Supratik Kar

List of Publications by Year
in descending order

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119 papers	4,445 citations	126708 33 h-index	114278 63 g-index
126 all docs	126 docs citations	126 times ranked	3661 citing authors

#	Article	IF	Citations
1	On a simple approach for determining applicability domain of QSAR models. Chemometrics and Intelligent Laboratory Systems, 2015, 145, 22-29.	1.8	534
2	Comparative Studies on Some Metrics for External Validation of QSPR Models. Journal of Chemical Information and Modeling, 2012, 52, 396-408.	2.5	399
3	Some case studies on application of â€œr_m²â€•metrics for judging quality of quantitative structureâ€“activity relationship predictions: Emphasis on scaling of response data. Journal of Computational Chemistry, 2013, 34, 1071-1082.	1.5	366
4	A Primer on QSAR/QSPR Modeling. Springer Briefs in Molecular Science, 2015, , .	0.1	197
5	Green Chemistry in the Synthesis of Pharmaceuticals. Chemical Reviews, 2022, 122, 3637-3710.	23.0	155
6	Periodic table-based descriptors to encode cytotoxicity profile of metal oxide nanoparticles: A mechanistic QSTR approach. Ecotoxicology and Environmental Safety, 2014, 107, 162-169.	2.9	103
7	How far can virtual screening take us in drug discovery?. Expert Opinion on Drug Discovery, 2013, 8, 245-261.	2.5	102
8	Open access in silico tools to predict the ADMET profiling of drug candidates. Expert Opinion on Drug Discovery, 2020, 15, 1473-1487.	2.5	99
9	QSAR modeling of toxicity of diverse organic chemicals to Daphnia magna using 2D and 3D descriptors. Journal of Hazardous Materials, 2010, 177, 344-351.	6.5	92
10	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
11	How Precise Are Our Quantitative Structureâ€“Activity Relationship Derived Predictions for New Query Chemicals?. ACS Omega, 2018, 3, 11392-11406.	1.6	88
12	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. Green Chemistry, 2020, 22, 1458-1516.	4.6	86
13	Exploration of Computational Approaches to Predict the Toxicity of Chemical Mixtures. Toxics, 2019, 7, 15.	1.6	84
14	On further application of r as a metric for validation of QSAR models. Journal of Chemometrics, 2010, 24, 22-33.	0.7	82
15	Endocrine-disrupting activity of per- and polyfluoroalkyl substances: Exploring combined approaches of ligand and structure based modeling. Chemosphere, 2017, 184, 514-523.	4.2	79
16	Nano-quantitative structureâ€“activity relationship modeling using easily computable and interpretable descriptors for uptake of magnetofluorescent engineered nanoparticles in pancreatic cancer cells. Toxicology in Vitro, 2014, 28, 600-606.	1.1	77
17	Statistical Methods in QSAR/QSPR. Springer Briefs in Molecular Science, 2015, , 37-59.	0.1	75
18	First report on interspecies quantitative correlation of ecotoxicity of pharmaceuticals. Chemosphere, 2010, 81, 738-747.	4.2	67

