfection Byproducts: A Combined Experimental and Computational Study. SSRN Electronic Journal, 0, , .	0.4	0
1143	Chemical Property Relation Guided Few-Shot Molecular Property Prediction. , 2022, , .		0
1144	Batched Bayesian Optimization for Drug Design in Noisy Environments. Journal of Chemical Information and Modeling, 2022, 62, 3970-3981.	2.5	11
1145	Discovery and Design of Radiopharmaceuticals by In silico Methods. Current Radiopharmaceuticals, 2022, 15, 271-319.	0.3	3
1146	Quantitative Structure Activity Relationship (QSAR) Investigations and Molecular Docking Analysis of Plasmodium Protein Farnesyltransferase Inhibitors as Potent Antimalarial Agents. Jordan Journal of Pharmaceutical Sciences, 2022, 15, 315-340.	0.2	0
1147	A Perspective Study on the RTK, PI3K, Bâ€Raf, CDK and the Multiâ€Protein Targeting in Medicinal Chemistry. Chemistry and Biodiversity, 2022, 19, .	1.0	2
1148	Machine Learning and Computational Chemistry for the Endocannabinoid System. Methods in Molecular Biology, 2023, , 477-493.	0.4	2

#	Article	IF	Citations
1149	Development of a Deep Learning Generative Neural Network for Computer-Aided Design of Potential SARS-Cov-2 Inhibitors. Mathematical Biology and Bioinformatics, 2022, 17, 188-207.	0.1	2
1150	FP-GNN: a versatile deep learning architecture for enhanced molecular property prediction. Briefings in Bioinformatics, 2022, 23, .	3.2	28
1151	Computer-Aided Drug Design Boosts RAS Inhibitor Discovery. Molecules, 2022, 27, 5710.	1.7	6
1153	Protein Function Analysis through Machine Learning. Biomolecules, 2022, 12, 1246.	1.8	8
1154	Cytotoxicity of nitrogenous disinfection byproducts: A combined experimental and computational study. Science of the Total Environment, 2023, 856, 159273.	3.9	15
1157	O data, where art thou? Revolutionizing data sharing to advance our sustainability goals through smart chemical innovation. IScience, 2022, 25, 105256.	1.9	6
1158	Exploring the Gallic and Cinnamic Acids Chimeric Derivatives as Anticancer Agents over HeLa Cell Line: An in silico and inâ€...vitro Study. Molecular Informatics, 2023, 42, .	1.4	5
1159	Evaluating molecular fingerprint-based models of drug side effects against a statistical control. Drug Discovery Today, 2022, 27, 103364.	3.2	3
1160	Automated retention time prediction of new psychoactive substances in gas chromatography. Procedia Computer Science, 2022, 207, 654-663.	1.2	3
1161	Supramolecular assembly in designing co-crystals of fumaric acid and pyrimidine/picolinate derivatives. Green Chemistry Letters and Reviews, 2022, 15, 825-836.	2.1	5
1162	Quantitative Framework for Bench-to-Bedside Cancer Research. Cancers, 2022, 14, 5254.	1.7	0
1163	Improving VAE based molecular representations for compound property prediction. Journal of Cheminformatics, 2022, 14, .	2.8	3
1164	Antibiotics degradation by advanced oxidation process (AOPs): Recent advances in ecotoxicity and antibiotic-resistance genes induction of degradation products. Chemosphere, 2023, 311, 136977.	4.2	62
1165	Review on Compounds Isolated from Eriocaulaceae Family and Evaluation of Biological Activities by Machine Learning. Molecules, 2022, 27, 7186.	1.7	0
1167	Generative and reinforcement learning approaches for the automated de novo design of bioactive compounds. Communications Chemistry, 2022, 5, .	2.0	12
1168	In Silico Investigations into the Selectivity of Psychoactive and New Psychoactive Substances in Monoamine Transporters. ACS Omega, 2022, 7, 38311-38321.	1.6	0
1170	Artificial intelligence for antiviral drug discovery in low resourced settings: A perspective. Frontiers in Drug Discovery, 0, 2, .	1.1	3
1171	Accurate Prediction of Epigenetic Multi-Targets with Graph Neural Network-Based Feature Extraction. International Journal of Molecular Sciences, 2022, 23, 13347.	1.8	3