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19	Introduction of rm2(rank) metric incorporating rank-order predictions as an additional tool for validation of QSAR/QSPR models. Chemometrics and Intelligent Laboratory Systems, 2012, 118, 200-210.	1.8	67
20	Pharmacophore mapping-based virtual screening followed by molecular docking studies in search of potential acetylcholinesterase inhibitors as anti-Alzheimer's agents. BioSystems, 2014, 116, 10-20.	0.9	64
21	Applicability Domain: A Step Toward Confident Predictions and Decidability for QSAR Modeling. Methods in Molecular Biology, 2018, 1800, 141-169.	0.4	61
22	Therapeutics for COVID-19: from computation to practicesâ€"where we are, where we are heading to. Molecular Diversity, 2021, 25, 625-659.	2.1	53
23	Prediction reliability of QSAR models: an overview of various validation tools. Archives of Toxicology, 2022, 96, 1279-1295.	1.9	49
24	Electronic Structure and Optical Properties of Designed Photo-Efficient Indoline-Based Dye-Sensitizers with Dâ€"Aâ^Ï€â€"A Framework. Journal of Physical Chemistry C, 2019, 123, 3309-3320.	1.5	46
25	Extrapolating between toxicity endpoints of metal oxide nanoparticles: Predicting toxicity to Escherichia coli and human keratinocyte cell line (HaCaT) with Nano-QTTR. Ecotoxicology and Environmental Safety, 2016, 126, 238-244.	2.9	44
26	Insight into the optoelectronic properties of designed solar cells efficient tetrahydroquinoline dye-sensitizers on TiO2(101) surface: first principles approach. Scientific Reports, 2018, 8, 10997.	1.6	44
27	InÂvitro and in silico modeling of perfluoroalkyl substances mixture toxicity in an amphibian fibroblast cell line. Chemosphere, 2019, 233, 25-33.	4.2	44
28	Risk assessment for ecotoxicity of pharmaceuticals â€“ an emerging issue. Expert Opinion on Drug Safety, 2012, 11, 235-274.	1.0	43
29	In silico designing of power conversion efficient organic lead dyes for solar cells using todays innovative approaches to assure renewable energy for future. Npj Computational Materials, 2017, 3, .	3.5	43
30	First report on development of quantitative interspecies structureâ€"carcinogenicity relationship models and exploring discriminatory features for rodent carcinogenicity of diverse organic chemicals using OECD guidelines. Chemosphere, 2012, 87, 339-355.	4.2	42
31	The rm2 metrics and regression through origin approach: Reliable and useful validation tools for predictive QSAR models (Commentary on â€˜Is regression through origin useful in external validation of) Tj ETQq1 1 0.784314 rgBT /Ov	1.9	41
32	QSAR with quantum topological molecular similarity indices: toxicity of aromatic aldehydes toTetrahymena pyriformis. SAR and QSAR in Environmental Research, 2010, 21, 149-168.	1.0	36
33	Validation of QSAR Models. , 2015, , 231-289.		36
34	Revealing the Photophysical Mechanism of N,Nâ€²-Diphenyl-aniline Based Sensitizers with the Dâ€"Dâ^Ï€â€"A Framework: Theoretical Insights. ACS Sustainable Chemistry and Engineering, 2020, 8, 13328-13341.	3.2	36
35	Chemometric modeling of power conversion efficiency of organic dyes in dye sensitized solar cells for the future renewable energy. Nano Energy, 2020, 70, 104537.	8.2	35
36	Impact of Pharmaceuticals on the Environment: Risk Assessment Using QSAR Modeling Approach. Methods in Molecular Biology, 2018, 1800, 395-443.	0.4	32

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37	QSAR of phytochemicals for the design of better drugs. Expert Opinion on Drug Discovery, 2012, 7, 877-902.	2.5	31
38	Inhibitors or toxins? Large library target-specific screening of fullerene-based nanoparticles for drug design purpose. Nanoscale, 2017, 9, 10263-10276.	2.8	29
39	Second generation periodic table-based descriptors to encode toxicity of metal oxide nanoparticles to multiple species: QSTR modeling for exploration of toxicity mechanisms. Environmental Science: Nano, 2018, 5, 2742-2760.	2.2	26
40	Quantitative structure-property relationship model leading to virtual screening of fullerene derivatives: Exploring structural attributes critical for photoconversion efficiency of polymer solar cell acceptors. Nano Energy, 2016, 26, 677-691.	8.2	25
41	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
42	Development and validation of a robust QSAR model for prediction of carcinogenicity of drugs. Indian Journal of Biochemistry and Biophysics, 2011, 48, 111-22.	0.2	24
43	Single or mixture halogenated chemicals? Risk assessment and developmental toxicity prediction on zebrafish embryos based on weighted descriptors approach. Chemosphere, 2018, 210, 588-596.	4.2	23
44	Toward comprehension of multiple human cells uptake of engineered nano metal oxides: quantitative inter cell line uptake specificity (QICLUS) modeling. Nanotoxicology, 2019, 13, 14-34.	1.6	23
45	Selected Statistical Methods in QSAR. , 2015, , 191-229.		22
46	Synthesis and characterization of pyrrolo[1,2-a]quinoline derivatives for their larvicidal activity against Anopheles arabiensis. Structural Chemistry, 2020, 31, 1533-1543.	1.0	22
47	Background of QSAR and Historical Developments. , 2015, , 1-46.		21
48	Protein reliability analysis and virtual screening of natural inhibitors for SARS-CoV-2 main protease (M^{pro}) through docking, molecular mechanic & dynamic, and ADMET profiling. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6810-6827.	2.0	21
49	Development of classification and regression based QSAR models to predict rodent carcinogenic potency using oral slope factor. Ecotoxicology and Environmental Safety, 2012, 82, 85-95.	2.9	20
50	QSAR/QSPR Modeling: Introduction. Springer Briefs in Molecular Science, 2015, , 1-36.	0.1	20
51	Other Related Techniques. , 2015, , 357-425.		20
52	Can Toxicity for Different Species be Correlated?. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 23-51.	1.1	20
53	First report on predictive chemometric modeling, 3D-toxicophore mapping and in silico screening of in vitro basal cytotoxicity of diverse organic chemicals. Toxicology in Vitro, 2013, 27, 597-608.	1.1	19
54	Evaluating the cytotoxicity of a large pool of metal oxide nanoparticles to Escherichia coli: Mechanistic understanding through InÂVitro and In Silico studies. Chemosphere, 2021, 264, 128428.	4.2	19

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55	Recent Advances of Computational Modeling for Predicting Drug Metabolism: A Perspective. Current Drug Metabolism, 2018, 18, 1106-1122.	0.7	19
56	Development of classification- and regression-based QSAR models andin silicoscreening of skin sensitisation potential of diverse organic chemicals. Molecular Simulation, 2014, 40, 261-274.	0.9	17
57	Power Conversion Efficiency of Arylamine Organic Dyes for Dye-Sensitized Solar Cells (DSSCs) Explicit to Cobalt Electrolyte: Understanding the Structural Attributes Using a Direct QSPR Approach. Computation, 2017, 5, 2.	1.0	17
58	QSAR modeling of adipose/blood partition coefficients of Alcohols, PCBs, PBDEs, PCDDs and PAHs: A data gap filling approach. Environment International, 2018, 121, 1193-1203.	4.8	17
59	Development and validation of regression-based QSAR models for quantification of contributions of molecular fragments to skin sensitization potency of diverse organic chemicals. SAR and QSAR in Environmental Research, 2013, 24, 1009-1023.	1.0	15
60	Chemical Information and Descriptors. , 2015, , 47-80.		15
61	In Silico Models for Ecotoxicity of Pharmaceuticals. Methods in Molecular Biology, 2016, 1425, 237-304.	0.4	15
62	Optoelectronic Properties of C60 and C70 Fullerene Derivatives: Designing and Evaluating Novel Candidates for Efficient P3HT Polymer Solar Cells. Materials, 2019, 12, 2282.	1.3	15
63	In Silico Tools and Software to Predict ADMET of New Drug Candidates. Methods in Molecular Biology, 2022, 2425, 85-115.	0.4	15
64	Computational Chemistry. , 2015, , 151-189.		14
65	On Applications of QSARs in Food and Agricultural Sciences: History and Critical Review of Recent Developments. Challenges and Advances in Computational Chemistry and Physics, 2017, , 203-302.	0.6	14
66	Recent Advances of In-Silico Modeling of Potent Antagonists for the Adenosine Receptors. Current Pharmaceutical Design, 2019, 25, 750-773.	0.9	14
67	Application of Artificial Intelligence and Machine Learning Techniques in Classifying Extent of Dementia Across Alzheimer's Image Data. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 29-46.	1.1	13
68	Prediction of hERG Potassium Channel Blocking Actions Using Combination of Classification and Regression Based Models: A Mixed Descriptors Approach. Molecular Informatics, 2012, 31, 879-894.	1.4	11
69	Prediction of Milk/Plasma Concentration Ratios of Drugs and Environmental Pollutants Using In Silico Tools: Classification and Regression Based QSARs and Pharmacophore Mapping. Molecular Informatics, 2013, 32, 693-705.	1.4	11
70	From Animal to Human: Interspecies Analysis Provides a Novel Way of Ascertaining and Fighting COVID-19. Innovation(China), 2020, 1, 100021.	5.2	11
71	Importance of Applicability Domain of QSAR Models. Advances in Chemical and Materials Engineering Book Series, 2015, , 180-211.	0.2	11
72	Geometry optimization of steroid sulfatase inhibitors - the influence on the free binding energy with STS. Structural Chemistry, 2017, 28, 1017-1032.	1.0	10