#	Article	IF	Citations
1172	The role of computational toxicology in the risk assessment of food products. , 2023, , 643-659.		1
1173	A comprehensive evaluation of liposome/water partition coefficient prediction models based on the Technique for Order Preference by Similarity to an Ideal Solution (TOPSIS) method: Challenges from different descriptor dimension reduction methods and machine learning algorithms. Journal of Hazardous Materials, 2023, 443, 130181.	6.5	1
1174	DNN-PP: A novel Deep Neural Network approach and its applicability in drug-related property prediction. Expert Systems With Applications, 2023, 213, 119055.	4.4	8
1175	Quantitative Structureâ€“Toxicity Relationship in Bioactive Molecules from a Conceptual DFT Perspective. Pharmaceuticals, 2022, 15, 1383.	1.7	2
1176	Application of Computational Biology and Artificial Intelligence in Drug Design. International Journal of Molecular Sciences, 2022, 23, 13568.	1.8	17
1177	Electrochemoinformatics as an Emerging Scientific Field for Designing Materials and Electrochemical Energy Storage and Conversion Devicesâ€”An Application in Battery Science and Technology. Advanced Energy Materials, 2022, 12, .	10.2	4
1178	Less is more: Vital roles of bioactive equivalency in assessing food quality. EFood, 2022, 3, .	1.7	0
1179	A review of quantitative structure-activity relationship modelling approaches to predict the toxicity of mixtures. Computational Toxicology, 2023, 25, 100251.	1.8	7
1180	Efficient design of peptide-binding polymers using active learning approaches. Journal of Controlled Release, 2023, 353, 903-914.	4.8	2
1181	Improved graphâ€based multitask learning model with sparse sharing for quantitative structureâ€“property relationship prediction of drug molecules. AICHE Journal, 2023, 69, .	1.8	1
1182	Cheminformatics analysis of chemicals that increase estrogen and progesterone synthesis for a breast cancer hazard assessment. Scientific Reports, 2022, 12, .	1.6	2
1183	DeepPROTACs is a deep learning-based targeted degradation predictor for PROTACs. Nature Communications, 2022, 13, .	5.8	23
1184	Relevance of Machine Learning to Predict the Inhibitory Activity of Small Thiazole Chemicals on Estrogen Receptor. Current Computer-Aided Drug Design, 2023, 19, 37-50.	0.8	0
1185	Pharmacophore Synergism in Diverse Scaffold Clinches in Aurora Kinase B. International Journal of Molecular Sciences, 2022, 23, 14527.	1.8	0
1186	Antibiotic discovery in the artificial intelligence era. Annals of the New York Academy of Sciences, 2023, 1519, 74-93.	1.8	13
1187	3CLpro inhibitors: DEL-based molecular generation. Frontiers in Pharmacology, 0, 13, .	1.6	1
1189	Artificial intelligence systems for the design of magic shotgun drugs. Artificial Intelligence in the Life Sciences, 2022, , 100055.	1.6	1
1190	HiGNN: A Hierarchical Informative Graph Neural Network for Molecular Property Prediction Equipped with Feature-Wise Attention. Journal of Chemical Information and Modeling, 2023, 63, 43-55.	2.5	9

#	Article	IF	Citations
1191	Predicting CO₂ Absorption in Ionic Liquids with Molecular Descriptors and Explainable Graph Neural Networks. ACS Sustainable Chemistry and Engineering, 2022, 10, 16681-16691.	3.2	9
1192	SIRT2i_Predictor: A Machine Learning-Based Tool to Facilitate the Discovery of Novel SIRT2 Inhibitors. Pharmaceuticals, 2023, 16, 127.	1.7	1
1193	A comparison between 2D and 3D descriptors in QSAR modeling based on bioâ€active conformations. Molecular Informatics, 2023, 42, .	1.4	2
1194	Computational Approaches for Identifying Therapeutic Potential of Phytocompounds. Sustainable Development and Biodiversity, 2023, , 531-555.	1.4	0
1195	Prediction of drug-induced mitochondrial dysfunction using succinate-cytochrome c reductase activity, QSAR and molecular docking. Toxicology, 2023, 485, 153412.	2.0	7
1196	QSAR Studies, Molecular Docking, Molecular Dynamics, Synthesis, and Biological Evaluation of Novel Quinolinone-Based Thiosemicarbazones against Mycobacterium tuberculosis. Antibiotics, 2023, 12, 61.	1.5	6
1197	AI and Big Data for Drug Discovery. Integrated Science, 2022, , 121-138.	0.1	0
1199	Machine Learning and Deep Learning Applications to Evaluate Mutagenicity. Computational Methods in Engineering & the Sciences, 2023, , 447-461.	0.3	0
1200	Comprehensive assessment of nine target prediction web services: which should we choose for target fishing?. Briefings in Bioinformatics, 2023, 24, .	3.2	6
1201	Applicability Domain Characterization for Machine Learning QSAR Models. Computational Methods in Engineering & the Sciences, 2023, , 323-353.	0.3	2
1202	Identification of Structural Alerts by Machine Learning and Their Applications in Toxicology. Computational Methods in Engineering & the Sciences, 2023, , 479-495.	0.3	0
1203	Computational screening of phytochemicals for anti-cancer drug discovery. , 2023, , 313-334.		1
1204	Recent advances in the area of plant-based anti-cancer drug discovery using computational approaches. Molecular Diversity, 0, , .	2.1	7
1205	From Structural Alerts to Signature Fragment Alerts: A Case Study on Pyrrolizidine Alkaloids. Chemical Research in Toxicology, 2023, 36, 213-229.	1.7	0
1206	Molecular Toxicity Virtual Screening Applying a Quantized Computational SNN-Based Framework. Molecules, 2023, 28, 1342.	1.7	1
1207	Machine Learning-Based QSAR Models and Structural Alerts for Prediction of Mitochondrial Dysfunction. Computational Methods in Engineering & the Sciences, 2023, , 433-446.	0.3	0
1208	Drug discovery: Standing on the shoulders of giants. , 2023, , 207-338.		0
1209	Doctoral and professional programs. , 2023, , 169-196.		0