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73	Lead Hopping for PfDHODH Inhibitors as Antimalarials Based on Pharmacophore Mapping, Molecular Docking and Comparative Binding Energy Analysis (COMBINE): A Threeâ€Layered Virtual Screening Approach. Molecular Informatics, 2012, 31, 711-718.	1.4	9
74	Is intraspecies QSTR model answer to toxicity data gap filling: Ecotoxicity modeling of chemicals to avian species. Science of the Total Environment, 2020, 738, 139858.	3.9	9
75	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
76	Identification of potential antivirals against 3CLpro enzyme for the treatment of SARS-CoV-2: A multi-step virtual screening study. SAR and QSAR in Environmental Research, 2022, 33, 357-386.	1.0	9
77	Repurposing FDA approved drugs as possible anti-SARS-CoV-2 medications using ligand-based computational approaches: sum of ranking difference-based model selection. Structural Chemistry, 2022, 33, 1741-1753.	1.0	9
78	Linear discriminant analysis for skin sensitisation potential of diverse organic chemicals. Molecular Simulation, 2013, 39, 432-441.	0.9	8
79	Introduction to 3D-QSAR. , 2015, , 291-317.		8
80	Quantification of contributions of molecular fragments for eye irritation of organic chemicals using QSAR study. Computers in Biology and Medicine, 2014, 48, 102-108.	3.9	7
81	Newer QSAR Techniques. , 2015, , 319-356.		7
82	Synthesis and anthelmintic activity of some novel (E)-2-methyl/propyl-4-(2-(substitutedbenzylidene)hydrazinyl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidines. Medicinal Chemistry Research, 2020, 29, 1600-1610.	1.1	7
83	Current Status in the Design and Development of Agonists and Antagonists of Adenosine A3 Receptor as Potential Therapeutic Agents. Current Pharmaceutical Design, 2019, 25, 2772-2787.	0.9	7
84	Is clay-polycation adsorbent future of the greener society? In silico modeling approach with comprehensive virtual screening. Chemosphere, 2019, 220, 1108-1117.	4.2	6
85	Preliminary Screening of COVID-19 Infection Employing Machine Learning Techniques From Simple Blood Profile. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 35-47.	1.1	6
86	Ecotoxicity Databases for QSAR Modeling. Methods in Pharmacology and Toxicology, 2020, , 709-758.	0.1	6
87	How to Judge Predictive Quality of Classification and Regression Based QSAR Models?. , 2015, , 71-120.		6
88	Exploring Simple, Interpretable, and Predictive QSPR Model of Fullerene C60 Solubility in Organic Solvents. Journal of Nanotoxicology and Nanomedicine, 2017, 2, 28-43.	0.7	6
89	Predictive Chemometric Modeling and Three-Dimensional Toxicophore Mapping of Diverse Organic Chemicals Causing Bioluminescent Repression of the Bacterium Genus Pseudomonas. Industrial & Engineering Chemistry Research, 2013, 52, 17648-17657.	1.8	5
90	Classical QSAR. , 2015, , 81-102.		5