#	Article	IF	Citations
1211	Towards Arginase Inhibition: Hybrid SAR Protocol for Property Mapping of Chlorinated N-arylcinnamamides. International Journal of Molecular Sciences, 2023, 24, 3611.	1.8	0
1212	Characterization of oxidative damage induced by nanoparticles via mechanism-driven machine learning approaches. Science of the Total Environment, 2023, 871, 162103.	3.9	2
1213	QSAR-based virtual screening of traditional Chinese medicine for the identification of mitotic kinesin Eg5 inhibitors. Computational Biology and Chemistry, 2023, 104, 107865.	1.1	6
1214	Prediction of KRASG12C inhibitors using conjoint fingerprint and machine learning-based QSAR models. Journal of Molecular Graphics and Modelling, 2023, 122, 108466.	1.3	3
1215	Data driven toxicity assessment of organic chemicals against Gammarus species using QSAR approach. Chemosphere, 2023, 328, 138433.	4.2	4
1216	Methods for Biodegradability and Toxicity Assessment of Ionic Liquid. , 2022, , 888-893.		0
1217	Quantum-Mechanical Approach to Predicting the Carcinogenic Potency of N-Nitroso Impurities in Pharmaceuticals. Chemical Research in Toxicology, 2023, 36, 291-304.	1.7	6
1219	Rational design of stapled antimicrobial peptides. Amino Acids, 2023, 55, 421-442.	1.2	8
1220	Computer-Aided drug design of new 2-amino-thiophene derivatives as anti-leishmanial agents. European Journal of Medicinal Chemistry, 2023, 250, 115223.	2.6	7
1221	Modeling structureâ€“activity relationships with machine learning to identify GSK3-targeted small molecules as potential COVID-19 therapeutics. Frontiers in Endocrinology, 0, 14, .	1.5	1
1222	Quantitative Structure-Activity Relationship (QSAR) modelling of the activity of anti-colorectal cancer agents featuring quantum chemical predictors and interaction terms. Results in Chemistry, 2023, 5, 100888.	0.9	2
1223	Small Data Can Play a Big Role in Chemical Discovery. Angewandte Chemie - International Edition, 2023, 62, .	7.2	5
1224	Small Data Can Play a Big Role in Chemical Discovery. Angewandte Chemie, 2023, 135, .	1.6	1
1225	Application of Computing as a High-Practicability and -Efficiency Auxiliary Tool in Nanodrugs Discovery. Pharmaceutics, 2023, 15, 1064.	2.0	3
1226	In silico modeling revealed phytomolecules derived from Cymbopogon citratus (DC.) leaf extract as promising candidates for malaria therapy. Journal of Biomolecular Structure and Dynamics, 2024, 42, 101-118.	2.0	3
1227	Serverless Prediction of Peptide Properties with Recurrent Neural Networks. Journal of Chemical Information and Modeling, 2023, 63, 2546-2553.	2.5	8
1228	2D, 3D-QSAR study and docking of vascular endothelial growth factor receptor 3 (VEGFR3) inhibitors for potential treatment of retinoblastoma. Frontiers in Pharmacology, 0, 14, .	1.6	2
1229	Computational Tools for Drug Discovery of Anticancer Therapy. Biological and Medical Physics Series, 2023, , 887-904.	0.3	0

#	Article	IF	Citations
1230	Predictive in silico models for aquatic toxicity of cosmetic and personal care additive mixtures. Water Research, 2023, 236, 119981.	5.3	5
1231	Identification of Promising Inhibitory Heterocyclic Compounds Against Acetylcholinesterase Using QSAR, ADMET, Biological Activity, and Molecular Docking. Computational Biology and Chemistry, 2023, , 107872.	1.1	4
1233	The pursuit of natural medicineâ€"a current perspective. , 2023, , 173-192.		0
1234	Quantitative structure-activity relationship and its application to cancer therapy. , 2023, , 91-99.		0
1235	2Dâ€Quantitative structureâ€"activity relationship modeling for risk assessment of pharmacotherapy applied during pregnancy. Journal of Applied Toxicology, 2023, 43, 1436-1446.	1.4	7
1236	Quantitative structureâ€"activity relationship and artificial neural network-based results for designing corrosion inhibitors. , 2023, , 509-524.		1
1237	Computational approaches streamlining drug discovery. Nature, 2023, 616, 673-685.	13.7	117
1242	Quantum similarity description of a unique classical and quantum QSPR algorithm in molecular spaces: the connection with Boolean hypercubes, algorithmic intelligence, and GÃ¶del's incompleteness theorems. , 2023, , 505-572.		0
1243	Chemical space and molecular descriptors for QSAR studies. , 2023, , 303-327.		0
1244	Quantitative structure-activity relationships (QSARs) in medicinal chemistry. , 2023, , 3-38.		0
1248	Molecular modelling of the thermophysical properties of fluids: expectations, limitations, gaps and opportunities. Physical Chemistry Chemical Physics, 2023, 25, 12607-12628.	1.3	5
1249	Prediction of retention in liquid chromatography. , 2023, , 795-819.		0
1258	Structure-related relationship: Plant-derived antidiabetic compounds. Studies in Natural Products Chemistry, 2023, , 241-295.	0.8	0
1263	Bioinformatics and Biostatistics in Precision Medicine. , 2023, , 189-235.		1
1264	Modeling of BACE-1 Inhibitors as Anti-Alzheimerâ€™s Agents. Neuromethods, 2023, , 99-125.	0.2	0
1282	Role of Natural products in Drug discovery. , 2023, , 1-5.		0
1283	Machine learningâ€"based QSAR for safety evaluation of environmental chemicals. , 2023, , 89-99.		0
1288	Approaches for In Silico Validation of Safety (Toxicity) Data for Cosmetics. , 2023, , 187-210.		0

#	Article	IF	Citations
1292	Molecular Compounds Proposal for Drug-Resistant Tuberculosis in the Drug Discovery Process. , 2023, , .		0
1302	Quantum Chemical and Informatics-Based Approaches for Probing Biomolecular Systems Toxicology. , 2024, , 193-201.		0
1306	Novel enzymatic tools for Câ€“C bond formation through the development of new-to-nature biocatalysis. Advances in Catalysis, 2023, , .	0.1	0
1309	In Silico Insights Toward the Exploration of Adenosine Receptors Ligand Recognition. Topics in Medicinal Chemistry, 2023, , 275-315.	0.4	0
1313	Advances in QSAR through artificial intelligence and machine learning methods. , 2023, , 101-116.		1
1314	Advances of the QSAR approach as an alternative strategy in the environmental risk assessment. , 2023, , 117-137.		1
1315	Corrosion management using computational simulations. , 2023, , 399-423.		0
1319	Computational and Informatics Methodologies in Drug Discovery, with Focus on Natural Products. , 2023, , 1-22.		0
1321	An Introduction to Machine Learning in Molecular Sciences. Challenges and Advances in Computational Chemistry and Physics, 2023, , 1-19.	0.6	0
1333	PRACTICAL APPLICATIONS OF MACHINE LEARNING FOR ANTI-INFECTIVE DRUG DISCOVERY. Medicinal Chemistry Reviews, 0, , 345-375.	0.1	0
1338	In Silico Approaches in Pesticides. Engineering Materials, 2024, , 335-351.	0.3	0
1345	Tuberculosis Drug Discovery Estimation Process by Using Machine and Deep Learning Models. Communications in Computer and Information Science, 2024, , 43-53.	0.4	0
1351	Free Energy Estimation for Drug Discovery: Background and Perspectives. , 2023, , 310-345.		0
1352	Machine Learning Modeling Predicting Vascular Endothelial Growth Factor Receptor 2 (VEGFR2) Inhibitors Structure-Activity Relationships Using Quantum DFT Descriptors. , 2023, , .		0
1361	Graph Neural Networks for the Prediction of Molecular Structureâ€“Property Relationships. , 2023, , 159-181.		0
1363	Anesthetic drug discovery with computer-aided drug design and machine learning. , 2024, 2, .		0
1368	The pursuit of accurate predictive models of the bioactivity of small molecules. Chemical Science, 2024, 15, 1938-1952.	3.7	2
1388	Are We Moving Towards a More Sustainable World? Insights from Patent Analysis of Chemical Inventions. SpringerBriefs in Economics, 2024, , 39-59.	0.1	0

#	Article	IF	Citations
1392	AI Deep Learning Generative Models for Drug Discovery. , 2024, , 461-475.		0
1396	Future of Regulatory Safety Assessment. , 2023, , 1-26.		0
1399	Computational Methods for Predictive Toxicology: In Silico Toxicology. , 2024, , 85-97.		0