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91	Predictive toxicity modelling of benzodiazepine drugs using multiplein silicoapproaches: descriptor-based QSTR, group-based QSTR and 3D-toxicophore mapping. Molecular Simulation, 2015, 41, 345-355.	0.9	5
92	A comprehensive computational analysis of cathinone and its metabolites using quantum mechanical approaches and docking studies. Structural Chemistry, 2016, 27, 1291-1302.	1.0	5
93	“Prediction Reliability Indicator”: A new tool to judge the quality of predictions from QSAR models for new query compounds. , 0, , .		5
94	Computational approaches in assessments of mixture toxicity. Current Opinion in Toxicology, 2022, 29, 31-35.	2.6	5
95	Conformational analysis, energy profile, and structural-electronic properties evaluation of mephedrone derivatives employing quantum-mechanical models. Structural Chemistry, 2017, 28, 791-799.	1.0	4
96	Predicting Thermal Conductivity Enhancement of Al2O3/Water and CuO/Water Nanofluids Using Quantitative Structure-Property Relationship Approach. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 18-27.	1.1	4
97	Ecotoxicological QSARs of Mixtures. Methods in Pharmacology and Toxicology, 2020, , 437-475.	0.1	4
98	Future Avenues. , 2015, , 455-462.		3
99	SAR and QSAR in Drug Discovery and Chemical Designâ€"Some Examples. , 2015, , 427-453.		3
100	Chemometric Modeling of the Ecotoxicity of Industrial Chemicals to an Avian Species Anas Platyrhynchos. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 1-16.	1.1	3
101	In Silico Meets In Vitro Techniques in ADMET Profiling of Drug Discovery (Part I). Current Drug Metabolism, 2020, 21, 745-745.	0.7	3
102	Newer Directions in QSAR/QSPR. Springer Briefs in Molecular Science, 2015, , 105-121.	0.1	2
103	QSAR and machine learning modeling of toxicity of nanomaterials: a risk assessment approach. , 2021, , 417-441.		2
104	Editorial: Exploration of Natural Product Leads for Multitarget-Based Treatment of Cancerâ€"Computational to Experimental Journey. Frontiers in Pharmacology, 2022, 13, 850151.	1.6	2
105	Drug Databases for Development of Therapeutics Against Coronaviruses. Methods in Pharmacology and Toxicology, 2021, , 761.	0.1	1
106	In Silico Meets In Vitro Techniques in ADMET Profiling of Drug Discovery (Part II). Current Drug Metabolism, 2021, 22, 502-502.	0.7	1
107	Importance of Applicability Domain of QSAR Models. , 2017, , 1012-1043.		1
108	Computational Methods of Interspecies Nanotoxicity Extrapolation: A Step toward the Future. , 2019, , 401-435.		1

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109	In Vitro and In Silico Study of Cytotoxicity of Metal Oxide Nanoparticles towards Escherichia coli. , 0, , .		1
110	On Error Measures for Validation and Uncertainty Estimation of Predictive QSAR Models. , 2019, , 437-493.		1
111	Distribution of Cancer Patients According to Time Taken From Starting Day of Symptoms to Reporting at a Regional Cancer Institute in Eastern India. Asian Pacific Journal of Cancer Prevention, 2001, 2, 281-286.	0.5	1
112	Topological QSAR. , 2015, , 103-149.		0
113	Theoretical study of formate, tartrate, tartronate, and glycolate production from 6-carbon trioxylate intermediate in the citric acid cycle. Journal of Molecular Modeling, 2019, 25, 347.	0.8	0
114	Application of QSPR Modeling in Designing and Prediction of Power Conversion-Efficient Solar Cell. Challenges and Advances in Computational Chemistry and Physics, 2021, , 167-186.	0.6	0
115	Computational Screening of Organic Dye-Sensitizers for Dye-Sensitized Solar Cells: DFT/TDDFT Approach. Challenges and Advances in Computational Chemistry and Physics, 2021, , 187-205.	0.6	0
116	QSAR/QSPR Methods. Springer Briefs in Molecular Science, 2015, , 61-103.	0.1	0
117	Intelligent consensus predictor: Towards more precise predictions for external set compounds. , 0, , .		0
118	Ecotoxicological assessment of pharmaceuticals using computational toxicology approaches: QSTR and interspecies QTTR modelling. , 0, , .		0
119	Can Toxicity for Different Species Be Correlated?. , 0, , 339-371.		0